



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:37 AM UTC

PDB ID : 1T5E / pdb_00001t5e
Title : The structure of MexA
Authors : Higgins, M.K.; Bokma, E.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on : 2004-05-04
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

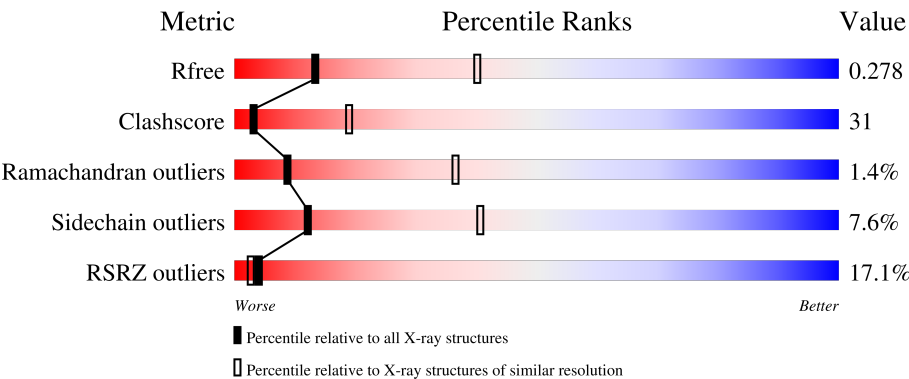
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	18% 32%28% 36%
1	B	360	13% 34%27% 36%
1	C	360	10% 34%27% 36%
1	D	360	12% 32%27% 36%
1	E	360	5% 34%27% 36%

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Mol	Chain	Length	Quality of chain
1	F	360	
1	G	360	
1	H	360	
1	I	360	
1	J	360	
1	K	360	
1	L	360	
1	M	360	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	361	-	-	X	X
2	GOL	B	361	-	-	-	X
2	GOL	J	361	-	-	X	-
3	3GR	C	361	-	-	-	X
3	3GR	D	361	-	-	-	X
3	3GR	E	361	-	-	-	X
3	3GR	F	361	-	-	X	X
3	3GR	G	361	-	-	-	X
3	3GR	H	361	-	-	-	X
3	3GR	I	361	-	-	X	-
3	3GR	K	361	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23101 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multidrug resistance protein mexA.

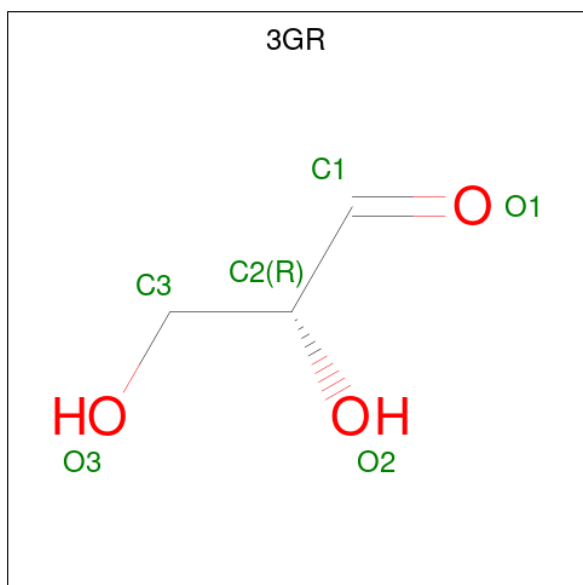
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	B	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	C	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	D	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	E	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	F	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	G	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	H	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	I	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	J	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	K	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	L	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	M	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

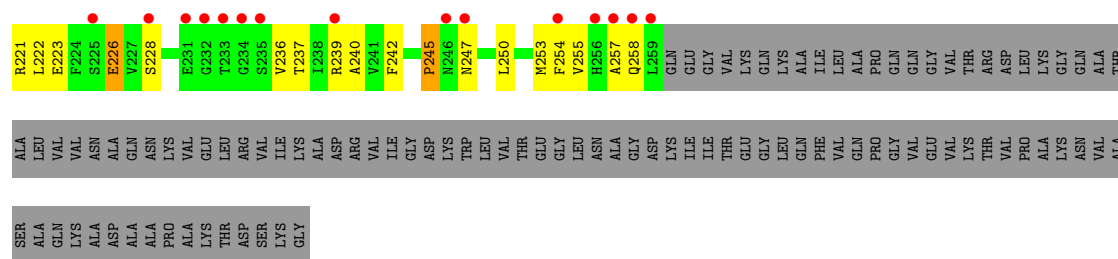


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		

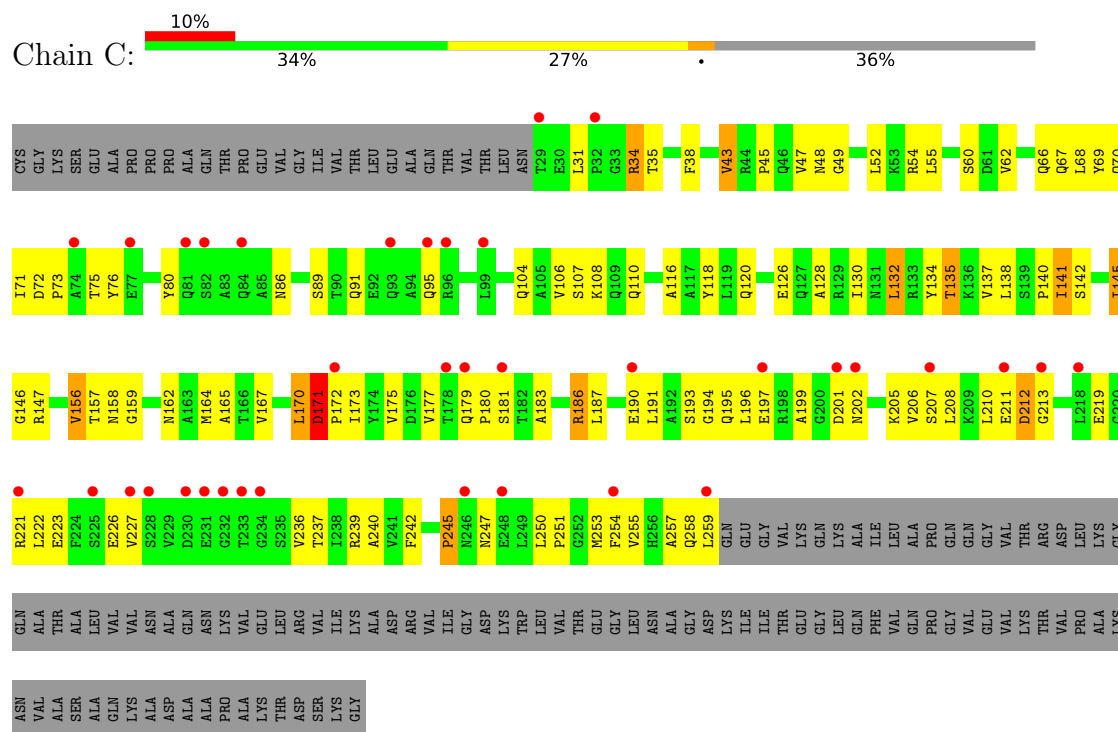
- Molecule 3 is D-Glyceraldehyde (CCD ID: 3GR) (formula: $C_3H_6O_3$).



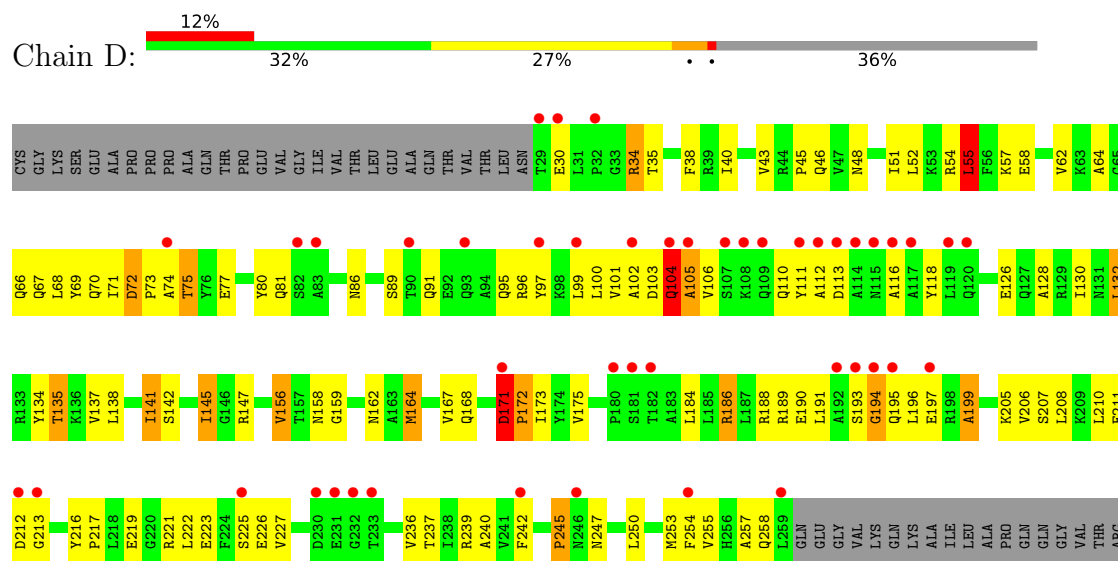
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	I	1	Total 6	C 3	O 3	0	0
3	K	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0

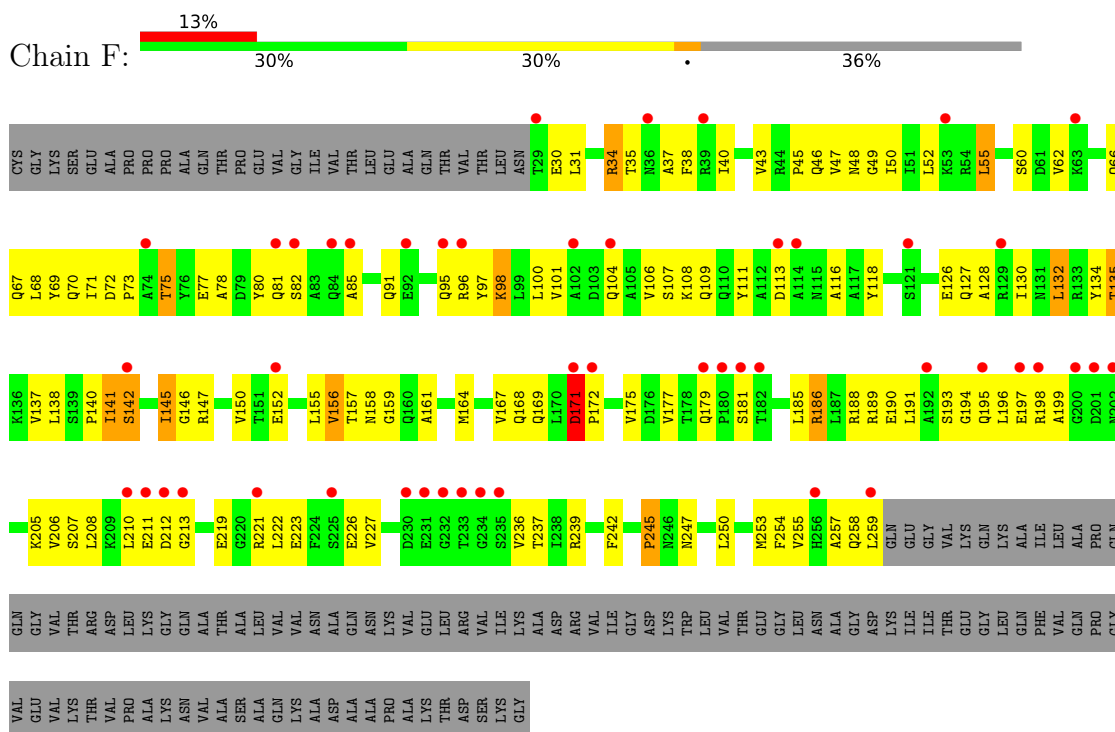


- Molecule 1: Multidrug resistance protein mexA

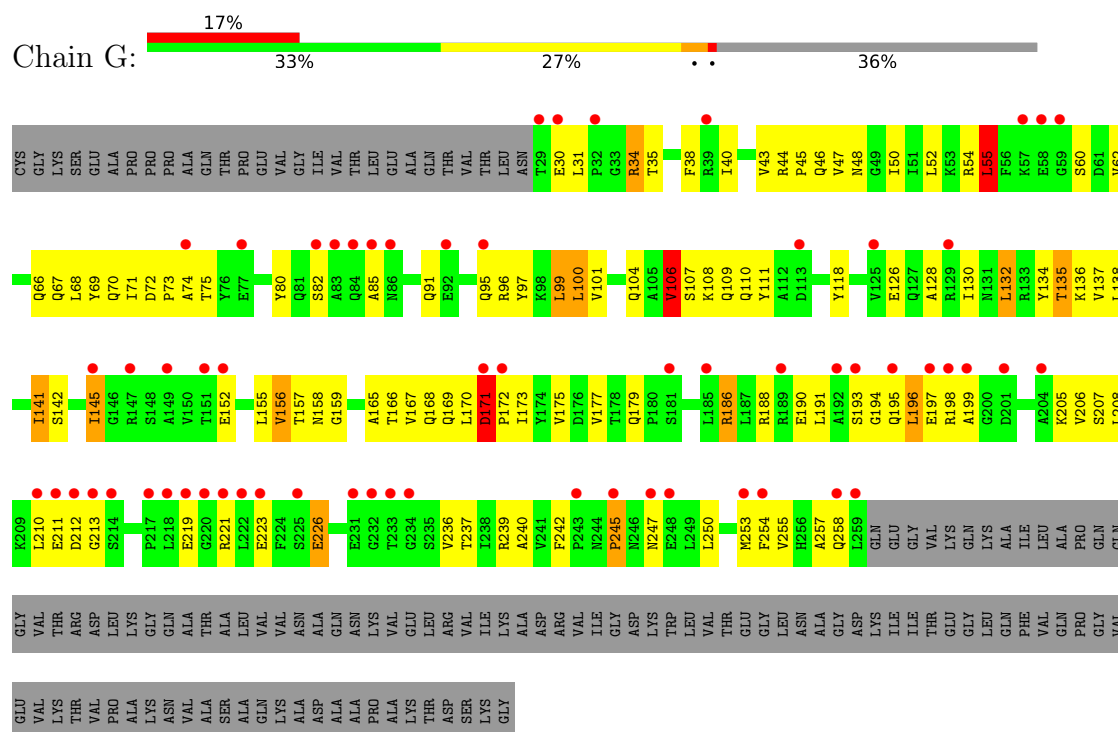


- Molecule 1: Multidrug resistance protein mexA

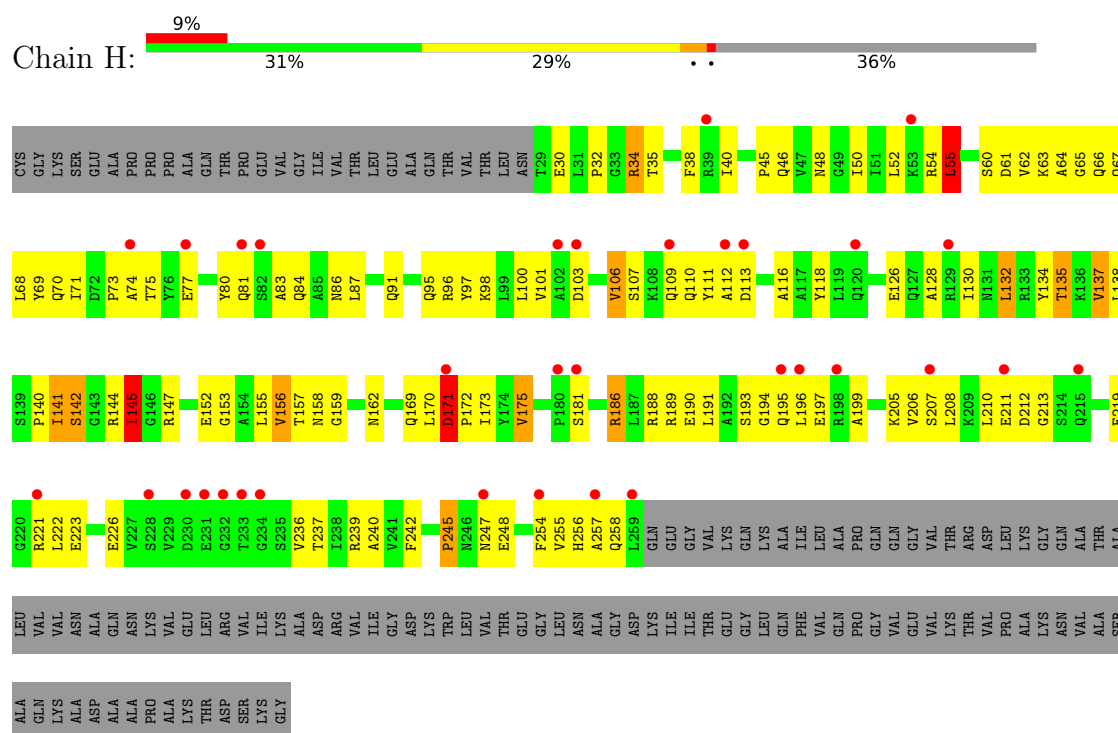




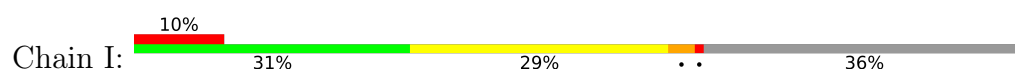
- Molecule 1: Multidrug resistance protein mexA

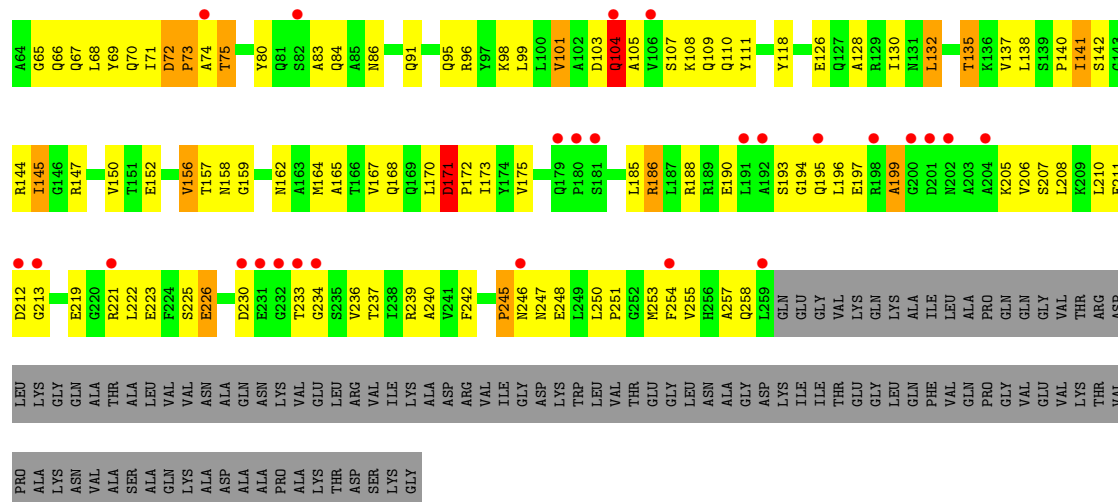


- Molecule 1: Multidrug resistance protein mexA

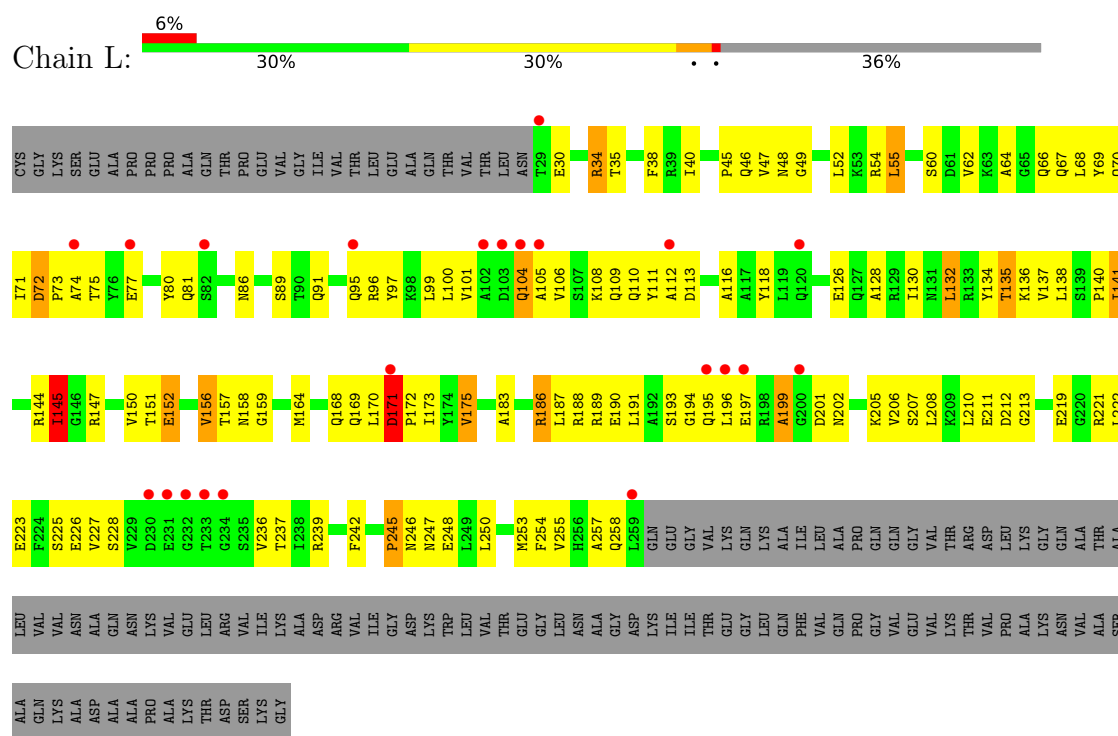


- Molecule 1: Multidrug resistance protein mexA

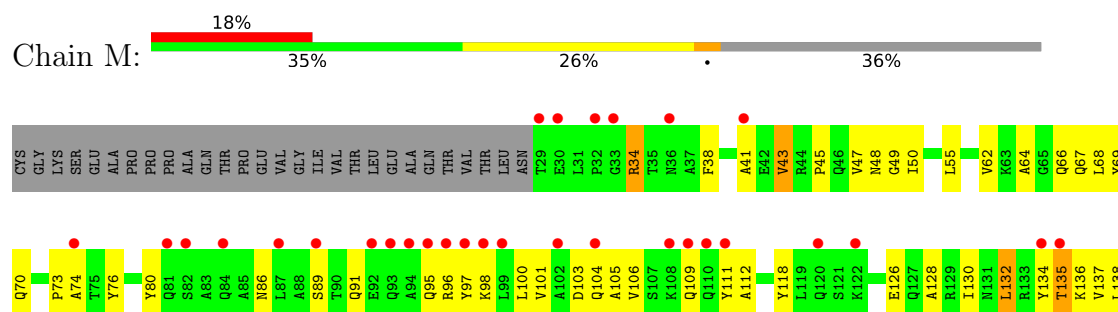


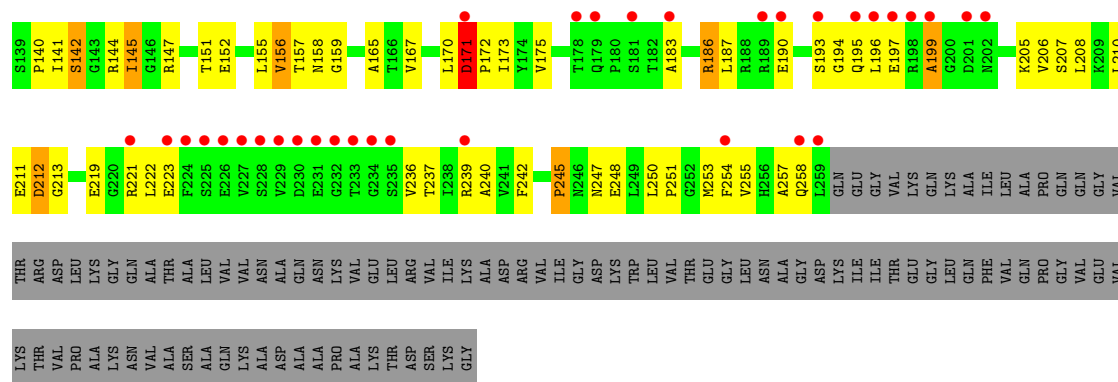


• Molecule 1: Multidrug resistance protein mexA



• Molecule 1: Multidrug resistance protein mexA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.55Å 183.59Å 213.31Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	95.00 – 3.00 95.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (95.00-3.00) 98.9 (95.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.285 0.268 , 0.278	Depositor DCC
R_{free} test set	9310 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23101	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 3GR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.73	1/1795 (0.1%)	0.99	8/2434 (0.3%)
1	B	0.48	0/1795	1.05	8/2434 (0.3%)
1	C	0.51	0/1795	1.03	9/2434 (0.4%)
1	D	0.53	1/1795 (0.1%)	1.12	13/2434 (0.5%)
1	E	0.59	0/1795	1.12	10/2434 (0.4%)
1	F	0.48	0/1795	1.06	9/2434 (0.4%)
1	G	0.45	0/1795	1.02	6/2434 (0.2%)
1	H	0.58	0/1795	1.14	11/2434 (0.5%)
1	I	0.61	0/1795	1.12	9/2434 (0.4%)
1	J	0.74	0/1795	1.19	11/2434 (0.5%)
1	K	0.66	0/1795	1.16	13/2434 (0.5%)
1	L	0.61	0/1795	1.15	13/2434 (0.5%)
1	M	0.48	0/1795	1.06	9/2434 (0.4%)
All	All	0.58	2/23335 (0.0%)	1.09	129/31642 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	C-N	-25.67	1.00	1.33
1	D	164	MET	SD-CE	-5.75	1.65	1.79

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	171	ASP	CA-C-N	-12.84	106.19	119.93
1	J	171	ASP	C-N-CA	-12.84	106.19	119.93
1	H	171	ASP	CA-C-N	-12.34	106.72	119.93
1	H	171	ASP	C-N-CA	-12.34	106.72	119.93
1	E	171	ASP	CA-C-N	-11.51	107.61	119.93
1	E	171	ASP	C-N-CA	-11.51	107.61	119.93
1	K	171	ASP	CA-C-N	-11.15	108.00	119.93
1	K	171	ASP	C-N-CA	-11.15	108.00	119.93
1	G	171	ASP	CA-C-N	-11.05	108.10	119.93
1	G	171	ASP	C-N-CA	-11.05	108.10	119.93
1	L	171	ASP	CA-C-N	-10.93	108.24	119.93
1	L	171	ASP	C-N-CA	-10.93	108.24	119.93
1	D	171	ASP	CA-C-N	-10.49	108.71	119.93
1	D	171	ASP	C-N-CA	-10.49	108.71	119.93
1	I	171	ASP	CA-C-N	-9.82	109.42	119.93
1	I	171	ASP	C-N-CA	-9.82	109.42	119.93
1	F	171	ASP	CA-C-N	-9.79	109.46	119.93
1	F	171	ASP	C-N-CA	-9.79	109.46	119.93
1	B	171	ASP	CA-C-N	-9.68	107.74	119.84
1	B	171	ASP	C-N-CA	-9.68	107.74	119.84
1	M	171	ASP	CA-C-N	-9.46	109.01	119.98
1	M	171	ASP	C-N-CA	-9.46	109.01	119.98
1	L	175	VAL	CB-CA-C	8.94	120.60	110.41
1	H	175	VAL	CB-CA-C	8.54	120.14	110.41
1	L	72	ASP	CA-C-N	8.40	129.46	120.47
1	L	72	ASP	C-N-CA	8.40	129.46	120.47
1	J	213	GLY	N-CA-C	-8.18	104.83	113.58
1	A	171	ASP	CA-C-N	-8.15	109.65	119.84
1	A	171	ASP	C-N-CA	-8.15	109.65	119.84
1	I	213	GLY	N-CA-C	-8.02	105.00	113.58
1	K	213	GLY	N-CA-C	-8.00	105.02	113.58
1	C	171	ASP	CA-C-N	-7.92	109.93	119.84
1	C	171	ASP	C-N-CA	-7.92	109.93	119.84
1	C	213	GLY	N-CA-C	-7.90	105.13	113.58
1	B	213	GLY	N-CA-C	-7.77	105.27	113.58
1	E	213	GLY	N-CA-C	-7.68	105.36	113.58
1	E	175	VAL	CB-CA-C	7.51	118.97	110.41
1	D	213	GLY	N-CA-C	-7.51	105.55	113.58
1	J	175	VAL	CB-CA-C	7.45	118.90	110.41
1	K	101	VAL	N-CA-C	-7.35	102.20	113.16
1	L	213	GLY	N-CA-C	-7.19	105.89	113.58
1	F	213	GLY	N-CA-C	-7.01	106.08	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	213	GLY	N-CA-C	-7.00	106.09	113.58
1	H	213	GLY	N-CA-C	-6.90	106.20	113.58
1	M	213	GLY	N-CA-C	-6.69	106.42	113.58
1	J	245	PRO	N-CA-C	-6.59	99.79	110.40
1	A	213	GLY	N-CA-C	-6.57	106.55	113.58
1	K	72	ASP	CA-C-N	6.44	128.29	120.94
1	K	72	ASP	C-N-CA	6.44	128.29	120.94
1	J	162	ASN	N-CA-C	6.38	119.92	110.48
1	K	239	ARG	N-CA-C	6.34	119.23	108.90
1	H	199	ALA	N-CA-C	-6.33	105.02	114.64
1	K	75	THR	N-CA-C	6.33	119.12	111.40
1	B	199	ALA	N-CA-C	-6.29	105.08	114.64
1	I	145	ILE	CB-CA-C	-6.28	102.96	111.63
1	E	245	PRO	N-CA-C	-6.28	100.29	110.40
1	B	239	ARG	N-CA-C	6.15	119.42	109.40
1	B	49	GLY	N-CA-C	6.02	118.70	110.69
1	J	239	ARG	N-CA-C	5.99	119.16	109.40
1	M	199	ALA	N-CA-C	-5.98	105.55	114.64
1	I	245	PRO	N-CA-C	-5.96	100.80	110.40
1	M	239	ARG	N-CA-C	5.96	119.18	109.59
1	A	239	ARG	N-CA-C	5.94	119.09	109.40
1	C	239	ARG	N-CA-C	5.94	119.09	109.40
1	E	239	ARG	N-CA-C	5.94	119.08	109.40
1	C	49	GLY	N-CA-C	5.92	118.56	110.69
1	L	49	GLY	N-CA-C	5.92	119.09	110.63
1	G	239	ARG	N-CA-C	5.90	119.02	109.40
1	A	199	ALA	N-CA-C	-5.89	105.69	114.64
1	K	245	PRO	N-CA-C	-5.89	100.92	110.40
1	C	199	ALA	N-CA-C	-5.88	105.70	114.64
1	G	199	ALA	N-CA-C	-5.86	105.73	114.64
1	J	199	ALA	N-CA-C	-5.82	105.79	114.64
1	E	199	ALA	N-CA-C	-5.81	105.80	114.64
1	K	162	ASN	N-CA-C	5.76	118.62	110.50
1	M	49	GLY	N-CA-C	5.75	118.85	110.63
1	F	49	GLY	N-CA-C	5.73	118.31	110.69
1	D	162	ASN	N-CA-C	5.71	118.73	110.28
1	D	105	ALA	N-CA-C	-5.71	105.41	112.38
1	D	104	GLN	N-CA-C	-5.71	105.05	113.72
1	I	152	GLU	N-CA-C	-5.69	103.02	110.53
1	D	72	ASP	CA-C-N	5.67	127.40	120.94
1	D	72	ASP	C-N-CA	5.67	127.40	120.94
1	H	142	SER	N-CA-C	-5.65	99.97	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	245	PRO	N-CA-C	-5.63	101.33	110.40
1	I	71	ILE	N-CA-C	-5.62	100.32	108.36
1	L	105	ALA	N-CA-C	-5.59	105.18	112.23
1	M	142	SER	N-CA-C	-5.59	100.07	109.07
1	M	245	PRO	N-CA-C	-5.57	101.44	110.40
1	L	199	ALA	N-CA-C	-5.54	106.22	114.64
1	L	239	ARG	N-CA-C	5.54	118.42	109.40
1	D	245	PRO	N-CA-C	-5.50	101.54	110.40
1	H	239	ARG	N-CA-C	5.49	118.35	109.40
1	I	239	ARG	N-CA-C	5.47	118.40	109.59
1	I	199	ALA	N-CA-C	-5.44	106.37	114.64
1	B	245	PRO	N-CA-C	-5.44	101.26	112.47
1	E	105	ALA	N-CA-C	-5.42	106.44	113.16
1	J	141	ILE	N-CA-CB	-5.41	105.62	112.60
1	D	199	ALA	N-CA-C	-5.40	106.43	114.64
1	F	239	ARG	N-CA-C	5.40	118.29	109.59
1	L	245	PRO	N-CA-C	-5.40	101.35	112.47
1	E	145	ILE	CB-CA-C	-5.39	104.19	111.63
1	D	172	PRO	N-CA-C	-5.38	102.49	111.26
1	H	245	PRO	N-CA-C	-5.35	101.78	110.40
1	D	75	THR	N-CA-C	5.35	117.93	111.40
1	G	245	PRO	N-CA-C	-5.34	101.81	110.40
1	M	212	ASP	N-CA-C	-5.34	105.54	111.36
1	K	199	ALA	N-CA-C	-5.31	106.56	114.64
1	D	239	ARG	N-CA-C	5.30	118.04	109.40
1	H	145	ILE	CB-CA-C	-5.30	104.32	111.63
1	K	233	THR	N-CA-C	-5.28	107.50	114.31
1	C	245	PRO	N-CA-C	-5.27	101.62	112.47
1	J	51	ILE	CB-CA-C	-5.27	105.61	111.35
1	L	152	GLU	N-CA-C	-5.26	103.59	110.53
1	B	103	ASP	N-CA-C	-5.23	107.20	113.21
1	F	199	ALA	N-CA-C	-5.21	106.72	114.64
1	J	125	VAL	CB-CA-C	-5.16	105.29	112.04
1	C	162	ASN	N-CA-C	5.14	118.09	110.48
1	H	162	ASN	N-CA-C	5.13	118.08	110.48
1	L	145	ILE	CB-CA-C	-5.12	104.57	111.63
1	A	135	THR	N-CA-C	-5.11	106.14	112.38
1	C	212	ASP	N-CA-C	-5.10	105.80	111.36
1	E	152	GLU	N-CA-C	-5.07	103.84	110.53
1	A	245	PRO	N-CA-C	-5.07	102.03	112.47
1	K	152	GLU	N-CA-C	-5.05	103.86	110.53
1	H	152	GLU	N-CA-C	-5.05	103.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	98	LYS	N-CA-C	-5.04	105.67	111.07
1	A	212	ASP	N-CA-C	-5.03	105.88	111.36
1	F	161	ALA	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	THR	Mainchain
1	I	111	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1771	0	1774	118	1
1	B	1771	0	1775	110	0
1	C	1771	0	1775	104	0
1	D	1771	0	1775	119	1
1	E	1771	0	1775	107	0
1	F	1771	0	1775	113	0
1	G	1771	0	1775	123	0
1	H	1771	0	1775	118	0
1	I	1771	0	1775	121	0
1	J	1771	0	1775	116	0
1	K	1771	0	1775	125	0
1	L	1771	0	1775	134	0
1	M	1771	0	1775	112	0
2	A	6	0	8	5	0
2	B	6	0	5	3	0
2	J	6	0	5	6	0
2	M	6	0	5	3	0
3	C	6	0	5	2	0
3	D	6	0	5	0	0
3	E	6	0	5	2	0
3	F	6	0	5	4	0
3	G	6	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	6	0	5	2	0
3	I	6	0	5	4	0
3	K	6	0	5	3	0
3	L	6	0	5	1	0
All	All	23101	0	23142	1440	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1440) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:GLY:HA3	3:F:361:3GR:O2	1.37	1.24
1:M:70:GLN:HE22	1:M:135:THR:HG23	1.08	1.15
1:A:70:GLN:HE22	1:A:135:THR:HG23	1.18	1.07
1:F:91:GLN:HG2	1:F:95:GLN:HE21	1.21	1.05
1:J:91:GLN:HG2	1:J:95:GLN:HE21	1.16	1.04
1:J:147:ARG:N	2:J:361:GOL:O2	1.89	1.04
1:B:91:GLN:HG2	1:B:95:GLN:HE21	1.22	1.03
1:B:55:LEU:HD12	1:B:67:GLN:HG2	1.38	1.02
1:G:91:GLN:HG2	1:G:95:GLN:HE21	1.21	1.02
1:I:171:ASP:HB3	1:I:172:PRO:HD3	1.43	1.01
1:F:171:ASP:HB3	1:F:172:PRO:HD3	1.41	1.01
1:K:107:SER:HB3	1:K:110:GLN:HG3	1.42	0.99
1:K:91:GLN:HG2	1:K:95:GLN:HE21	1.22	0.99
1:C:91:GLN:HG2	1:C:95:GLN:HE21	1.27	0.99
1:K:52:LEU:HD13	1:K:72:ASP:HB2	1.44	0.98
1:I:91:GLN:HG2	1:I:95:GLN:HE21	1.25	0.98
1:E:91:GLN:HG2	1:E:95:GLN:HE21	1.25	0.98
1:L:91:GLN:HG2	1:L:95:GLN:HE21	1.26	0.98
1:A:91:GLN:HG2	1:A:95:GLN:HE21	1.26	0.97
1:C:171:ASP:HB3	1:C:172:PRO:HD3	1.44	0.97
1:D:91:GLN:HG2	1:D:95:GLN:HE21	1.26	0.97
1:G:48:ASN:ND2	1:G:158:ASN:H	1.64	0.96
2:A:361:GOL:O1	1:B:228:SER:HB3	1.65	0.96
1:M:91:GLN:HG2	1:M:95:GLN:HE21	1.30	0.95
1:D:171:ASP:HB3	1:D:172:PRO:HD3	1.46	0.95
1:G:107:SER:H	1:G:110:GLN:HE21	1.15	0.95
1:C:146:GLY:HA3	3:C:361:3GR:O1	1.65	0.94
1:A:48:ASN:ND2	1:A:158:ASN:H	1.66	0.94
1:G:132:LEU:O	1:G:135:THR:HB	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ASP:HB3	1:E:172:PRO:HD3	1.48	0.93
1:B:132:LEU:O	1:B:135:THR:HB	1.68	0.93
1:C:132:LEU:O	1:C:135:THR:HB	1.69	0.92
1:M:48:ASN:ND2	1:M:158:ASN:H	1.68	0.92
1:G:171:ASP:HB3	1:G:172:PRO:CD	2.00	0.92
1:H:91:GLN:HG2	1:H:95:GLN:HE21	1.31	0.92
1:K:132:LEU:O	1:K:135:THR:HB	1.69	0.91
1:L:132:LEU:O	1:L:135:THR:HB	1.71	0.91
1:H:62:VAL:HG23	1:H:66:GLN:CD	1.96	0.90
1:I:146:GLY:HA3	3:I:361:3GR:O2	1.72	0.90
1:K:108:LYS:HD2	1:L:96:ARG:HD2	1.53	0.90
1:L:48:ASN:ND2	1:L:158:ASN:H	1.70	0.90
1:K:171:ASP:HB3	1:K:172:PRO:CD	2.00	0.90
1:H:48:ASN:ND2	1:H:158:ASN:H	1.70	0.89
1:H:132:LEU:O	1:H:135:THR:HB	1.71	0.89
1:L:62:VAL:HG21	1:L:68:LEU:HD21	1.54	0.89
1:J:132:LEU:O	1:J:135:THR:HB	1.72	0.89
1:M:70:GLN:NE2	1:M:135:THR:HG23	1.87	0.89
1:M:147:ARG:N	2:M:361:GOL:O1	2.04	0.89
1:L:171:ASP:HB3	1:L:172:PRO:CD	2.02	0.89
1:D:132:LEU:O	1:D:135:THR:HB	1.74	0.88
1:A:171:ASP:HB3	1:A:172:PRO:CD	2.03	0.88
1:G:107:SER:OG	1:G:110:GLN:HG3	1.74	0.88
1:K:48:ASN:ND2	1:K:158:ASN:H	1.72	0.88
1:B:171:ASP:HB3	1:B:172:PRO:CD	2.04	0.87
1:D:48:ASN:ND2	1:D:158:ASN:H	1.72	0.87
1:F:171:ASP:HB3	1:F:172:PRO:CD	2.05	0.87
1:I:132:LEU:O	1:I:135:THR:HB	1.75	0.86
1:M:171:ASP:HB3	1:M:172:PRO:CD	2.04	0.86
1:J:52:LEU:HD13	1:J:72:ASP:HB2	1.57	0.86
1:A:70:GLN:NE2	1:A:135:THR:HG23	1.91	0.86
1:B:145:ILE:HG23	1:B:167:VAL:HG22	1.56	0.86
1:I:34:ARG:HH11	1:I:34:ARG:HB3	1.41	0.85
1:C:62:VAL:HG21	1:C:68:LEU:HD21	1.57	0.85
1:J:91:GLN:HG2	1:J:95:GLN:NE2	1.92	0.85
1:M:55:LEU:HD12	1:M:67:GLN:HG2	1.56	0.85
1:F:62:VAL:HG21	1:F:68:LEU:HD21	1.57	0.85
1:F:85:ALA:HB2	1:G:82:SER:HB2	1.57	0.85
1:B:48:ASN:ND2	1:B:158:ASN:H	1.74	0.85
1:G:62:VAL:HG21	1:G:68:LEU:HD21	1.58	0.85
1:A:62:VAL:HG21	1:A:68:LEU:HD21	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:132:LEU:O	1:M:135:THR:HB	1.77	0.84
1:E:62:VAL:HG21	1:E:68:LEU:HD21	1.57	0.84
1:E:132:LEU:O	1:E:135:THR:HB	1.76	0.84
1:E:186:ARG:HH11	1:E:186:ARG:HB3	1.41	0.84
1:I:171:ASP:HB3	1:I:172:PRO:CD	2.07	0.84
1:B:34:ARG:HH11	1:B:34:ARG:HB3	1.41	0.83
1:L:52:LEU:HD13	1:L:72:ASP:HB2	1.57	0.83
1:C:34:ARG:HB3	1:C:34:ARG:HH11	1.42	0.83
1:B:70:GLN:HE22	1:B:135:THR:HG23	1.41	0.83
1:G:34:ARG:HH11	1:G:34:ARG:HB3	1.43	0.83
1:H:171:ASP:HB3	1:H:172:PRO:CD	2.07	0.83
1:E:55:LEU:HD12	1:E:67:GLN:HG2	1.61	0.83
1:F:48:ASN:ND2	1:F:158:ASN:H	1.75	0.82
1:F:37:ALA:HB3	1:F:40:ILE:HD11	1.59	0.82
1:C:38:PHE:HB2	1:C:172:PRO:O	1.77	0.82
1:H:62:VAL:HG23	1:H:66:GLN:OE1	1.80	0.82
1:K:91:GLN:HG2	1:K:95:GLN:NE2	1.93	0.82
1:I:186:ARG:HH11	1:I:186:ARG:HB3	1.45	0.82
1:J:62:VAL:HG21	1:J:68:LEU:HD21	1.61	0.82
1:I:91:GLN:HG2	1:I:95:GLN:NE2	1.95	0.81
1:B:62:VAL:HG21	1:B:68:LEU:HD21	1.61	0.81
1:L:158:ASN:HD22	1:L:159:GLY:N	1.77	0.81
1:D:52:LEU:HD13	1:D:72:ASP:HB2	1.62	0.81
1:E:171:ASP:O	1:E:172:PRO:C	2.18	0.81
1:L:55:LEU:HD12	1:L:67:GLN:HG2	1.60	0.81
1:J:34:ARG:HB3	1:J:34:ARG:HH11	1.44	0.81
1:G:171:ASP:O	1:G:172:PRO:C	2.22	0.81
1:I:48:ASN:ND2	1:I:158:ASN:H	1.79	0.81
1:J:48:ASN:ND2	1:J:158:ASN:H	1.79	0.81
1:E:171:ASP:HB3	1:E:172:PRO:CD	2.09	0.80
1:H:70:GLN:HE22	1:H:135:THR:HG23	1.47	0.80
1:H:158:ASN:HD22	1:H:159:GLY:N	1.79	0.80
1:I:62:VAL:HG21	1:I:68:LEU:HD21	1.64	0.80
1:A:132:LEU:O	1:A:135:THR:HB	1.81	0.80
1:C:171:ASP:HB3	1:C:172:PRO:CD	2.10	0.80
1:F:91:GLN:HG2	1:F:95:GLN:NE2	1.97	0.80
1:L:34:ARG:HH11	1:L:34:ARG:HB3	1.44	0.80
1:D:62:VAL:HG21	1:D:68:LEU:HD21	1.62	0.80
1:E:48:ASN:ND2	1:E:158:ASN:H	1.78	0.80
1:J:186:ARG:HH11	1:J:186:ARG:HB3	1.47	0.79
1:M:62:VAL:HG23	1:M:66:GLN:CD	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLN:HG2	1:B:95:GLN:NE2	1.97	0.79
1:D:171:ASP:HB3	1:D:172:PRO:CD	2.11	0.79
1:A:34:ARG:HH11	1:A:34:ARG:HB3	1.46	0.79
1:G:91:GLN:HG2	1:G:95:GLN:NE2	1.96	0.79
1:A:55:LEU:HD12	1:A:67:GLN:HG2	1.64	0.79
1:L:130:ILE:HD12	1:M:74:ALA:HB1	1.65	0.79
1:F:62:VAL:HG23	1:F:66:GLN:CD	2.09	0.78
1:B:62:VAL:HG23	1:B:66:GLN:CD	2.09	0.78
1:K:62:VAL:HG21	1:K:68:LEU:HD21	1.65	0.78
1:M:34:ARG:HH11	1:M:34:ARG:HB3	1.47	0.78
1:K:34:ARG:HH11	1:K:34:ARG:HB3	1.47	0.78
1:D:34:ARG:HH11	1:D:34:ARG:HB3	1.49	0.78
1:E:34:ARG:HB3	1:E:34:ARG:HH11	1.47	0.78
1:B:106:VAL:HG13	1:B:110:GLN:OE1	1.84	0.78
1:D:46:GLN:HB2	1:D:134:TYR:CD2	2.19	0.78
1:G:109:GLN:OE1	1:H:96:ARG:NH2	2.17	0.78
1:J:171:ASP:HB3	1:J:172:PRO:CD	2.14	0.77
1:L:70:GLN:HE22	1:L:135:THR:HG23	1.48	0.77
1:B:186:ARG:HH11	1:B:186:ARG:HB3	1.48	0.77
1:G:186:ARG:HH11	1:G:186:ARG:HB3	1.48	0.77
1:K:62:VAL:HG23	1:K:66:GLN:CD	2.08	0.77
1:D:62:VAL:HG23	1:D:66:GLN:CD	2.10	0.77
1:H:171:ASP:O	1:H:172:PRO:C	2.21	0.77
1:J:171:ASP:O	1:J:172:PRO:C	2.21	0.77
1:G:145:ILE:HD12	1:G:145:ILE:H	1.50	0.77
1:M:186:ARG:HB3	1:M:186:ARG:HH11	1.48	0.77
1:G:62:VAL:HG23	1:G:66:GLN:CD	2.09	0.77
1:L:186:ARG:HH11	1:L:186:ARG:HB3	1.47	0.77
1:E:91:GLN:HG2	1:E:95:GLN:NE2	1.99	0.77
1:C:91:GLN:HG2	1:C:95:GLN:NE2	2.00	0.77
1:E:62:VAL:HG23	1:E:66:GLN:CD	2.10	0.77
1:C:55:LEU:HD12	1:C:67:GLN:HG2	1.67	0.76
1:D:186:ARG:HH11	1:D:186:ARG:HB3	1.48	0.76
1:J:62:VAL:HG23	1:J:66:GLN:CD	2.10	0.76
1:K:70:GLN:HE22	1:K:135:THR:HG23	1.50	0.76
1:F:52:LEU:HD13	1:F:72:ASP:HB2	1.68	0.76
1:I:171:ASP:O	1:I:172:PRO:C	2.26	0.76
1:L:62:VAL:HG23	1:L:66:GLN:CD	2.11	0.76
1:H:34:ARG:HH11	1:H:34:ARG:HB3	1.51	0.75
1:E:38:PHE:HB2	1:E:172:PRO:O	1.86	0.75
1:I:206:VAL:HG11	1:I:257:ALA:HB1	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:VAL:HG23	1:M:66:GLN:OE1	1.85	0.75
1:F:145:ILE:HD12	1:F:145:ILE:H	1.49	0.75
1:I:62:VAL:HG23	1:I:66:GLN:CD	2.12	0.75
1:A:101:VAL:HG13	1:A:106:VAL:HG23	1.69	0.75
1:H:62:VAL:HG21	1:H:68:LEU:HD21	1.68	0.74
1:G:171:ASP:HB3	1:G:172:PRO:HD2	1.69	0.74
1:G:107:SER:N	1:G:110:GLN:HE21	1.84	0.74
1:C:145:ILE:HG23	1:C:167:VAL:HG22	1.70	0.74
1:D:158:ASN:HD22	1:D:159:GLY:N	1.85	0.74
1:C:48:ASN:ND2	1:C:158:ASN:H	1.85	0.74
1:L:171:ASP:O	1:L:172:PRO:C	2.30	0.74
1:D:38:PHE:HB2	1:D:172:PRO:O	1.88	0.74
1:K:171:ASP:O	1:K:172:PRO:C	2.28	0.74
1:M:38:PHE:HB2	1:M:172:PRO:O	1.87	0.74
1:M:62:VAL:HG21	1:M:68:LEU:HD21	1.68	0.74
1:D:48:ASN:HD21	1:D:158:ASN:H	1.35	0.74
1:B:38:PHE:HB2	1:B:172:PRO:O	1.88	0.74
1:G:55:LEU:HD12	1:G:67:GLN:HG2	1.69	0.73
1:I:45:PRO:HG3	1:I:156:VAL:HG22	1.70	0.73
1:I:65:GLY:O	1:I:138:LEU:HD22	1.88	0.73
1:K:147:ARG:HB2	3:K:361:3GR:O3	1.88	0.73
1:A:91:GLN:HG2	1:A:95:GLN:NE2	2.03	0.73
1:J:106:VAL:HG13	1:J:110:GLN:HB2	1.69	0.73
1:F:34:ARG:HH11	1:F:34:ARG:HB3	1.53	0.73
1:F:101:VAL:HG21	1:F:111:TYR:HB2	1.69	0.73
1:I:70:GLN:HE22	1:I:135:THR:HG23	1.53	0.73
1:H:100:LEU:HB3	1:H:106:VAL:HB	1.70	0.73
1:D:110:GLN:C	1:D:112:ALA:H	1.96	0.73
1:D:91:GLN:HG2	1:D:95:GLN:NE2	2.03	0.73
1:F:171:ASP:O	1:F:172:PRO:C	2.27	0.73
1:H:55:LEU:HD12	1:H:67:GLN:HG2	1.70	0.73
2:A:361:GOL:O1	1:B:228:SER:CB	2.36	0.73
1:B:70:GLN:NE2	1:B:135:THR:HG23	2.02	0.73
1:E:158:ASN:HD22	1:E:159:GLY:N	1.86	0.73
1:C:62:VAL:HG23	1:C:66:GLN:CD	2.14	0.72
1:K:188:ARG:NH2	1:L:246:ASN:O	2.17	0.72
1:C:67:GLN:HA	1:C:138:LEU:HD23	1.71	0.72
1:A:158:ASN:HD22	1:A:159:GLY:N	1.88	0.72
1:E:145:ILE:HG23	1:E:167:VAL:HG22	1.71	0.72
1:F:71:ILE:O	1:F:73:PRO:HD3	1.89	0.72
1:B:171:ASP:O	1:B:172:PRO:C	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ARG:HH11	1:C:186:ARG:HB3	1.54	0.72
1:D:103:ASP:C	1:D:105:ALA:H	1.97	0.72
1:B:30:GLU:HG2	1:B:258:GLN:HG2	1.72	0.72
1:L:147:ARG:N	3:L:361:3GR:O3	2.22	0.72
1:M:70:GLN:HE22	1:M:135:THR:CG2	1.97	0.72
1:A:186:ARG:HB3	1:A:186:ARG:HH11	1.55	0.72
1:I:147:ARG:N	3:I:361:3GR:O2	2.22	0.72
1:E:206:VAL:HG11	1:E:257:ALA:HB1	1.72	0.71
1:M:158:ASN:HD22	1:M:159:GLY:N	1.88	0.71
1:H:126:GLU:O	1:H:130:ILE:HG12	1.90	0.71
1:L:101:VAL:HG11	1:L:108:LYS:HG2	1.71	0.71
1:L:38:PHE:HB2	1:L:172:PRO:O	1.88	0.71
1:A:38:PHE:HB2	1:A:172:PRO:O	1.90	0.71
1:G:38:PHE:HB2	1:G:172:PRO:O	1.90	0.71
1:F:146:GLY:CA	3:F:361:3GR:O2	2.29	0.71
1:H:186:ARG:HB3	1:H:186:ARG:HH11	1.53	0.70
1:I:145:ILE:HD12	1:I:145:ILE:H	1.56	0.70
1:L:91:GLN:HG2	1:L:95:GLN:NE2	2.03	0.70
1:A:104:GLN:HG3	1:G:104:GLN:OE1	1.91	0.70
1:H:91:GLN:HG2	1:H:95:GLN:NE2	2.06	0.70
1:D:52:LEU:HD22	1:D:72:ASP:HA	1.72	0.70
1:L:100:LEU:HB3	1:L:106:VAL:HG23	1.72	0.70
1:B:62:VAL:HG23	1:B:66:GLN:OE1	1.91	0.70
1:K:186:ARG:HH11	1:K:186:ARG:HB3	1.56	0.70
1:M:170:LEU:HD21	1:M:251:PRO:HD3	1.74	0.70
1:J:55:LEU:HD12	1:J:67:GLN:HG2	1.73	0.70
1:J:245:PRO:C	1:J:247:ASN:H	2.00	0.70
1:M:145:ILE:HG23	1:M:167:VAL:HG22	1.72	0.70
1:E:45:PRO:HG3	1:E:156:VAL:HG22	1.73	0.70
1:J:206:VAL:HG11	1:J:257:ALA:HB1	1.71	0.70
1:L:101:VAL:HG21	1:L:111:TYR:HB2	1.73	0.70
1:M:245:PRO:C	1:M:247:ASN:H	2.00	0.70
1:A:62:VAL:HG23	1:A:66:GLN:CD	2.16	0.69
1:C:70:GLN:HE22	1:C:135:THR:HG23	1.54	0.69
1:E:70:GLN:HE22	1:E:135:THR:HG23	1.57	0.69
1:H:45:PRO:HG3	1:H:156:VAL:HG22	1.72	0.69
1:D:126:GLU:O	1:D:130:ILE:HG12	1.92	0.69
1:F:206:VAL:HG11	1:F:257:ALA:HB1	1.74	0.69
1:C:45:PRO:HG3	1:C:156:VAL:HG22	1.75	0.69
1:M:67:GLN:HA	1:M:138:LEU:HD23	1.75	0.69
1:F:197:GLU:OE2	1:F:205:LYS:HD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:PRO:C	1:F:247:ASN:H	2.00	0.69
1:K:158:ASN:HD22	1:K:159:GLY:N	1.90	0.69
1:H:206:VAL:HG11	1:H:257:ALA:HB1	1.75	0.69
1:K:62:VAL:HG23	1:K:66:GLN:OE1	1.93	0.69
1:A:48:ASN:HD21	1:A:158:ASN:H	1.37	0.69
1:B:70:GLN:HE22	1:B:135:THR:CG2	2.05	0.69
1:B:245:PRO:C	1:B:247:ASN:H	2.01	0.69
1:G:67:GLN:HA	1:G:138:LEU:HD23	1.74	0.69
1:A:245:PRO:C	1:A:247:ASN:H	2.01	0.69
1:B:206:VAL:HG11	1:B:257:ALA:HB1	1.75	0.69
1:E:104:GLN:HG2	1:K:108:LYS:HB2	1.74	0.69
1:F:186:ARG:HH11	1:F:186:ARG:HB3	1.57	0.69
1:A:45:PRO:HG3	1:A:156:VAL:HG22	1.73	0.69
1:F:132:LEU:O	1:F:135:THR:HB	1.92	0.69
1:B:67:GLN:HA	1:B:138:LEU:HD23	1.75	0.69
1:G:245:PRO:C	1:G:247:ASN:H	2.02	0.69
1:D:100:LEU:HB3	1:D:106:VAL:HG23	1.75	0.68
1:G:107:SER:H	1:G:110:GLN:NE2	1.90	0.68
1:J:45:PRO:HG3	1:J:156:VAL:HG22	1.74	0.68
1:K:52:LEU:HD22	1:K:72:ASP:HA	1.76	0.68
1:B:146:GLY:HA3	2:B:361:GOL:H12	1.75	0.68
1:I:109:GLN:NE2	1:J:96:ARG:HH21	1.91	0.68
1:I:245:PRO:C	1:I:247:ASN:H	2.00	0.68
1:H:145:ILE:HD12	1:H:145:ILE:H	1.58	0.68
1:E:52:LEU:HD13	1:E:72:ASP:HB2	1.76	0.68
1:J:67:GLN:OE1	1:J:136:LYS:HD3	1.92	0.68
1:D:171:ASP:O	1:D:172:PRO:C	2.34	0.68
1:K:206:VAL:HG11	1:K:257:ALA:HB1	1.76	0.68
1:L:45:PRO:HG3	1:L:156:VAL:HG22	1.74	0.68
1:M:91:GLN:HG2	1:M:95:GLN:NE2	2.06	0.68
1:E:99:LEU:O	1:E:102:ALA:HB3	1.94	0.67
1:F:145:ILE:HG23	1:F:167:VAL:HG22	1.75	0.67
1:A:206:VAL:HG11	1:A:257:ALA:HB1	1.77	0.67
1:F:38:PHE:HB2	1:F:172:PRO:O	1.95	0.67
1:A:107:SER:OG	1:A:110:GLN:HG3	1.94	0.67
1:J:38:PHE:HB2	1:J:172:PRO:O	1.95	0.67
1:H:46:GLN:HB2	1:H:134:TYR:CD2	2.30	0.67
1:H:147:ARG:N	3:H:361:3GR:O2	2.26	0.66
1:K:55:LEU:HD12	1:K:67:GLN:HG2	1.77	0.66
1:B:45:PRO:HG3	1:B:156:VAL:HG22	1.77	0.66
1:L:70:GLN:NE2	1:L:135:THR:HG23	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:HB3	1:A:172:PRO:HD2	1.76	0.66
1:K:70:GLN:NE2	1:K:135:THR:HG23	2.09	0.66
1:C:245:PRO:C	1:C:247:ASN:H	2.02	0.66
1:I:158:ASN:HD22	1:I:159:GLY:N	1.93	0.66
1:B:126:GLU:O	1:B:130:ILE:HG12	1.95	0.66
1:F:67:GLN:HA	1:F:138:LEU:HD23	1.78	0.66
1:L:245:PRO:C	1:L:247:ASN:H	2.04	0.66
1:D:97:TYR:O	1:D:101:VAL:HG23	1.96	0.66
1:G:226:GLU:HG3	1:H:144:ARG:HE	1.61	0.66
1:M:147:ARG:HD2	2:M:361:GOL:H12	1.76	0.66
1:G:48:ASN:HD22	1:G:158:ASN:H	1.44	0.66
1:I:38:PHE:HB2	1:I:172:PRO:O	1.95	0.66
1:M:100:LEU:HB3	1:M:106:VAL:HG23	1.77	0.66
1:K:107:SER:HB3	1:K:110:GLN:CG	2.21	0.65
1:D:45:PRO:HG3	1:D:156:VAL:HG22	1.77	0.65
1:A:40:ILE:HG12	1:A:168:GLN:HG2	1.76	0.65
1:K:48:ASN:HD21	1:K:158:ASN:H	1.44	0.65
1:C:106:VAL:HG22	1:C:110:GLN:HB2	1.78	0.65
1:F:126:GLU:O	1:F:130:ILE:HG12	1.96	0.65
1:H:35:THR:HG22	1:H:175:VAL:HG22	1.79	0.65
1:H:97:TYR:O	1:H:101:VAL:HG23	1.96	0.65
1:M:48:ASN:O	1:M:76:TYR:OH	2.07	0.65
1:A:145:ILE:HG23	1:A:167:VAL:HG22	1.79	0.65
1:C:171:ASP:O	1:C:172:PRO:C	2.37	0.65
1:D:245:PRO:C	1:D:247:ASN:H	2.05	0.65
1:G:101:VAL:HG21	1:G:111:TYR:HB2	1.79	0.65
1:J:145:ILE:HG23	1:J:167:VAL:HG22	1.77	0.65
1:L:188:ARG:HH21	1:M:248:GLU:HA	1.61	0.65
1:C:48:ASN:ND2	1:C:157:THR:HA	2.12	0.65
1:E:38:PHE:CD2	1:E:169:GLN:NE2	2.65	0.65
1:D:97:TYR:HA	1:D:106:VAL:HG21	1.79	0.65
1:A:70:GLN:HE22	1:A:135:THR:CG2	2.04	0.65
1:E:248:GLU:HB3	1:F:185:LEU:HD21	1.79	0.65
1:D:110:GLN:C	1:D:112:ALA:N	2.55	0.65
1:H:48:ASN:HD21	1:H:158:ASN:H	1.45	0.64
1:L:206:VAL:HG11	1:L:257:ALA:HB1	1.79	0.64
1:E:186:ARG:O	1:E:190:GLU:HG3	1.97	0.64
1:L:126:GLU:O	1:L:130:ILE:HG12	1.97	0.64
1:A:126:GLU:O	1:A:130:ILE:HG12	1.97	0.64
1:C:52:LEU:HD13	1:C:72:ASP:HB2	1.77	0.64
1:E:38:PHE:HD2	1:E:169:GLN:NE2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ILE:HG23	1:G:167:VAL:HG22	1.78	0.64
1:K:186:ARG:HD3	1:K:190:GLU:OE2	1.97	0.64
1:L:35:THR:HG22	1:L:175:VAL:HG22	1.79	0.64
1:C:145:ILE:HD12	1:C:145:ILE:H	1.63	0.64
1:J:144:ARG:HG3	1:J:144:ARG:HH11	1.63	0.64
1:L:189:ARG:NH2	1:M:212:ASP:OD1	2.28	0.64
1:C:197:GLU:OE2	1:C:205:LYS:HD2	1.98	0.64
1:D:71:ILE:O	1:D:73:PRO:HD3	1.97	0.64
1:G:206:VAL:HG11	1:G:257:ALA:HB1	1.79	0.64
1:I:52:LEU:HD13	1:I:72:ASP:HB2	1.80	0.64
1:L:38:PHE:HD2	1:L:169:GLN:NE2	1.95	0.63
1:E:186:ARG:HH11	1:E:186:ARG:CB	2.11	0.63
1:H:30:GLU:HG2	1:H:258:GLN:HG2	1.79	0.63
1:G:186:ARG:HD3	1:G:190:GLU:OE2	1.98	0.63
1:K:67:GLN:HA	1:K:138:LEU:HD23	1.80	0.63
1:M:206:VAL:HG11	1:M:257:ALA:HB1	1.81	0.63
1:G:40:ILE:HG12	1:G:168:GLN:HG2	1.81	0.63
1:M:197:GLU:OE2	1:M:205:LYS:HD2	1.98	0.63
1:B:186:ARG:O	1:B:190:GLU:HG3	1.98	0.63
1:F:70:GLN:HE22	1:F:135:THR:HG23	1.64	0.63
1:K:54:ARG:HD2	1:K:54:ARG:O	1.99	0.63
1:D:206:VAL:HG11	1:D:257:ALA:HB1	1.80	0.63
1:F:146:GLY:HA3	3:F:361:3GR:HA	1.60	0.63
1:H:70:GLN:NE2	1:H:135:THR:HG23	2.13	0.63
1:J:52:LEU:HD22	1:J:72:ASP:HA	1.81	0.63
1:M:186:ARG:HH11	1:M:186:ARG:CB	2.12	0.63
1:B:48:ASN:ND2	1:B:157:THR:HA	2.13	0.62
1:C:206:VAL:HG11	1:C:257:ALA:HB1	1.80	0.62
1:C:107:SER:OG	1:C:110:GLN:HG3	1.98	0.62
1:E:126:GLU:O	1:E:130:ILE:HG12	2.00	0.62
1:G:31:LEU:HB3	1:G:177:VAL:CG1	2.29	0.62
1:K:126:GLU:O	1:K:130:ILE:HG12	1.99	0.62
1:A:171:ASP:O	1:A:172:PRO:C	2.39	0.62
1:H:245:PRO:C	1:H:247:ASN:H	2.05	0.62
1:M:171:ASP:HB3	1:M:172:PRO:HD2	1.81	0.62
1:E:106:VAL:HG13	1:E:110:GLN:HB2	1.79	0.62
1:F:145:ILE:HD12	1:F:145:ILE:N	2.15	0.62
1:K:38:PHE:HB2	1:K:172:PRO:O	1.99	0.62
1:A:30:GLU:HG2	1:A:258:GLN:HG2	1.80	0.62
1:E:62:VAL:HG23	1:E:66:GLN:OE1	2.00	0.62
1:D:221:ARG:HD3	1:D:223:GLU:OE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:ARG:O	1:I:99:LEU:HB3	1.98	0.62
1:K:245:PRO:C	1:K:247:ASN:H	2.06	0.62
1:L:38:PHE:CD2	1:L:169:GLN:NE2	2.68	0.62
1:F:186:ARG:HD3	1:F:190:GLU:OE2	1.99	0.62
1:E:30:GLU:HG2	1:E:258:GLN:HG2	1.82	0.62
1:E:48:ASN:HD21	1:E:158:ASN:H	1.47	0.62
1:F:45:PRO:HG3	1:F:156:VAL:HG22	1.82	0.61
1:G:48:ASN:ND2	1:G:158:ASN:N	2.44	0.61
1:F:158:ASN:HD22	1:F:159:GLY:N	1.98	0.61
1:K:43:VAL:HG23	1:K:165:ALA:O	2.00	0.61
1:C:208:LEU:HB2	1:C:242:PHE:CE2	2.36	0.61
1:G:145:ILE:HD12	1:G:145:ILE:N	2.15	0.61
1:I:228:SER:HB3	2:J:361:GOL:H2	1.82	0.61
1:A:186:ARG:O	1:A:190:GLU:HG3	2.01	0.61
1:L:95:GLN:O	1:L:99:LEU:HD13	2.00	0.61
1:H:67:GLN:HA	1:H:138:LEU:HD23	1.81	0.61
1:J:186:ARG:O	1:J:190:GLU:HG3	2.00	0.61
1:C:186:ARG:HD3	1:C:190:GLU:OE2	1.99	0.61
1:M:48:ASN:HD21	1:M:158:ASN:H	1.43	0.61
1:H:112:ALA:HB1	1:I:92:GLU:HG3	1.83	0.61
1:H:188:ARG:HH21	1:I:248:GLU:HA	1.66	0.61
1:I:145:ILE:HD12	1:I:145:ILE:N	2.15	0.61
1:L:158:ASN:HD22	1:L:158:ASN:C	2.04	0.61
1:L:208:LEU:HB2	1:L:242:PHE:CE2	2.36	0.61
1:A:47:VAL:HG22	1:A:76:TYR:CZ	2.36	0.61
1:F:48:ASN:HD21	1:F:158:ASN:H	1.49	0.61
1:I:109:GLN:NE2	1:J:96:ARG:NH2	2.48	0.61
1:J:188:ARG:NH2	1:K:246:ASN:O	2.34	0.61
1:I:197:GLU:OE2	1:I:205:LYS:HD2	2.01	0.61
1:L:40:ILE:O	1:M:151:THR:HB	2.01	0.60
1:B:158:ASN:HD22	1:B:159:GLY:N	1.99	0.60
1:E:221:ARG:HD3	1:E:223:GLU:OE2	2.01	0.60
1:J:144:ARG:HG3	1:J:144:ARG:NH1	2.16	0.60
1:K:186:ARG:O	1:K:190:GLU:HG3	2.00	0.60
1:L:145:ILE:HD12	1:L:145:ILE:H	1.66	0.60
1:M:45:PRO:HG3	1:M:156:VAL:HG22	1.83	0.60
1:E:245:PRO:C	1:E:247:ASN:H	2.08	0.60
1:I:185:LEU:HD21	1:J:248:GLU:HB3	1.83	0.60
1:G:71:ILE:O	1:G:73:PRO:HD3	2.02	0.60
1:M:91:GLN:HG3	1:M:118:TYR:CE1	2.37	0.60
1:B:186:ARG:HD3	1:B:190:GLU:OE2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:SER:HA	1:G:82:SER:OG	2.01	0.60
1:G:145:ILE:HG23	1:G:167:VAL:CG2	2.32	0.60
1:J:146:GLY:HA3	2:J:361:GOL:H12	1.83	0.60
1:I:186:ARG:HH11	1:I:186:ARG:CB	2.13	0.60
1:B:100:LEU:HB3	1:B:106:VAL:HG23	1.83	0.60
1:G:158:ASN:HD22	1:G:159:GLY:N	2.00	0.60
1:I:55:LEU:N	1:I:55:LEU:HD23	2.17	0.60
1:L:171:ASP:HB3	1:L:172:PRO:HD2	1.83	0.60
1:C:106:VAL:HG23	1:C:110:GLN:CD	2.27	0.59
1:G:62:VAL:HG23	1:G:66:GLN:OE1	2.01	0.59
1:H:107:SER:OG	1:H:110:GLN:HG3	2.02	0.59
1:L:101:VAL:CG2	1:L:111:TYR:HB2	2.31	0.59
1:M:171:ASP:O	1:M:172:PRO:C	2.41	0.59
1:D:100:LEU:HD21	1:K:103:ASP:HB3	1.84	0.59
1:G:48:ASN:HD21	1:G:158:ASN:H	1.45	0.59
1:M:211:GLU:HB3	1:M:254:PHE:O	2.01	0.59
1:C:186:ARG:O	1:C:190:GLU:HG3	2.01	0.59
1:D:186:ARG:O	1:D:190:GLU:HG3	2.03	0.59
1:A:208:LEU:HD11	1:A:255:VAL:HG21	1.85	0.59
1:D:55:LEU:HD12	1:D:67:GLN:HG2	1.84	0.59
1:D:103:ASP:C	1:D:105:ALA:N	2.58	0.59
1:G:126:GLU:O	1:G:130:ILE:HG12	2.03	0.59
1:I:146:GLY:CA	3:I:361:3GR:O2	2.50	0.59
1:L:48:ASN:HD21	1:L:158:ASN:H	1.44	0.59
1:J:231:GLU:HG2	1:K:251:PRO:HB2	1.84	0.59
1:A:29:THR:HG22	1:A:30:GLU:N	2.17	0.59
1:H:140:PRO:O	1:H:141:ILE:HD12	2.03	0.59
1:L:186:ARG:O	1:L:190:GLU:HG3	2.01	0.59
1:C:206:VAL:HG13	1:C:258:GLN:O	2.02	0.59
1:J:62:VAL:HG23	1:J:66:GLN:OE1	2.01	0.59
1:M:101:VAL:CG2	1:M:111:TYR:HB2	2.33	0.59
1:M:186:ARG:O	1:M:190:GLU:HG3	2.03	0.59
1:G:197:GLU:OE2	1:G:205:LYS:HD2	2.03	0.59
1:L:226:GLU:HG3	1:M:144:ARG:HE	1.68	0.59
1:A:145:ILE:HD12	1:A:145:ILE:H	1.66	0.58
1:C:54:ARG:O	1:C:54:ARG:HG2	2.03	0.58
1:E:158:ASN:HD22	1:E:159:GLY:H	1.49	0.58
1:H:189:ARG:NH2	1:I:212:ASP:OD1	2.32	0.58
1:I:70:GLN:NE2	1:I:135:THR:HG23	2.18	0.58
1:I:228:SER:CB	2:J:361:GOL:H2	2.33	0.58
1:J:126:GLU:O	1:J:130:ILE:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:101:VAL:HG21	1:M:111:TYR:HB2	1.85	0.58
1:A:144:ARG:NE	1:B:226:GLU:OE2	2.36	0.58
1:A:211:GLU:HB3	1:A:254:PHE:O	2.03	0.58
1:B:208:LEU:HB2	1:B:242:PHE:CE2	2.39	0.58
1:C:170:LEU:HD11	1:C:251:PRO:HD3	1.85	0.58
1:J:185:LEU:HD21	1:K:248:GLU:HB3	1.86	0.58
1:K:103:ASP:C	1:K:105:ALA:H	2.10	0.58
1:L:91:GLN:HG3	1:L:118:TYR:CE1	2.38	0.58
1:B:221:ARG:HD3	1:B:223:GLU:OE2	2.02	0.58
1:E:95:GLN:O	1:E:99:LEU:HD13	2.02	0.58
1:F:147:ARG:HD2	3:F:361:3GR:O3	2.03	0.58
1:D:96:ARG:HG2	1:D:100:LEU:HD12	1.84	0.58
1:D:158:ASN:HD22	1:D:159:GLY:H	1.49	0.58
1:D:208:LEU:HD11	1:D:255:VAL:HG21	1.85	0.58
1:L:62:VAL:HG23	1:L:66:GLN:NE2	2.18	0.58
1:F:30:GLU:HG2	1:F:258:GLN:HG2	1.84	0.58
1:F:62:VAL:HG23	1:F:66:GLN:NE2	2.18	0.58
1:H:186:ARG:HD3	1:H:190:GLU:OE2	2.04	0.58
1:I:62:VAL:HG23	1:I:66:GLN:OE1	2.03	0.58
1:J:109:GLN:OE1	1:K:96:ARG:NH2	2.37	0.58
1:M:208:LEU:HB2	1:M:242:PHE:CE2	2.38	0.58
1:G:206:VAL:HG13	1:G:258:GLN:O	2.04	0.58
1:C:104:GLN:HB2	1:I:108:LYS:HE3	1.85	0.58
1:E:147:ARG:N	3:E:361:3GR:O2	2.34	0.58
1:H:100:LEU:CB	1:H:106:VAL:HB	2.33	0.58
1:I:71:ILE:O	1:I:73:PRO:HD3	2.03	0.58
1:D:104:GLN:HE22	1:J:104:GLN:HE22	1.50	0.58
1:E:147:ARG:H	3:E:361:3GR:HA	1.52	0.58
1:F:35:THR:HG22	1:F:175:VAL:HG22	1.86	0.58
1:D:62:VAL:CG1	1:D:145:ILE:HG13	2.33	0.58
1:F:186:ARG:O	1:F:190:GLU:HG3	2.02	0.58
1:G:50:ILE:HD13	1:G:155:LEU:HA	1.85	0.58
1:E:145:ILE:HD12	1:E:145:ILE:H	1.69	0.57
1:G:52:LEU:HD13	1:G:72:ASP:HB2	1.85	0.57
1:L:186:ARG:HD3	1:L:190:GLU:OE2	2.04	0.57
1:G:31:LEU:HB3	1:G:177:VAL:HG11	1.84	0.57
1:L:197:GLU:OE2	1:L:205:LYS:HD2	2.04	0.57
1:C:70:GLN:NE2	1:C:135:THR:HG23	2.19	0.57
1:H:211:GLU:HB3	1:H:254:PHE:O	2.04	0.57
1:I:107:SER:OG	1:I:110:GLN:HG3	2.04	0.57
1:J:67:GLN:HA	1:J:138:LEU:HD23	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:VAL:HG13	1:L:258:GLN:O	2.05	0.57
1:M:98:LYS:HA	1:M:111:TYR:CE1	2.39	0.57
1:A:62:VAL:CG1	1:A:145:ILE:HG13	2.35	0.57
1:A:91:GLN:HG3	1:A:118:TYR:CE1	2.39	0.57
1:H:171:ASP:HB3	1:H:172:PRO:HD2	1.85	0.57
1:H:197:GLU:OE2	1:H:205:LYS:HD2	2.04	0.57
1:I:55:LEU:HD12	1:I:67:GLN:HG2	1.87	0.57
1:K:171:ASP:HB3	1:K:172:PRO:HD3	1.82	0.57
1:E:67:GLN:HA	1:E:138:LEU:HD23	1.87	0.57
1:G:186:ARG:HH11	1:G:186:ARG:CB	2.18	0.57
1:L:210:LEU:C	1:L:212:ASP:H	2.12	0.57
1:M:101:VAL:HG21	1:M:111:TYR:CG	2.39	0.57
1:E:206:VAL:HG21	1:E:222:LEU:HB2	1.86	0.57
1:F:108:LYS:HE3	1:L:104:GLN:NE2	2.20	0.57
1:I:54:ARG:HD2	1:I:54:ARG:O	2.05	0.57
1:J:186:ARG:HH11	1:J:186:ARG:CB	2.17	0.57
1:B:48:ASN:HD21	1:B:158:ASN:H	1.49	0.57
1:C:126:GLU:O	1:C:130:ILE:HG12	2.03	0.57
1:C:211:GLU:HB3	1:C:254:PHE:O	2.04	0.57
1:H:91:GLN:HG3	1:H:118:TYR:CE1	2.40	0.57
1:L:101:VAL:HG21	1:L:111:TYR:CB	2.33	0.57
1:L:186:ARG:HH11	1:L:186:ARG:CB	2.18	0.57
1:A:221:ARG:HD3	1:A:223:GLU:OE2	2.04	0.57
1:D:67:GLN:HA	1:D:138:LEU:HD23	1.85	0.57
1:H:71:ILE:O	1:H:73:PRO:HD3	2.04	0.57
1:I:48:ASN:HD21	1:I:157:THR:HG23	1.70	0.57
1:J:145:ILE:HD12	1:J:145:ILE:H	1.69	0.57
1:J:208:LEU:HD11	1:J:255:VAL:HG21	1.87	0.57
1:A:67:GLN:HA	1:A:138:LEU:HD23	1.87	0.57
1:B:197:GLU:OE2	1:B:205:LYS:HD2	2.04	0.57
1:K:108:LYS:CD	1:L:96:ARG:HD2	2.30	0.57
1:K:171:ASP:HB3	1:K:172:PRO:HD2	1.87	0.56
1:K:221:ARG:HD3	1:K:223:GLU:OE2	2.04	0.56
1:H:109:GLN:NE2	1:H:110:GLN:HG3	2.20	0.56
1:I:186:ARG:O	1:I:190:GLU:HG3	2.04	0.56
1:C:158:ASN:HD22	1:C:159:GLY:N	2.04	0.56
1:E:147:ARG:HG3	1:F:227:VAL:HG12	1.87	0.56
1:L:86:ASN:O	1:L:89:SER:HB3	2.06	0.56
1:B:171:ASP:HB3	1:B:172:PRO:HD2	1.83	0.56
1:C:71:ILE:O	1:C:73:PRO:HD3	2.05	0.56
1:D:145:ILE:HG23	1:D:167:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ALA:HA	1:G:85:ALA:HB1	1.88	0.56
1:I:37:ALA:HB3	1:I:40:ILE:HD11	1.86	0.56
1:D:62:VAL:HG23	1:D:66:GLN:OE1	2.05	0.56
1:G:97:TYR:HD2	1:G:106:VAL:HG11	1.70	0.56
1:I:186:ARG:HD3	1:I:190:GLU:OE2	2.06	0.56
1:M:126:GLU:O	1:M:130:ILE:HG12	2.06	0.56
1:L:211:GLU:HB3	1:L:254:PHE:O	2.06	0.56
1:A:47:VAL:HG22	1:A:76:TYR:OH	2.06	0.56
1:B:211:GLU:HB3	1:B:254:PHE:O	2.05	0.56
1:E:91:GLN:HG3	1:E:118:TYR:CE1	2.41	0.56
1:G:208:LEU:HD11	1:G:255:VAL:HG21	1.88	0.56
1:K:147:ARG:CB	3:K:361:3GR:O3	2.54	0.56
1:L:206:VAL:HG12	1:L:207:SER:N	2.19	0.56
1:B:144:ARG:HG3	1:B:144:ARG:HH11	1.71	0.56
1:C:48:ASN:HD22	1:C:157:THR:HA	1.70	0.56
1:D:208:LEU:HB2	1:D:242:PHE:CE2	2.41	0.56
1:E:35:THR:HG22	1:E:175:VAL:HG22	1.87	0.56
1:A:210:LEU:C	1:A:212:ASP:H	2.14	0.56
1:F:211:GLU:HB3	1:F:254:PHE:O	2.06	0.56
1:G:141:ILE:HG23	1:G:142:SER:N	2.20	0.56
1:I:141:ILE:HG23	1:I:142:SER:N	2.21	0.56
1:J:206:VAL:HG21	1:J:222:LEU:HB2	1.87	0.56
1:M:109:GLN:O	1:M:112:ALA:HB3	2.05	0.56
1:G:208:LEU:HB2	1:G:242:PHE:CE2	2.41	0.56
1:J:30:GLU:HG2	1:J:258:GLN:HG2	1.88	0.56
1:C:52:LEU:HD22	1:C:72:ASP:HA	1.88	0.55
1:M:141:ILE:CG2	1:M:142:SER:N	2.70	0.55
1:G:186:ARG:O	1:G:190:GLU:HG3	2.06	0.55
1:J:158:ASN:HD22	1:J:159:GLY:N	2.03	0.55
1:L:221:ARG:HD3	1:L:223:GLU:OE2	2.06	0.55
1:M:210:LEU:C	1:M:212:ASP:H	2.14	0.55
1:D:250:LEU:O	1:D:253:MET:HG3	2.07	0.55
1:M:250:LEU:O	1:M:253:MET:HG3	2.06	0.55
1:B:55:LEU:CD1	1:B:67:GLN:HG2	2.27	0.55
1:B:206:VAL:HG13	1:B:258:GLN:O	2.06	0.55
1:C:35:THR:HG22	1:C:175:VAL:HG22	1.87	0.55
1:E:48:ASN:ND2	1:E:157:THR:HA	2.21	0.55
1:G:45:PRO:HG3	1:G:156:VAL:HG22	1.87	0.55
1:H:145:ILE:HD12	1:H:145:ILE:N	2.21	0.55
1:K:45:PRO:HG3	1:K:156:VAL:HG22	1.88	0.55
1:J:48:ASN:HD21	1:J:158:ASN:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:ASP:HB3	1:J:172:PRO:HD3	1.88	0.55
1:L:71:ILE:O	1:L:73:PRO:HD3	2.06	0.55
1:C:62:VAL:HG23	1:C:66:GLN:OE1	2.06	0.55
1:D:211:GLU:HB3	1:D:254:PHE:O	2.06	0.55
1:L:158:ASN:C	1:L:158:ASN:ND2	2.63	0.55
1:A:208:LEU:HD11	1:A:255:VAL:CG2	2.36	0.55
1:C:147:ARG:HG3	1:D:227:VAL:HG12	1.87	0.55
1:F:48:ASN:ND2	1:F:157:THR:HA	2.22	0.55
1:I:245:PRO:C	1:I:247:ASN:N	2.65	0.55
1:J:70:GLN:HE22	1:J:135:THR:HG23	1.72	0.55
1:K:145:ILE:H	1:K:145:ILE:HD12	1.72	0.55
1:M:64:ALA:HB2	1:M:141:ILE:C	2.32	0.55
1:F:206:VAL:HG12	1:F:207:SER:N	2.20	0.55
1:H:137:VAL:HG12	1:H:137:VAL:O	2.07	0.55
1:J:34:ARG:HH11	1:J:34:ARG:CB	2.18	0.55
1:J:62:VAL:CG1	1:J:145:ILE:HG13	2.37	0.55
1:A:96:ARG:NH2	1:B:109:GLN:NE2	2.55	0.55
1:B:102:ALA:C	1:B:104:GLN:H	2.14	0.55
1:E:51:ILE:HD11	1:E:164:MET:HE3	1.88	0.55
1:H:158:ASN:HD22	1:H:158:ASN:C	2.10	0.54
1:H:208:LEU:HD11	1:H:255:VAL:HG21	1.88	0.54
1:K:55:LEU:N	1:K:55:LEU:HD23	2.22	0.54
1:D:206:VAL:HG13	1:D:258:GLN:O	2.07	0.54
1:E:211:GLU:HB3	1:E:254:PHE:O	2.07	0.54
1:K:98:LYS:O	1:K:101:VAL:HG12	2.07	0.54
1:B:186:ARG:HH11	1:B:186:ARG:CB	2.19	0.54
1:L:40:ILE:HG12	1:L:168:GLN:HG2	1.90	0.54
1:A:101:VAL:CG1	1:A:106:VAL:HG23	2.37	0.54
1:B:35:THR:HG22	1:B:175:VAL:HG22	1.89	0.54
1:I:34:ARG:HH11	1:I:34:ARG:CB	2.15	0.54
1:L:70:GLN:HE22	1:L:135:THR:CG2	2.17	0.54
1:A:197:GLU:OE2	1:A:205:LYS:HD2	2.07	0.54
1:F:60:SER:O	1:F:145:ILE:HD12	2.07	0.54
1:I:48:ASN:HD22	1:I:157:THR:HA	1.73	0.54
1:L:99:LEU:HD12	1:L:99:LEU:N	2.23	0.54
1:C:210:LEU:C	1:C:212:ASP:H	2.15	0.54
1:E:170:LEU:O	1:E:171:ASP:O	2.26	0.54
1:E:171:ASP:O	1:E:173:ILE:N	2.40	0.54
1:B:48:ASN:HD22	1:B:157:THR:HA	1.73	0.54
1:D:197:GLU:OE2	1:D:205:LYS:HD2	2.07	0.54
1:D:208:LEU:HD11	1:D:255:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:VAL:CG2	1:G:111:TYR:HB2	2.38	0.54
1:I:48:ASN:ND2	1:I:157:THR:HG23	2.22	0.54
1:M:141:ILE:HG23	1:M:142:SER:N	2.22	0.54
1:K:71:ILE:O	1:K:73:PRO:HD3	2.08	0.54
1:M:62:VAL:CG1	1:M:145:ILE:HG13	2.38	0.54
1:M:206:VAL:HG12	1:M:207:SER:N	2.23	0.54
1:A:109:GLN:O	1:A:112:ALA:HB3	2.08	0.54
1:C:108:LYS:HG3	1:I:104:GLN:HB3	1.89	0.54
1:C:208:LEU:HD11	1:C:255:VAL:HG21	1.90	0.54
1:D:30:GLU:HG2	1:D:258:GLN:HG2	1.90	0.54
1:D:145:ILE:HD12	1:D:145:ILE:H	1.72	0.54
1:D:186:ARG:HD3	1:D:190:GLU:OE2	2.07	0.54
1:F:206:VAL:O	1:F:219:GLU:HB2	2.08	0.54
1:J:221:ARG:HD3	1:J:223:GLU:OE2	2.08	0.54
1:K:99:LEU:N	1:K:99:LEU:HD12	2.23	0.54
1:M:144:ARG:HG3	1:M:144:ARG:HH11	1.73	0.54
1:A:186:ARG:HD3	1:A:190:GLU:OE2	2.07	0.54
1:L:206:VAL:HG21	1:L:222:LEU:HB2	1.90	0.54
1:M:97:TYR:O	1:M:101:VAL:HG23	2.07	0.54
1:A:141:ILE:HG23	1:A:142:SER:N	2.23	0.53
1:D:186:ARG:HH11	1:D:186:ARG:CB	2.20	0.53
1:K:70:GLN:HE22	1:K:135:THR:CG2	2.17	0.53
1:C:221:ARG:HD3	1:C:223:GLU:OE2	2.08	0.53
1:C:245:PRO:C	1:C:247:ASN:N	2.66	0.53
1:B:140:PRO:O	1:B:141:ILE:HD12	2.09	0.53
1:D:236:VAL:HG12	1:D:237:THR:N	2.24	0.53
1:M:134:TYR:C	1:M:136:LYS:N	2.65	0.53
1:A:48:ASN:HD22	1:A:158:ASN:H	1.53	0.53
1:A:206:VAL:HG13	1:A:258:GLN:O	2.07	0.53
1:K:111:TYR:C	1:K:111:TYR:CD2	2.86	0.53
1:K:210:LEU:C	1:K:212:ASP:H	2.14	0.53
1:G:236:VAL:HG12	1:G:237:THR:N	2.23	0.53
1:D:210:LEU:C	1:D:212:ASP:H	2.16	0.53
1:G:221:ARG:HD3	1:G:223:GLU:OE2	2.09	0.53
1:M:101:VAL:HG21	1:M:111:TYR:CB	2.38	0.53
1:I:208:LEU:HD11	1:I:255:VAL:HG21	1.89	0.53
1:K:35:THR:HG22	1:K:175:VAL:HG22	1.91	0.53
1:F:62:VAL:CG1	1:F:145:ILE:HG13	2.39	0.53
1:F:96:ARG:O	1:F:100:LEU:HG	2.09	0.53
1:K:206:VAL:HG12	1:K:207:SER:N	2.24	0.53
1:M:96:ARG:O	1:M:100:LEU:HD13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:VAL:HG13	1:E:258:GLN:O	2.09	0.53
1:F:98:LYS:HG3	1:F:111:TYR:OH	2.08	0.53
1:I:70:GLN:HE21	1:I:73:PRO:HD3	1.73	0.53
1:J:48:ASN:ND2	1:J:157:THR:HA	2.24	0.53
1:A:158:ASN:HD22	1:A:158:ASN:C	2.15	0.52
1:E:144:ARG:HG3	1:E:144:ARG:HH11	1.74	0.52
1:E:197:GLU:OE2	1:E:205:LYS:HD2	2.10	0.52
1:I:206:VAL:HG13	1:I:258:GLN:O	2.08	0.52
1:J:186:ARG:HD3	1:J:190:GLU:OE2	2.09	0.52
1:A:147:ARG:HD2	2:A:361:GOL:C1	2.39	0.52
1:D:110:GLN:OE1	1:D:110:GLN:HA	2.09	0.52
1:G:211:GLU:HB3	1:G:254:PHE:O	2.09	0.52
1:H:221:ARG:HD3	1:H:223:GLU:OE2	2.09	0.52
1:K:103:ASP:C	1:K:105:ALA:N	2.68	0.52
1:L:110:GLN:C	1:L:112:ALA:N	2.63	0.52
1:M:236:VAL:HG12	1:M:237:THR:N	2.24	0.52
1:A:29:THR:CG2	1:A:30:GLU:N	2.71	0.52
1:D:40:ILE:HG12	1:D:168:GLN:HG2	1.92	0.52
1:F:50:ILE:HD13	1:F:155:LEU:HA	1.91	0.52
1:F:141:ILE:HG23	1:F:142:SER:N	2.25	0.52
1:C:48:ASN:HD21	1:C:157:THR:CG2	2.21	0.52
1:F:80:TYR:HA	1:F:128:ALA:HB1	1.91	0.52
1:H:145:ILE:H	1:H:145:ILE:CD1	2.18	0.52
1:B:48:ASN:ND2	1:B:158:ASN:N	2.52	0.52
1:B:206:VAL:HG12	1:B:207:SER:N	2.25	0.52
1:C:141:ILE:CG2	1:C:142:SER:N	2.72	0.52
1:F:38:PHE:HD2	1:F:169:GLN:OE1	1.93	0.52
1:G:208:LEU:HD11	1:G:255:VAL:CG2	2.40	0.52
1:L:48:ASN:ND2	1:L:158:ASN:N	2.50	0.52
1:L:245:PRO:C	1:L:247:ASN:N	2.67	0.52
1:A:104:GLN:HB2	1:G:108:LYS:CD	2.39	0.52
1:C:70:GLN:HE22	1:C:135:THR:CG2	2.22	0.52
1:E:104:GLN:HE22	1:K:104:GLN:HA	1.75	0.52
1:J:206:VAL:HG13	1:J:258:GLN:O	2.09	0.52
1:L:62:VAL:CG1	1:L:145:ILE:HG13	2.40	0.52
1:A:51:ILE:HD11	1:A:164:MET:HE3	1.91	0.52
1:A:96:ARG:NH2	1:B:109:GLN:CD	2.67	0.52
1:A:147:ARG:HD2	2:A:361:GOL:H12	1.92	0.52
1:A:208:LEU:HB2	1:A:242:PHE:CE2	2.45	0.52
1:F:206:VAL:HG13	1:F:258:GLN:O	2.08	0.52
1:G:145:ILE:H	1:G:145:ILE:CD1	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:45:PRO:HD3	1:L:164:MET:SD	2.48	0.52
1:M:221:ARG:HD3	1:M:223:GLU:OE2	2.10	0.52
1:B:208:LEU:HD11	1:B:255:VAL:HG21	1.91	0.52
1:E:46:GLN:HB2	1:E:134:TYR:CD2	2.44	0.52
1:E:52:LEU:HD22	1:E:72:ASP:HA	1.91	0.52
1:F:221:ARG:HD3	1:F:223:GLU:OE2	2.10	0.52
1:K:83:ALA:O	1:K:86:ASN:N	2.43	0.52
1:M:48:ASN:HD22	1:M:158:ASN:H	1.50	0.52
1:B:51:ILE:HD11	1:B:164:MET:HE3	1.91	0.52
1:C:146:GLY:CA	3:C:361:3GR:O1	2.49	0.52
1:E:144:ARG:HG3	1:E:144:ARG:NH1	2.25	0.52
1:I:206:VAL:HG12	1:I:207:SER:N	2.24	0.52
1:I:208:LEU:HB2	1:I:242:PHE:CE2	2.44	0.52
1:K:208:LEU:HD11	1:K:255:VAL:HG21	1.90	0.52
1:L:67:GLN:HE22	1:L:136:LYS:HD3	1.74	0.52
1:A:210:LEU:C	1:A:212:ASP:N	2.68	0.52
1:G:106:VAL:HG13	1:G:110:GLN:HB2	1.92	0.52
1:I:48:ASN:ND2	1:I:157:THR:HA	2.25	0.52
1:I:62:VAL:CG1	1:I:145:ILE:HG13	2.40	0.52
1:I:211:GLU:HB3	1:I:254:PHE:O	2.10	0.52
1:L:48:ASN:ND2	1:L:157:THR:HA	2.24	0.52
1:A:48:ASN:O	1:A:76:TYR:OH	2.25	0.51
1:B:144:ARG:HG3	1:B:144:ARG:NH1	2.24	0.51
1:D:51:ILE:HD11	1:D:164:MET:HE3	1.91	0.51
1:D:141:ILE:HG23	1:D:142:SER:N	2.25	0.51
1:A:147:ARG:HD2	2:A:361:GOL:O1	2.09	0.51
1:D:95:GLN:O	1:D:99:LEU:HD13	2.11	0.51
1:L:130:ILE:CG2	1:L:134:TYR:HE1	2.23	0.51
1:M:206:VAL:HG21	1:M:222:LEU:HB2	1.91	0.51
1:A:175:VAL:HB	1:A:240:ALA:HB3	1.92	0.51
1:E:208:LEU:HD11	1:E:255:VAL:HG21	1.93	0.51
1:I:141:ILE:CG2	1:I:142:SER:N	2.73	0.51
1:J:140:PRO:O	1:J:141:ILE:HD12	2.11	0.51
1:L:250:LEU:O	1:L:253:MET:HG3	2.09	0.51
1:M:47:VAL:HG22	1:M:76:TYR:CZ	2.44	0.51
1:A:35:THR:HG22	1:A:175:VAL:HG22	1.92	0.51
1:A:104:GLN:CB	1:G:108:LYS:HD2	2.41	0.51
1:C:48:ASN:ND2	1:C:157:THR:HG23	2.26	0.51
1:C:145:ILE:HD12	1:C:145:ILE:N	2.23	0.51
1:D:34:ARG:HH11	1:D:34:ARG:CB	2.22	0.51
1:D:97:TYR:HB3	1:D:106:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:TYR:HA	1:J:128:ALA:HB1	1.93	0.51
1:C:250:LEU:O	1:C:253:MET:HG3	2.10	0.51
1:D:55:LEU:N	1:D:55:LEU:HD23	2.25	0.51
1:G:206:VAL:HG12	1:G:207:SER:N	2.25	0.51
1:H:70:GLN:HE22	1:H:135:THR:CG2	2.20	0.51
1:I:208:LEU:HD11	1:I:255:VAL:CG2	2.41	0.51
1:B:145:ILE:HD12	1:B:145:ILE:H	1.74	0.51
1:B:210:LEU:C	1:B:212:ASP:H	2.17	0.51
1:C:206:VAL:HG12	1:C:207:SER:N	2.25	0.51
1:D:158:ASN:ND2	1:D:159:GLY:N	2.57	0.51
1:F:97:TYR:O	1:F:101:VAL:HG23	2.10	0.51
1:J:210:LEU:C	1:J:212:ASP:H	2.18	0.51
1:C:69:TYR:CD1	1:C:164:MET:HE2	2.46	0.51
1:E:206:VAL:HG12	1:E:207:SER:N	2.24	0.51
1:F:245:PRO:C	1:F:247:ASN:N	2.65	0.51
1:I:70:GLN:NE2	1:I:73:PRO:HD3	2.26	0.51
1:I:210:LEU:C	1:I:212:ASP:H	2.18	0.51
1:L:140:PRO:O	1:L:141:ILE:HD12	2.10	0.51
1:L:206:VAL:O	1:L:219:GLU:HB2	2.10	0.51
1:M:62:VAL:HG12	1:M:145:ILE:HG13	1.93	0.51
1:C:183:ALA:O	1:C:187:LEU:HG	2.11	0.51
1:E:246:ASN:O	1:F:188:ARG:NH2	2.37	0.51
1:H:69:TYR:HB2	1:H:137:VAL:HB	1.91	0.51
1:L:210:LEU:C	1:L:212:ASP:N	2.68	0.51
1:D:62:VAL:HG12	1:D:145:ILE:HG13	1.92	0.51
1:E:34:ARG:HH11	1:E:34:ARG:CB	2.19	0.51
1:E:151:THR:HB	1:F:40:ILE:O	2.10	0.51
1:F:71:ILE:O	1:F:73:PRO:CD	2.59	0.51
1:F:208:LEU:HB2	1:F:242:PHE:CE2	2.45	0.51
1:K:107:SER:CB	1:K:110:GLN:HG3	2.29	0.51
1:M:144:ARG:HG3	1:M:144:ARG:NH1	2.26	0.51
1:A:48:ASN:ND2	1:A:158:ASN:N	2.48	0.51
1:E:236:VAL:HG12	1:E:237:THR:N	2.25	0.51
1:I:126:GLU:O	1:I:130:ILE:HG12	2.10	0.51
1:K:210:LEU:C	1:K:212:ASP:N	2.68	0.51
1:L:171:ASP:HB3	1:L:172:PRO:HD3	1.87	0.51
1:B:141:ILE:HG23	1:B:142:SER:N	2.26	0.50
1:C:48:ASN:HD21	1:C:157:THR:HG23	1.74	0.50
1:D:96:ARG:NH2	1:E:109:GLN:OE1	2.45	0.50
1:D:100:LEU:CD2	1:K:103:ASP:HB3	2.42	0.50
1:D:113:ASP:O	1:D:116:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ILE:H	1:I:145:ILE:CD1	2.17	0.50
1:I:146:GLY:HA3	3:I:361:3GR:HA	1.75	0.50
1:K:197:GLU:OE2	1:K:205:LYS:HD2	2.11	0.50
1:A:206:VAL:HG12	1:A:207:SER:N	2.25	0.50
1:E:158:ASN:ND2	1:E:159:GLY:N	2.58	0.50
1:F:145:ILE:H	1:F:145:ILE:CD1	2.13	0.50
1:J:171:ASP:O	1:J:173:ILE:N	2.43	0.50
1:J:245:PRO:C	1:J:247:ASN:N	2.65	0.50
1:K:185:LEU:HD21	1:L:248:GLU:HB3	1.93	0.50
1:L:46:GLN:CD	1:L:134:TYR:CE2	2.90	0.50
1:M:145:ILE:HD12	1:M:145:ILE:H	1.76	0.50
1:M:183:ALA:O	1:M:187:LEU:HG	2.11	0.50
1:F:101:VAL:CG2	1:F:111:TYR:HB2	2.39	0.50
1:A:73:PRO:O	1:A:74:ALA:C	2.53	0.50
1:A:236:VAL:HG12	1:A:237:THR:N	2.25	0.50
1:B:215:GLN:HE22	1:B:258:GLN:HE22	1.58	0.50
1:E:186:ARG:HD3	1:E:190:GLU:OE2	2.10	0.50
1:K:40:ILE:O	1:L:151:THR:HB	2.12	0.50
1:K:158:ASN:HD22	1:K:159:GLY:H	1.57	0.50
1:G:193:SER:C	1:G:195:GLN:H	2.20	0.50
1:C:43:VAL:HG23	1:C:165:ALA:O	2.11	0.50
1:D:206:VAL:HG12	1:D:207:SER:N	2.26	0.50
1:H:158:ASN:C	1:H:158:ASN:ND2	2.68	0.50
1:H:208:LEU:HD11	1:H:255:VAL:CG2	2.42	0.50
1:I:116:ALA:O	1:I:120:GLN:HG3	2.11	0.50
1:J:145:ILE:HD12	1:J:145:ILE:N	2.26	0.50
1:E:101:VAL:HG23	1:E:106:VAL:O	2.12	0.50
1:F:186:ARG:HH11	1:F:186:ARG:CB	2.24	0.50
1:F:210:LEU:C	1:F:212:ASP:H	2.20	0.50
1:H:62:VAL:HG23	1:H:66:GLN:NE2	2.27	0.50
1:C:208:LEU:HD11	1:C:255:VAL:CG2	2.41	0.50
1:F:236:VAL:HG12	1:F:237:THR:N	2.27	0.50
1:H:38:PHE:HB2	1:H:172:PRO:O	2.12	0.50
1:J:35:THR:HG22	1:J:175:VAL:HG22	1.93	0.50
1:B:91:GLN:HG3	1:B:118:TYR:CE1	2.47	0.49
1:E:210:LEU:C	1:E:212:ASP:H	2.18	0.49
1:F:55:LEU:N	1:F:55:LEU:HD23	2.27	0.49
1:G:245:PRO:C	1:G:247:ASN:N	2.67	0.49
1:H:141:ILE:HG23	1:H:142:SER:N	2.27	0.49
1:H:186:ARG:O	1:H:190:GLU:HG3	2.12	0.49
1:J:208:LEU:HD11	1:J:255:VAL:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:ASN:HD22	1:L:159:GLY:H	1.60	0.49
1:M:80:TYR:HA	1:M:128:ALA:HB1	1.94	0.49
1:M:208:LEU:HD11	1:M:255:VAL:HG21	1.94	0.49
1:B:147:ARG:HB2	2:B:361:GOL:O2	2.12	0.49
1:D:73:PRO:O	1:D:74:ALA:C	2.52	0.49
1:F:101:VAL:HG21	1:F:111:TYR:CB	2.40	0.49
1:K:140:PRO:O	1:K:141:ILE:HD12	2.12	0.49
1:L:170:LEU:O	1:L:171:ASP:O	2.30	0.49
1:M:170:LEU:HD21	1:M:251:PRO:CD	2.42	0.49
1:A:62:VAL:HG23	1:A:66:GLN:OE1	2.12	0.49
1:F:208:LEU:HD11	1:F:255:VAL:HG21	1.94	0.49
1:L:34:ARG:HH11	1:L:34:ARG:CB	2.19	0.49
1:L:48:ASN:HD22	1:L:157:THR:HA	1.76	0.49
1:M:73:PRO:O	1:M:74:ALA:C	2.54	0.49
1:B:236:VAL:HG12	1:B:237:THR:N	2.28	0.49
1:K:51:ILE:HD11	1:K:164:MET:HE3	1.94	0.49
1:L:201:ASP:O	1:L:202:ASN:HB2	2.13	0.49
1:C:141:ILE:HG23	1:C:142:SER:N	2.27	0.49
1:D:210:LEU:C	1:D:212:ASP:N	2.71	0.49
1:J:55:LEU:HD23	1:J:55:LEU:N	2.27	0.49
1:J:208:LEU:HB2	1:J:242:PHE:CE2	2.47	0.49
1:K:206:VAL:HG21	1:K:222:LEU:HB2	1.94	0.49
1:K:211:GLU:HB3	1:K:254:PHE:O	2.12	0.49
1:D:110:GLN:O	1:D:112:ALA:N	2.46	0.49
1:G:91:GLN:HG3	1:G:118:TYR:CE1	2.47	0.49
1:G:48:ASN:ND2	1:G:157:THR:HG23	2.27	0.49
1:G:206:VAL:O	1:G:219:GLU:HB2	2.13	0.49
1:K:73:PRO:O	1:K:74:ALA:C	2.55	0.49
1:H:83:ALA:O	1:H:86:ASN:N	2.46	0.49
1:J:197:GLU:OE2	1:J:205:LYS:HD2	2.12	0.49
1:J:236:VAL:HG21	1:K:250:LEU:HD12	1.94	0.49
1:K:62:VAL:CG1	1:K:145:ILE:HG13	2.43	0.49
1:K:208:LEU:HD11	1:K:255:VAL:CG2	2.43	0.49
1:B:171:ASP:O	1:B:173:ILE:N	2.45	0.49
1:D:103:ASP:O	1:D:104:GLN:HB3	2.12	0.49
1:G:62:VAL:CG1	1:G:145:ILE:HG13	2.43	0.49
1:H:158:ASN:ND2	1:H:159:GLY:N	2.56	0.49
1:H:206:VAL:HG21	1:H:222:LEU:HB2	1.95	0.49
1:I:226:GLU:HG3	1:J:144:ARG:HE	1.78	0.49
1:K:71:ILE:O	1:K:72:ASP:C	2.55	0.49
1:B:50:ILE:HD13	1:B:155:LEU:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:CD1	1:C:173:ILE:HD12	2.42	0.48
1:E:80:TYR:HA	1:E:128:ALA:HB1	1.93	0.48
1:G:141:ILE:CG2	1:G:142:SER:N	2.76	0.48
1:H:206:VAL:HG13	1:H:258:GLN:O	2.13	0.48
1:L:30:GLU:HG2	1:L:258:GLN:HG2	1.94	0.48
1:A:206:VAL:O	1:A:219:GLU:HB2	2.13	0.48
1:C:91:GLN:HG3	1:C:118:TYR:CE1	2.47	0.48
1:E:70:GLN:NE2	1:E:135:THR:HG23	2.25	0.48
1:H:245:PRO:C	1:H:247:ASN:N	2.69	0.48
1:J:210:LEU:C	1:J:212:ASP:N	2.71	0.48
1:L:46:GLN:HB2	1:L:134:TYR:CD2	2.48	0.48
1:M:140:PRO:O	1:M:141:ILE:HD12	2.13	0.48
1:D:101:VAL:C	1:D:103:ASP:H	2.21	0.48
1:E:65:GLY:O	1:E:138:LEU:HD22	2.13	0.48
1:G:191:LEU:C	1:G:191:LEU:HD13	2.38	0.48
1:K:245:PRO:C	1:K:247:ASN:N	2.70	0.48
1:K:99:LEU:N	1:K:99:LEU:CD1	2.77	0.48
1:K:145:ILE:HD12	1:K:145:ILE:N	2.28	0.48
1:A:141:ILE:CG2	1:A:142:SER:N	2.76	0.48
1:D:77:GLU:OE2	1:D:81:GLN:NE2	2.47	0.48
1:F:69:TYR:HB2	1:F:137:VAL:HB	1.95	0.48
1:G:69:TYR:HB2	1:G:137:VAL:HB	1.95	0.48
1:M:186:ARG:HD3	1:M:190:GLU:OE2	2.13	0.48
1:B:97:TYR:O	1:B:101:VAL:HG23	2.14	0.48
1:D:70:GLN:NE2	1:D:135:THR:HG23	2.28	0.48
1:J:236:VAL:CG2	1:K:250:LEU:HD12	2.43	0.48
1:M:134:TYR:C	1:M:136:LYS:H	2.20	0.48
1:D:91:GLN:HG3	1:D:118:TYR:CE1	2.49	0.48
1:E:96:ARG:NH2	1:F:109:GLN:OE1	2.46	0.48
1:F:37:ALA:HB3	1:F:40:ILE:CD1	2.36	0.48
1:G:188:ARG:HH21	1:H:248:GLU:HA	1.78	0.48
1:H:87:LEU:O	1:H:87:LEU:HD12	2.14	0.48
1:H:158:ASN:HD22	1:H:159:GLY:H	1.58	0.48
1:I:191:LEU:HD13	1:I:191:LEU:C	2.39	0.48
1:J:60:SER:O	1:J:145:ILE:HD12	2.14	0.48
1:L:67:GLN:HA	1:L:138:LEU:HD23	1.95	0.48
1:D:74:ALA:HB1	1:E:130:ILE:HD12	1.96	0.48
1:H:73:PRO:O	1:H:74:ALA:C	2.56	0.48
1:H:141:ILE:CG2	1:H:142:SER:N	2.77	0.48
1:H:191:LEU:HD13	1:H:191:LEU:C	2.39	0.48
1:K:69:TYR:HB2	1:K:137:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:ILE:HG23	1:K:167:VAL:HG22	1.95	0.48
1:A:186:ARG:HH11	1:A:186:ARG:CB	2.25	0.48
1:C:116:ALA:O	1:C:120:GLN:HG3	2.13	0.48
1:E:210:LEU:C	1:E:212:ASP:N	2.72	0.48
1:J:245:PRO:O	1:J:247:ASN:N	2.46	0.48
1:K:141:ILE:HG23	1:K:142:SER:N	2.28	0.48
1:K:230:ASP:O	1:K:234:GLY:N	2.45	0.48
1:L:52:LEU:HD22	1:L:72:ASP:HA	1.96	0.48
1:B:158:ASN:HD22	1:B:159:GLY:H	1.61	0.47
1:C:31:LEU:HD22	1:C:179:GLN:CD	2.39	0.47
1:E:71:ILE:O	1:E:72:ASP:C	2.57	0.47
1:G:60:SER:O	1:G:145:ILE:HD12	2.13	0.47
1:H:171:ASP:HB3	1:H:172:PRO:HD3	1.94	0.47
1:H:236:VAL:HG12	1:H:237:THR:N	2.29	0.47
1:L:145:ILE:HD12	1:L:145:ILE:N	2.29	0.47
1:M:206:VAL:O	1:M:219:GLU:HB2	2.14	0.47
1:M:210:LEU:C	1:M:212:ASP:N	2.69	0.47
1:B:210:LEU:C	1:B:212:ASP:N	2.71	0.47
1:E:48:ASN:HD22	1:E:157:THR:HA	1.79	0.47
1:I:236:VAL:HG12	1:I:237:THR:N	2.29	0.47
1:K:250:LEU:O	1:K:253:MET:HG3	2.14	0.47
1:M:103:ASP:O	1:M:105:ALA:N	2.47	0.47
1:C:34:ARG:HH11	1:C:34:ARG:CB	2.20	0.47
1:C:206:VAL:O	1:C:219:GLU:HB2	2.13	0.47
1:J:145:ILE:H	1:J:145:ILE:CD1	2.25	0.47
1:J:206:VAL:HG12	1:J:207:SER:N	2.28	0.47
1:L:69:TYR:HB2	1:L:137:VAL:HB	1.97	0.47
1:A:31:LEU:HB3	1:A:177:VAL:HG11	1.96	0.47
1:F:31:LEU:HB3	1:F:177:VAL:CG1	2.45	0.47
1:G:70:GLN:HE21	1:G:73:PRO:HD3	1.80	0.47
1:H:98:LYS:HB2	1:H:111:TYR:CE1	2.49	0.47
1:J:226:GLU:OE2	1:K:144:ARG:NE	2.48	0.47
1:L:48:ASN:ND2	1:L:157:THR:HG23	2.30	0.47
1:L:110:GLN:O	1:L:113:ASP:N	2.48	0.47
1:A:100:LEU:HB3	1:A:105:ALA:HB3	1.97	0.47
1:A:158:ASN:C	1:A:158:ASN:ND2	2.72	0.47
1:D:70:GLN:HE21	1:D:73:PRO:HD3	1.79	0.47
1:D:71:ILE:O	1:D:72:ASP:C	2.57	0.47
1:K:186:ARG:HH11	1:K:186:ARG:CB	2.25	0.47
1:A:171:ASP:HB3	1:A:172:PRO:HD3	1.94	0.47
1:C:80:TYR:HA	1:C:128:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ILE:CG2	1:D:142:SER:N	2.77	0.47
1:E:145:ILE:HD12	1:E:145:ILE:N	2.29	0.47
1:F:77:GLU:OE2	1:F:81:GLN:NE2	2.47	0.47
1:I:206:VAL:HG21	1:I:222:LEU:HB2	1.96	0.47
1:K:62:VAL:HG12	1:K:145:ILE:HG13	1.97	0.47
1:K:95:GLN:O	1:K:99:LEU:HD13	2.13	0.47
1:K:193:SER:C	1:K:195:GLN:H	2.23	0.47
1:M:158:ASN:HD22	1:M:158:ASN:C	2.18	0.47
1:B:206:VAL:O	1:B:219:GLU:HB2	2.15	0.47
1:F:70:GLN:NE2	1:F:135:THR:HG23	2.28	0.47
1:F:85:ALA:HB2	1:G:82:SER:CB	2.36	0.47
1:G:166:THR:HB	3:G:361:3GR:O1	2.15	0.47
1:H:206:VAL:HG12	1:H:207:SER:N	2.30	0.47
1:I:30:GLU:HG2	1:I:258:GLN:HG2	1.96	0.47
1:I:221:ARG:HD3	1:I:223:GLU:OE2	2.14	0.47
1:J:130:ILE:HG22	1:J:134:TYR:CE1	2.50	0.47
1:L:60:SER:O	1:L:145:ILE:HD12	2.15	0.47
1:L:73:PRO:O	1:L:74:ALA:C	2.54	0.47
1:L:245:PRO:O	1:L:247:ASN:N	2.48	0.47
1:M:208:LEU:HD11	1:M:255:VAL:CG2	2.45	0.47
1:C:147:ARG:NH2	1:D:237:THR:HG21	2.29	0.47
1:G:48:ASN:ND2	1:G:157:THR:HA	2.29	0.47
1:H:144:ARG:HG3	1:H:144:ARG:NH1	2.30	0.47
1:I:171:ASP:O	1:I:173:ILE:N	2.47	0.47
1:J:62:VAL:HG23	1:J:66:GLN:NE2	2.30	0.47
1:L:67:GLN:NE2	1:L:136:LYS:HD3	2.30	0.47
1:L:206:VAL:CG1	1:L:207:SER:N	2.78	0.47
1:D:245:PRO:C	1:D:247:ASN:N	2.68	0.47
1:E:145:ILE:H	1:E:145:ILE:CD1	2.25	0.47
1:F:69:TYR:CD1	1:F:164:MET:HE2	2.50	0.47
1:F:208:LEU:HD11	1:F:255:VAL:CG2	2.43	0.47
1:G:34:ARG:HH11	1:G:34:ARG:CB	2.19	0.47
1:H:171:ASP:O	1:H:173:ILE:N	2.47	0.47
1:J:111:TYR:C	1:J:111:TYR:CD2	2.92	0.47
1:K:65:GLY:O	1:K:138:LEU:HD22	2.14	0.47
1:E:43:VAL:HG23	1:E:165:ALA:O	2.15	0.47
1:E:140:PRO:O	1:E:141:ILE:HD12	2.15	0.47
1:J:211:GLU:HB3	1:J:254:PHE:O	2.14	0.47
1:K:236:VAL:HG12	1:K:237:THR:N	2.30	0.47
1:L:236:VAL:HG12	1:L:237:THR:N	2.30	0.47
1:A:97:TYR:CD1	1:A:114:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PRO:C	1:A:247:ASN:N	2.67	0.46
1:B:175:VAL:HB	1:B:240:ALA:HB3	1.97	0.46
1:I:48:ASN:HD21	1:I:158:ASN:H	1.58	0.46
1:I:193:SER:C	1:I:195:GLN:H	2.23	0.46
1:I:245:PRO:O	1:I:247:ASN:N	2.48	0.46
1:L:54:ARG:HD2	1:L:54:ARG:O	2.15	0.46
1:B:208:LEU:HD11	1:B:255:VAL:CG2	2.45	0.46
1:D:54:ARG:HD2	1:D:54:ARG:O	2.15	0.46
1:G:48:ASN:HD21	1:G:158:ASN:N	2.09	0.46
1:G:107:SER:HG	1:G:110:GLN:HG3	1.79	0.46
1:H:171:ASP:CB	1:H:172:PRO:CD	2.89	0.46
1:I:80:TYR:HA	1:I:128:ALA:HB1	1.96	0.46
1:B:147:ARG:HG3	1:C:227:VAL:HG12	1.96	0.46
1:G:38:PHE:HD2	1:G:169:GLN:NE2	2.13	0.46
1:G:250:LEU:O	1:G:253:MET:HG3	2.15	0.46
1:H:48:ASN:ND2	1:H:157:THR:HA	2.30	0.46
1:I:48:ASN:ND2	1:I:158:ASN:N	2.58	0.46
1:J:54:ARG:HD2	1:J:54:ARG:O	2.15	0.46
1:K:175:VAL:HB	1:K:240:ALA:HB3	1.97	0.46
1:M:175:VAL:HB	1:M:240:ALA:HB3	1.96	0.46
1:A:104:GLN:HB2	1:G:108:LYS:HD2	1.97	0.46
1:A:171:ASP:O	1:A:173:ILE:N	2.49	0.46
1:C:107:SER:H	1:C:110:GLN:HE21	1.63	0.46
1:J:67:GLN:CD	1:J:136:LYS:HD3	2.40	0.46
1:L:208:LEU:HD11	1:L:255:VAL:HG21	1.97	0.46
1:M:130:ILE:CG2	1:M:134:TYR:HE1	2.28	0.46
1:D:147:ARG:NH2	1:E:237:THR:HG21	2.29	0.46
1:F:31:LEU:HD22	1:F:179:GLN:CD	2.41	0.46
1:F:106:VAL:HG12	1:F:107:SER:N	2.30	0.46
1:M:158:ASN:ND2	1:M:159:GLY:N	2.62	0.46
1:C:69:TYR:HB2	1:C:137:VAL:HB	1.97	0.46
1:C:210:LEU:C	1:C:212:ASP:N	2.69	0.46
1:L:226:GLU:OE2	1:M:144:ARG:HD3	2.15	0.46
1:D:69:TYR:HB2	1:D:137:VAL:HB	1.96	0.46
1:F:62:VAL:HG23	1:F:66:GLN:OE1	2.15	0.46
1:M:171:ASP:O	1:M:173:ILE:N	2.49	0.46
1:F:206:VAL:CG1	1:F:207:SER:N	2.79	0.46
1:G:73:PRO:O	1:G:74:ALA:C	2.59	0.46
1:I:41:ALA:HB1	1:I:140:PRO:CG	2.46	0.46
1:I:67:GLN:HA	1:I:138:LEU:HD23	1.98	0.46
1:I:210:LEU:C	1:I:212:ASP:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:LYS:O	1:K:58:GLU:C	2.55	0.46
1:A:62:VAL:HG12	1:A:145:ILE:HG13	1.96	0.46
1:A:80:TYR:HA	1:A:128:ALA:HB1	1.97	0.46
1:D:70:GLN:HE22	1:D:135:THR:HG23	1.80	0.46
1:J:46:GLN:OE1	1:J:134:TYR:CE2	2.69	0.46
1:L:130:ILE:HG22	1:L:134:TYR:CE1	2.50	0.46
1:M:43:VAL:HG23	1:M:165:ALA:O	2.16	0.46
1:A:104:GLN:HB2	1:G:108:LYS:HD3	1.98	0.46
1:D:145:ILE:HD12	1:D:145:ILE:N	2.30	0.46
1:D:145:ILE:H	1:D:145:ILE:CD1	2.27	0.46
1:F:109:GLN:HE21	1:F:113:ASP:CG	2.24	0.46
1:G:46:GLN:OE1	1:G:134:TYR:CE2	2.69	0.46
1:K:48:ASN:HD22	1:K:158:ASN:H	1.56	0.46
1:K:206:VAL:O	1:K:219:GLU:HB2	2.16	0.46
1:M:100:LEU:HD12	1:M:100:LEU:N	2.31	0.46
1:C:186:ARG:HH11	1:C:186:ARG:CB	2.25	0.45
1:F:210:LEU:C	1:F:212:ASP:N	2.73	0.45
1:G:135:THR:HG22	1:G:136:LYS:HG3	1.96	0.45
1:K:208:LEU:HB2	1:K:242:PHE:CE2	2.50	0.45
1:L:171:ASP:O	1:L:173:ILE:N	2.49	0.45
1:M:48:ASN:HD21	1:M:158:ASN:N	2.12	0.45
1:G:210:LEU:C	1:G:212:ASP:H	2.23	0.45
1:I:158:ASN:HD22	1:I:158:ASN:C	2.23	0.45
1:L:62:VAL:HG23	1:L:66:GLN:OE1	2.16	0.45
1:M:158:ASN:HD22	1:M:159:GLY:H	1.63	0.45
1:M:158:ASN:C	1:M:158:ASN:ND2	2.72	0.45
1:C:107:SER:H	1:C:110:GLN:NE2	2.14	0.45
1:C:206:VAL:HG21	1:C:222:LEU:HB2	1.98	0.45
1:D:46:GLN:CD	1:D:134:TYR:CE2	2.94	0.45
1:D:80:TYR:HA	1:D:128:ALA:HB1	1.98	0.45
1:E:141:ILE:HG23	1:E:142:SER:N	2.32	0.45
1:G:193:SER:O	1:G:195:GLN:N	2.49	0.45
1:I:48:ASN:O	1:I:76:TYR:OH	2.25	0.45
1:J:91:GLN:HG3	1:J:118:TYR:CE1	2.51	0.45
1:K:109:GLN:OE1	1:L:96:ARG:NH2	2.50	0.45
1:B:250:LEU:O	1:B:253:MET:HG3	2.17	0.45
1:D:206:VAL:O	1:D:219:GLU:HB2	2.17	0.45
1:D:206:VAL:HG21	1:D:222:LEU:HB2	1.97	0.45
1:F:48:ASN:HD22	1:F:158:ASN:H	1.62	0.45
1:F:141:ILE:CG2	1:F:142:SER:N	2.78	0.45
1:G:236:VAL:HG12	1:G:237:THR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:ASP:O	1:J:116:ALA:HB3	2.16	0.45
1:L:158:ASN:ND2	1:L:159:GLY:N	2.55	0.45
1:M:86:ASN:O	1:M:89:SER:HB3	2.15	0.45
1:B:109:GLN:O	1:B:113:ASP:OD2	2.35	0.45
1:F:167:VAL:HG12	1:F:168:GLN:N	2.31	0.45
1:G:38:PHE:CD2	1:G:169:GLN:NE2	2.85	0.45
1:G:171:ASP:O	1:G:173:ILE:N	2.49	0.45
1:K:145:ILE:H	1:K:145:ILE:CD1	2.26	0.45
1:A:64:ALA:HB2	1:A:141:ILE:C	2.41	0.45
1:A:85:ALA:HB1	1:B:119:LEU:HB3	1.98	0.45
1:E:130:ILE:CG2	1:E:134:TYR:HE1	2.30	0.45
1:K:141:ILE:CG2	1:K:142:SER:N	2.80	0.45
1:E:62:VAL:HG23	1:E:66:GLN:NE2	2.32	0.45
1:K:206:VAL:HG13	1:K:258:GLN:O	2.17	0.45
1:M:245:PRO:O	1:M:247:ASN:N	2.49	0.45
1:B:245:PRO:C	1:B:247:ASN:N	2.66	0.45
1:C:31:LEU:HB3	1:C:177:VAL:HG11	1.99	0.45
1:I:46:GLN:HB2	1:I:134:TYR:CD2	2.51	0.45
1:I:206:VAL:O	1:I:219:GLU:HB2	2.17	0.45
1:M:193:SER:C	1:M:195:GLN:H	2.24	0.45
1:B:100:LEU:O	1:B:106:VAL:N	2.46	0.45
1:B:171:ASP:HB3	1:B:172:PRO:HD3	1.91	0.45
1:C:193:SER:C	1:C:195:GLN:H	2.25	0.45
1:H:38:PHE:CD2	1:H:169:GLN:NE2	2.84	0.45
1:I:100:LEU:C	1:I:106:VAL:HG12	2.42	0.45
1:I:140:PRO:O	1:I:141:ILE:HD12	2.16	0.45
1:K:60:SER:O	1:K:145:ILE:HD12	2.16	0.45
1:K:171:ASP:O	1:K:173:ILE:N	2.49	0.45
1:A:250:LEU:O	1:A:253:MET:HG3	2.17	0.44
1:D:100:LEU:O	1:D:106:VAL:HB	2.16	0.44
1:G:54:ARG:HD2	1:G:54:ARG:O	2.16	0.44
1:H:48:ASN:HD21	1:H:158:ASN:N	2.15	0.44
1:L:48:ASN:HD21	1:L:158:ASN:N	2.14	0.44
1:A:191:LEU:HD13	1:A:191:LEU:C	2.42	0.44
1:C:175:VAL:HB	1:C:240:ALA:HB3	1.99	0.44
1:D:100:LEU:HB2	1:D:106:VAL:HG21	1.99	0.44
1:F:48:ASN:HD22	1:F:157:THR:HA	1.81	0.44
1:F:250:LEU:O	1:F:253:MET:HG3	2.17	0.44
1:H:34:ARG:HH11	1:H:34:ARG:CB	2.24	0.44
1:H:40:ILE:O	1:I:151:THR:HB	2.17	0.44
1:H:48:ASN:HD22	1:H:158:ASN:H	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:PRO:O	1:H:247:ASN:N	2.51	0.44
1:E:68:LEU:HD11	1:E:139:SER:HB2	2.00	0.44
1:H:80:TYR:HA	1:H:128:ALA:HB1	1.98	0.44
1:I:71:ILE:O	1:I:72:ASP:C	2.58	0.44
1:I:195:GLN:O	1:I:195:GLN:HG2	2.17	0.44
1:J:201:ASP:O	1:J:202:ASN:HB2	2.16	0.44
1:A:245:PRO:O	1:A:247:ASN:N	2.50	0.44
1:D:97:TYR:CB	1:D:106:VAL:HG11	2.47	0.44
1:E:245:PRO:O	1:E:247:ASN:N	2.50	0.44
1:F:98:LYS:HG3	1:F:111:TYR:CZ	2.52	0.44
1:F:100:LEU:HB3	1:F:106:VAL:HG23	1.99	0.44
1:F:191:LEU:HD13	1:F:191:LEU:C	2.42	0.44
1:G:80:TYR:HA	1:G:128:ALA:HB1	1.99	0.44
1:K:80:TYR:HA	1:K:128:ALA:HB1	1.99	0.44
1:M:34:ARG:HH11	1:M:34:ARG:CB	2.25	0.44
1:G:35:THR:HG22	1:G:175:VAL:HG22	1.98	0.44
1:A:86:ASN:O	1:A:89:SER:HB3	2.18	0.44
1:A:145:ILE:HG23	1:A:167:VAL:CG2	2.47	0.44
1:B:250:LEU:HD12	1:C:236:VAL:HG21	1.98	0.44
1:I:109:GLN:O	1:I:112:ALA:HB3	2.17	0.44
1:I:186:ARG:HD2	1:I:186:ARG:C	2.43	0.44
1:J:236:VAL:HG12	1:J:237:THR:N	2.33	0.44
1:K:34:ARG:HH11	1:K:34:ARG:CB	2.22	0.44
1:A:145:ILE:HD12	1:A:145:ILE:N	2.32	0.44
1:B:206:VAL:HG21	1:B:222:LEU:HB2	1.99	0.44
1:C:140:PRO:O	1:C:141:ILE:HD12	2.17	0.44
1:F:206:VAL:HG22	1:F:259:LEU:CD2	2.48	0.44
1:I:73:PRO:O	1:I:74:ALA:C	2.60	0.44
1:K:52:LEU:HD12	1:K:52:LEU:HA	1.82	0.44
1:C:48:ASN:HD21	1:C:158:ASN:H	1.59	0.44
1:C:206:VAL:HG22	1:C:259:LEU:CD2	2.48	0.44
1:D:35:THR:HG22	1:D:175:VAL:HG22	2.00	0.44
1:D:97:TYR:O	1:D:106:VAL:HG11	2.18	0.44
1:G:158:ASN:ND2	1:G:159:GLY:N	2.66	0.44
1:I:158:ASN:ND2	1:I:159:GLY:N	2.64	0.44
1:C:236:VAL:HG12	1:C:237:THR:N	2.33	0.44
1:H:62:VAL:CG2	1:H:66:GLN:OE1	2.59	0.44
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.83	0.44
1:I:91:GLN:HG3	1:I:118:TYR:CE1	2.53	0.44
1:J:48:ASN:HD22	1:J:157:THR:HA	1.83	0.44
1:J:175:VAL:HB	1:J:240:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:SER:C	1:L:195:GLN:H	2.26	0.44
1:A:206:VAL:HG21	1:A:222:LEU:HB2	1.99	0.43
1:B:216:TYR:HA	1:B:217:PRO:HD2	1.85	0.43
1:C:145:ILE:H	1:C:145:ILE:CD1	2.22	0.43
1:D:86:ASN:O	1:D:89:SER:HB3	2.18	0.43
1:D:101:VAL:HA	1:D:106:VAL:O	2.17	0.43
1:E:208:LEU:HB2	1:E:242:PHE:CE2	2.53	0.43
1:E:245:PRO:C	1:E:247:ASN:N	2.73	0.43
1:F:31:LEU:HB3	1:F:177:VAL:HG11	2.00	0.43
1:F:46:GLN:HB2	1:F:134:TYR:CD2	2.52	0.43
1:F:91:GLN:HG3	1:F:118:TYR:CE1	2.53	0.43
1:F:158:ASN:HD22	1:F:158:ASN:C	2.23	0.43
1:G:31:LEU:HD22	1:G:179:GLN:CD	2.42	0.43
1:H:48:ASN:ND2	1:H:158:ASN:N	2.52	0.43
1:H:62:VAL:HG22	1:H:63:LYS:N	2.33	0.43
1:I:236:VAL:HG21	1:J:250:LEU:HD12	1.99	0.43
1:K:40:ILE:HG12	1:K:168:GLN:HG2	1.99	0.43
1:K:158:ASN:HD22	1:K:158:ASN:C	2.24	0.43
1:A:101:VAL:HG13	1:A:106:VAL:CG2	2.45	0.43
1:A:144:ARG:HE	1:B:226:GLU:HG3	1.83	0.43
1:A:186:ARG:HD2	1:A:186:ARG:C	2.43	0.43
1:C:69:TYR:CE1	1:C:164:MET:HE2	2.53	0.43
1:L:77:GLU:OE2	1:L:81:GLN:NE2	2.51	0.43
1:B:146:GLY:HA3	2:B:361:GOL:C1	2.46	0.43
1:B:245:PRO:O	1:B:247:ASN:N	2.51	0.43
1:E:69:TYR:HB2	1:E:137:VAL:HB	2.00	0.43
1:H:77:GLU:OE2	1:H:81:GLN:NE2	2.51	0.43
1:H:210:LEU:C	1:H:212:ASP:H	2.26	0.43
1:J:83:ALA:O	1:J:86:ASN:N	2.51	0.43
1:A:144:ARG:HE	1:B:226:GLU:CD	2.26	0.43
1:B:48:ASN:HD22	1:B:158:ASN:H	1.63	0.43
1:J:46:GLN:HB2	1:J:134:TYR:CD2	2.53	0.43
1:M:41:ALA:HB1	1:M:140:PRO:HG2	2.01	0.43
1:M:48:ASN:ND2	1:M:157:THR:HA	2.33	0.43
1:C:47:VAL:HG22	1:C:76:TYR:CZ	2.53	0.43
1:D:57:LYS:O	1:D:58:GLU:C	2.61	0.43
1:E:75:THR:HG23	1:F:127:GLN:HE22	1.83	0.43
1:F:140:PRO:O	1:F:141:ILE:HD12	2.18	0.43
1:G:210:LEU:C	1:G:212:ASP:N	2.75	0.43
1:I:250:LEU:O	1:I:253:MET:HG3	2.19	0.43
1:K:193:SER:O	1:K:195:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:N	1:B:99:LEU:HD22	2.34	0.43
1:C:106:VAL:CG2	1:C:110:GLN:HB2	2.47	0.43
1:D:104:GLN:NE2	1:J:104:GLN:HE22	2.13	0.43
1:D:171:ASP:O	1:D:173:ILE:N	2.52	0.43
1:E:184:LEU:HD13	1:E:188:ARG:HG3	2.00	0.43
1:F:104:GLN:HE22	1:L:108:LYS:HB2	1.84	0.43
1:G:44:ARG:HD2	1:H:153:GLY:O	2.18	0.43
1:H:64:ALA:HB2	1:H:141:ILE:C	2.43	0.43
1:H:107:SER:OG	1:H:109:GLN:NE2	2.51	0.43
1:H:147:ARG:N	3:H:361:3GR:HA	2.16	0.43
1:B:43:VAL:HG23	1:B:165:ALA:O	2.18	0.43
1:D:175:VAL:HB	1:D:240:ALA:HB3	2.01	0.43
1:E:104:GLN:NE2	1:K:104:GLN:HA	2.33	0.43
1:E:193:SER:C	1:E:195:GLN:H	2.26	0.43
1:G:175:VAL:HB	1:G:240:ALA:HB3	2.00	0.43
1:H:208:LEU:HB2	1:H:242:PHE:CE2	2.54	0.43
1:I:158:ASN:C	1:I:158:ASN:ND2	2.76	0.43
1:J:250:LEU:O	1:J:253:MET:HG3	2.19	0.43
1:K:101:VAL:C	1:K:103:ASP:H	2.26	0.43
1:A:96:ARG:HH22	1:B:109:GLN:NE2	2.17	0.43
1:B:193:SER:C	1:B:195:GLN:H	2.27	0.43
1:E:208:LEU:HD11	1:E:255:VAL:CG2	2.48	0.43
1:G:171:ASP:HB3	1:G:172:PRO:HD3	1.96	0.43
1:G:245:PRO:O	1:G:247:ASN:N	2.52	0.43
1:H:110:GLN:C	1:H:112:ALA:N	2.77	0.43
1:I:41:ALA:HB1	1:I:140:PRO:HG2	2.00	0.43
1:I:145:ILE:HG23	1:I:167:VAL:HG22	2.01	0.43
1:K:99:LEU:CD1	1:K:99:LEU:H	2.32	0.43
1:K:226:GLU:HG3	1:L:144:ARG:HE	1.84	0.43
1:L:144:ARG:HG3	1:L:144:ARG:HH11	1.83	0.43
1:L:191:LEU:C	1:L:191:LEU:HD13	2.44	0.43
1:B:141:ILE:CG2	1:B:142:SER:N	2.79	0.43
1:B:184:LEU:HD13	1:B:188:ARG:HG3	2.00	0.43
1:G:191:LEU:HD11	1:G:198:ARG:NH1	2.34	0.43
1:I:230:ASP:O	1:I:234:GLY:N	2.48	0.43
1:B:158:ASN:ND2	1:B:159:GLY:N	2.65	0.43
1:E:60:SER:O	1:E:145:ILE:HD12	2.19	0.43
1:I:158:ASN:HD22	1:I:159:GLY:H	1.65	0.43
1:I:175:VAL:HB	1:I:240:ALA:HB3	1.99	0.43
1:L:113:ASP:O	1:L:116:ALA:HB3	2.19	0.43
1:L:130:ILE:HG22	1:L:134:TYR:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:HG22	1:B:76:TYR:CZ	2.54	0.42
1:B:69:TYR:CD1	1:B:164:MET:HE2	2.54	0.42
1:B:170:LEU:O	1:B:171:ASP:O	2.37	0.42
1:F:245:PRO:O	1:F:247:ASN:N	2.51	0.42
1:G:206:VAL:CG1	1:G:207:SER:N	2.82	0.42
1:I:52:LEU:HD12	1:I:52:LEU:HA	1.92	0.42
1:K:103:ASP:O	1:K:105:ALA:N	2.52	0.42
1:B:46:GLN:HB2	1:B:134:TYR:CD2	2.53	0.42
1:F:113:ASP:O	1:F:116:ALA:HB3	2.19	0.42
1:K:83:ALA:O	1:K:84:GLN:C	2.62	0.42
1:K:91:GLN:HG3	1:K:118:TYR:CE1	2.53	0.42
1:K:170:LEU:HD21	1:K:251:PRO:CG	2.49	0.42
1:A:158:ASN:ND2	1:A:159:GLY:N	2.63	0.42
1:B:52:LEU:HD12	1:B:52:LEU:HA	1.80	0.42
1:B:186:ARG:C	1:B:186:ARG:HD2	2.44	0.42
1:C:245:PRO:O	1:C:247:ASN:N	2.52	0.42
1:D:158:ASN:HD22	1:D:158:ASN:C	2.24	0.42
1:E:206:VAL:O	1:E:219:GLU:HB2	2.19	0.42
1:F:62:VAL:HG12	1:F:145:ILE:HG13	2.00	0.42
1:H:38:PHE:HD2	1:H:169:GLN:NE2	2.16	0.42
1:H:55:LEU:HD23	1:H:55:LEU:N	2.33	0.42
1:H:101:VAL:HA	1:H:106:VAL:O	2.18	0.42
1:J:62:VAL:HG12	1:J:145:ILE:HG13	2.01	0.42
1:K:206:VAL:CG1	1:K:207:SER:N	2.83	0.42
1:B:71:ILE:O	1:B:72:ASP:C	2.63	0.42
1:D:46:GLN:OE1	1:D:134:TYR:CE2	2.73	0.42
1:F:206:VAL:CG1	1:F:258:GLN:H	2.33	0.42
1:H:206:VAL:O	1:H:219:GLU:HB2	2.19	0.42
1:I:227:VAL:HG12	1:J:147:ARG:HG3	2.01	0.42
1:J:106:VAL:HG13	1:J:110:GLN:CB	2.45	0.42
1:J:186:ARG:HD2	1:J:186:ARG:C	2.44	0.42
1:L:97:TYR:O	1:L:101:VAL:HG23	2.20	0.42
1:L:186:ARG:C	1:L:186:ARG:HD2	2.45	0.42
1:M:145:ILE:H	1:M:145:ILE:CD1	2.33	0.42
1:M:206:VAL:CG1	1:M:207:SER:N	2.82	0.42
1:A:48:ASN:HD21	1:A:158:ASN:N	2.09	0.42
1:A:50:ILE:HD13	1:A:155:LEU:HA	2.01	0.42
1:A:130:ILE:CG2	1:A:134:TYR:HE1	2.32	0.42
1:C:130:ILE:HG22	1:C:134:TYR:CE1	2.55	0.42
1:E:62:VAL:CG2	1:E:68:LEU:HD21	2.41	0.42
1:E:71:ILE:O	1:E:73:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:TYR:CE1	1:F:164:MET:HE2	2.54	0.42
1:I:144:ARG:NH1	1:I:144:ARG:HG3	2.35	0.42
1:J:71:ILE:O	1:J:72:ASP:C	2.62	0.42
1:J:206:VAL:O	1:J:219:GLU:HB2	2.19	0.42
1:C:180:PRO:O	1:C:181:SER:C	2.63	0.42
1:D:216:TYR:HA	1:D:217:PRO:HD2	1.87	0.42
1:E:245:PRO:O	1:E:246:ASN:HB2	2.20	0.42
1:G:96:ARG:O	1:G:99:LEU:HB2	2.18	0.42
1:G:101:VAL:HG21	1:G:111:TYR:CB	2.47	0.42
1:H:54:ARG:HD2	1:H:54:ARG:O	2.19	0.42
1:I:62:VAL:HG12	1:I:145:ILE:HG13	2.01	0.42
1:B:145:ILE:HD12	1:B:145:ILE:N	2.35	0.42
1:D:191:LEU:HD13	1:D:191:LEU:C	2.44	0.42
1:I:52:LEU:HD22	1:I:72:ASP:HA	2.00	0.42
1:L:101:VAL:HG13	1:L:106:VAL:O	2.20	0.42
1:A:31:LEU:HB3	1:A:177:VAL:CG1	2.50	0.42
1:A:34:ARG:HH11	1:A:34:ARG:CB	2.25	0.42
1:A:60:SER:O	1:A:145:ILE:HD12	2.20	0.42
1:B:199:ALA:HB2	1:B:205:LYS:N	2.35	0.42
1:C:171:ASP:O	1:C:173:ILE:N	2.53	0.42
1:C:186:ARG:HD2	1:C:186:ARG:C	2.44	0.42
1:C:191:LEU:HD13	1:C:191:LEU:C	2.44	0.42
1:F:206:VAL:HG21	1:F:222:LEU:HB2	2.02	0.42
1:G:171:ASP:CB	1:G:172:PRO:CD	2.84	0.42
1:H:60:SER:O	1:H:145:ILE:HD12	2.19	0.42
1:H:103:ASP:OD1	1:H:103:ASP:N	2.53	0.42
1:H:175:VAL:HB	1:H:240:ALA:HB3	2.02	0.42
1:L:99:LEU:N	1:L:99:LEU:CD1	2.82	0.42
1:B:113:ASP:O	1:B:116:ALA:HB3	2.19	0.42
1:E:77:GLU:OE2	1:E:81:GLN:NE2	2.53	0.42
1:G:190:GLU:CB	1:G:196:LEU:HD13	2.50	0.42
1:L:64:ALA:HB2	1:L:141:ILE:C	2.45	0.42
1:M:206:VAL:HG13	1:M:258:GLN:O	2.19	0.42
1:D:104:GLN:C	1:D:106:VAL:N	2.72	0.42
1:F:193:SER:C	1:F:195:GLN:H	2.27	0.42
1:G:70:GLN:HE22	1:G:135:THR:HG23	1.85	0.42
1:I:201:ASP:O	1:I:202:ASN:HB2	2.19	0.42
1:M:100:LEU:CB	1:M:106:VAL:HG23	2.47	0.42
1:M:101:VAL:HG21	1:M:111:TYR:CD1	2.55	0.42
1:A:104:GLN:HG2	1:G:104:GLN:HE22	1.84	0.41
1:A:183:ALA:O	1:A:187:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:SER:O	1:C:145:ILE:HD12	2.19	0.41
1:C:130:ILE:CG2	1:C:134:TYR:HE1	2.33	0.41
1:J:70:GLN:NE2	1:J:135:THR:HG23	2.35	0.41
1:L:145:ILE:H	1:L:145:ILE:CD1	2.25	0.41
1:B:193:SER:O	1:B:195:GLN:N	2.53	0.41
1:E:130:ILE:HG22	1:E:134:TYR:CE1	2.55	0.41
1:E:206:VAL:CG1	1:E:207:SER:N	2.83	0.41
1:F:75:THR:O	1:F:78:ALA:N	2.53	0.41
1:G:31:LEU:HD22	1:G:179:GLN:NE2	2.35	0.41
1:G:226:GLU:CG	1:H:144:ARG:HE	2.29	0.41
1:H:83:ALA:O	1:H:84:GLN:C	2.63	0.41
1:J:91:GLN:CG	1:J:95:GLN:HE21	2.07	0.41
1:J:99:LEU:O	1:J:102:ALA:HB3	2.20	0.41
1:J:146:GLY:HA3	2:J:361:GOL:C1	2.49	0.41
1:K:30:GLU:HG2	1:K:258:GLN:HG2	2.02	0.41
1:K:69:TYR:CD1	1:K:164:MET:HE2	2.55	0.41
1:M:48:ASN:ND2	1:M:158:ASN:N	2.50	0.41
1:A:31:LEU:HD22	1:A:179:GLN:CD	2.45	0.41
1:A:75:THR:O	1:A:78:ALA:N	2.54	0.41
1:B:103:ASP:O	1:B:104:GLN:C	2.62	0.41
1:B:206:VAL:CG1	1:B:207:SER:N	2.83	0.41
1:C:31:LEU:HB3	1:C:177:VAL:CG1	2.49	0.41
1:F:191:LEU:HD11	1:F:198:ARG:NH1	2.35	0.41
1:H:46:GLN:CD	1:H:134:TYR:CE2	2.98	0.41
1:H:193:SER:C	1:H:195:GLN:H	2.28	0.41
1:I:216:TYR:HA	1:I:217:PRO:HD2	1.85	0.41
1:J:70:GLN:HE21	1:J:73:PRO:HD3	1.85	0.41
1:J:146:GLY:HA3	2:J:361:GOL:O2	2.21	0.41
1:K:48:ASN:ND2	1:K:157:THR:HG23	2.35	0.41
1:M:199:ALA:HB2	1:M:205:LYS:N	2.36	0.41
1:B:48:ASN:HD21	1:B:158:ASN:N	2.14	0.41
1:D:158:ASN:ND2	1:D:158:ASN:C	2.78	0.41
1:E:92:GLU:OE1	1:E:96:ARG:NH1	2.53	0.41
1:H:50:ILE:HD13	1:H:155:LEU:HA	2.02	0.41
1:I:103:ASP:C	1:I:105:ALA:N	2.78	0.41
1:J:43:VAL:HG23	1:J:165:ALA:O	2.21	0.41
1:K:62:VAL:HG22	1:K:63:LYS:N	2.35	0.41
1:L:48:ASN:HD22	1:L:158:ASN:H	1.59	0.41
1:A:48:ASN:ND2	1:A:157:THR:HA	2.34	0.41
1:C:86:ASN:O	1:C:89:SER:HB3	2.21	0.41
1:C:201:ASP:O	1:C:202:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:O	1:D:106:VAL:N	2.54	0.41
1:D:100:LEU:CB	1:D:106:VAL:CG2	2.99	0.41
1:G:30:GLU:HA	1:G:257:ALA:O	2.20	0.41
1:I:135:THR:HG22	1:I:136:LYS:HG3	2.02	0.41
1:L:183:ALA:O	1:L:187:LEU:HG	2.21	0.41
1:A:206:VAL:CG1	1:A:207:SER:N	2.82	0.41
1:E:51:ILE:CD1	1:E:164:MET:HE3	2.50	0.41
1:H:110:GLN:C	1:H:112:ALA:H	2.28	0.41
1:H:186:ARG:HD2	1:H:186:ARG:C	2.46	0.41
1:J:65:GLY:O	1:J:138:LEU:HD22	2.20	0.41
1:J:71:ILE:O	1:J:73:PRO:HD3	2.21	0.41
1:L:80:TYR:HA	1:L:128:ALA:HB1	2.03	0.41
1:A:83:ALA:O	1:A:86:ASN:N	2.54	0.41
1:A:140:PRO:O	1:A:141:ILE:HD12	2.20	0.41
1:D:184:LEU:HD13	1:D:188:ARG:HG3	2.03	0.41
1:L:110:GLN:C	1:L:112:ALA:H	2.27	0.41
1:L:130:ILE:CG2	1:L:134:TYR:CE1	3.04	0.41
1:B:52:LEU:HD22	1:B:72:ASP:HA	2.02	0.41
1:D:193:SER:C	1:D:195:GLN:H	2.29	0.41
1:G:62:VAL:HG23	1:G:66:GLN:NE2	2.34	0.41
1:G:134:TYR:OH	1:H:74:ALA:HB3	2.20	0.41
1:I:46:GLN:OE1	1:I:134:TYR:CE2	2.73	0.41
1:K:39:ARG:C	1:K:40:ILE:HG13	2.46	0.41
1:K:130:ILE:HD12	1:L:74:ALA:HB1	2.03	0.41
1:L:110:GLN:O	1:L:111:TYR:C	2.63	0.41
1:M:47:VAL:HG22	1:M:76:TYR:OH	2.20	0.41
1:M:69:TYR:HB2	1:M:137:VAL:HB	2.03	0.41
1:M:145:ILE:HD12	1:M:145:ILE:N	2.35	0.41
1:A:206:VAL:HG22	1:A:259:LEU:HD21	2.01	0.41
1:C:206:VAL:CG1	1:C:207:SER:N	2.83	0.41
1:E:62:VAL:CG2	1:E:66:GLN:OE1	2.68	0.41
1:E:62:VAL:CG1	1:E:145:ILE:HG13	2.51	0.41
1:F:48:ASN:ND2	1:F:157:THR:HG23	2.35	0.41
1:G:170:LEU:O	1:G:171:ASP:O	2.39	0.41
1:H:48:ASN:HD22	1:H:157:THR:HA	1.84	0.41
1:I:206:VAL:CG1	1:I:207:SER:N	2.83	0.41
1:J:46:GLN:OE1	1:J:134:TYR:HE2	2.02	0.41
1:J:48:ASN:HD21	1:J:157:THR:HG23	1.85	0.41
1:J:87:LEU:CD2	1:J:125:VAL:HG21	2.51	0.41
1:J:87:LEU:HD23	1:J:125:VAL:HG21	2.03	0.41
1:J:189:ARG:O	1:J:192:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:193:SER:C	1:J:195:GLN:H	2.29	0.41
1:L:69:TYR:CD1	1:L:164:MET:HE2	2.56	0.41
1:L:199:ALA:HB2	1:L:205:LYS:N	2.36	0.41
1:M:41:ALA:HB1	1:M:140:PRO:CG	2.51	0.41
1:M:50:ILE:HD13	1:M:155:LEU:HA	2.03	0.41
1:C:106:VAL:CG2	1:C:110:GLN:CD	2.94	0.41
1:E:186:ARG:C	1:E:186:ARG:HD2	2.46	0.41
1:G:158:ASN:ND2	1:G:158:ASN:C	2.78	0.41
1:H:52:LEU:HD12	1:H:52:LEU:HA	1.81	0.41
1:H:170:LEU:O	1:H:171:ASP:O	2.38	0.41
1:I:40:ILE:HD12	1:I:168:GLN:HG2	2.02	0.41
1:I:193:SER:O	1:I:195:GLN:N	2.53	0.41
1:L:228:SER:HB3	2:M:361:GOL:H11	2.03	0.41
1:B:86:ASN:O	1:B:89:SER:HB3	2.22	0.40
1:D:64:ALA:HB2	1:D:141:ILE:C	2.46	0.40
1:D:206:VAL:CG1	1:D:207:SER:N	2.83	0.40
1:E:199:ALA:HB2	1:E:205:LYS:N	2.36	0.40
1:G:107:SER:N	1:G:110:GLN:NE2	2.58	0.40
1:H:32:PRO:HB3	1:H:256:HIS:CE1	2.56	0.40
1:J:141:ILE:HG23	1:J:142:SER:N	2.36	0.40
1:J:191:LEU:C	1:J:191:LEU:HD13	2.45	0.40
1:J:216:TYR:HA	1:J:217:PRO:HD2	1.87	0.40
1:L:227:VAL:HG12	1:M:147:ARG:HG3	2.03	0.40
1:M:140:PRO:C	1:M:141:ILE:HD12	2.46	0.40
1:A:193:SER:C	1:A:195:GLN:H	2.30	0.40
1:B:191:LEU:HD13	1:B:191:LEU:C	2.46	0.40
1:G:43:VAL:HG23	1:G:165:ALA:O	2.21	0.40
1:G:48:ASN:HD22	1:G:157:THR:HA	1.86	0.40
1:G:52:LEU:HA	1:G:52:LEU:HD12	1.84	0.40
1:I:174:TYR:CD2	1:I:239:ARG:HD3	2.57	0.40
1:K:199:ALA:HB2	1:K:205:LYS:N	2.36	0.40
1:M:193:SER:O	1:M:195:GLN:N	2.54	0.40
1:A:134:TYR:C	1:A:136:LYS:N	2.79	0.40
1:B:130:ILE:CG2	1:B:134:TYR:HE1	2.35	0.40
1:D:186:ARG:HD2	1:D:186:ARG:C	2.46	0.40
1:D:193:SER:O	1:D:195:GLN:N	2.54	0.40
1:M:171:ASP:HB3	1:M:172:PRO:HD3	1.92	0.40
1:A:145:ILE:H	1:A:145:ILE:CD1	2.26	0.40
1:B:47:VAL:HG22	1:B:76:TYR:OH	2.22	0.40
1:D:104:GLN:C	1:D:106:VAL:H	2.29	0.40
1:E:158:ASN:HD22	1:E:158:ASN:C	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:LEU:HD12	1:G:100:LEU:HA	1.85	0.40
1:H:65:GLY:O	1:H:138:LEU:HD22	2.21	0.40
1:J:73:PRO:O	1:J:74:ALA:C	2.65	0.40
1:K:147:ARG:N	3:K:361:3GR:O3	2.53	0.40
1:L:101:VAL:HG11	1:L:108:LYS:CG	2.47	0.40
1:L:109:GLN:HB3	1:M:96:ARG:CD	2.52	0.40
1:A:71:ILE:O	1:A:72:ASP:C	2.64	0.40
1:A:110:GLN:C	1:A:112:ALA:N	2.77	0.40
1:C:71:ILE:O	1:C:72:ASP:C	2.65	0.40
1:D:199:ALA:HB2	1:D:205:LYS:N	2.36	0.40
1:F:48:ASN:ND2	1:F:158:ASN:N	2.55	0.40
1:H:113:ASP:O	1:H:116:ALA:HB3	2.20	0.40
1:H:210:LEU:C	1:H:212:ASP:N	2.78	0.40
1:I:101:VAL:CG1	1:I:102:ALA:N	2.84	0.40
1:J:46:GLN:CD	1:J:134:TYR:CE2	3.00	0.40
1:J:69:TYR:HB2	1:J:137:VAL:HB	2.03	0.40
1:L:140:PRO:C	1:L:141:ILE:HD12	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:NH2	1:D:194:GLY:O[2_656]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	229/360 (64%)	207 (90%)	21 (9%)	1 (0%)	30 65
1	B	229/360 (64%)	203 (89%)	24 (10%)	2 (1%)	14 48
1	C	229/360 (64%)	209 (91%)	18 (8%)	2 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	229/360 (64%)	200 (87%)	24 (10%)	5 (2%)	5	26
1	E	229/360 (64%)	211 (92%)	15 (7%)	3 (1%)	9	38
1	F	229/360 (64%)	209 (91%)	17 (7%)	3 (1%)	9	38
1	G	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	7	32
1	H	229/360 (64%)	205 (90%)	19 (8%)	5 (2%)	5	26
1	I	229/360 (64%)	210 (92%)	16 (7%)	3 (1%)	9	38
1	J	229/360 (64%)	208 (91%)	17 (7%)	4 (2%)	7	32
1	K	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	7	32
1	L	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	7	32
1	M	229/360 (64%)	204 (89%)	22 (10%)	3 (1%)	9	38
All	All	2977/4680 (64%)	2681 (90%)	253 (8%)	43 (1%)	9	36

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	B	171	ASP
1	C	171	ASP
1	D	171	ASP
1	E	171	ASP
1	F	171	ASP
1	G	171	ASP
1	H	171	ASP
1	I	171	ASP
1	J	171	ASP
1	K	171	ASP
1	L	171	ASP
1	M	104	GLN
1	M	171	ASP
1	G	194	GLY
1	I	194	GLY
1	K	55	LEU
1	K	194	GLY
1	D	55	LEU
1	D	102	ALA
1	F	194	GLY
1	G	55	LEU
1	J	181	SER

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Mol	Chain	Res	Type
1	J	194	GLY
1	L	55	LEU
1	B	194	GLY
1	C	194	GLY
1	D	111	TYR
1	F	181	SER
1	H	137	VAL
1	I	55	LEU
1	J	55	LEU
1	L	104	GLN
1	L	194	GLY
1	M	194	GLY
1	E	194	GLY
1	H	55	LEU
1	H	181	SER
1	D	194	GLY
1	E	181	SER
1	G	106	VAL
1	K	104	GLN
1	H	194	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/287 (65%)	173 (93%)	13 (7%)	14	44
1	B	186/287 (65%)	174 (94%)	12 (6%)	15	47
1	C	186/287 (65%)	174 (94%)	12 (6%)	15	47
1	D	186/287 (65%)	171 (92%)	15 (8%)	11	38
1	E	186/287 (65%)	169 (91%)	17 (9%)	9	33
1	F	186/287 (65%)	169 (91%)	17 (9%)	9	33
1	G	186/287 (65%)	170 (91%)	16 (9%)	10	36
1	H	186/287 (65%)	173 (93%)	13 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	186/287 (65%)	173 (93%)	13 (7%)	14	44
1	J	186/287 (65%)	169 (91%)	17 (9%)	9	33
1	K	186/287 (65%)	170 (91%)	16 (9%)	10	36
1	L	186/287 (65%)	173 (93%)	13 (7%)	14	44
1	M	186/287 (65%)	177 (95%)	9 (5%)	23	57
All	All	2418/3731 (65%)	2235 (92%)	183 (8%)	12	41

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	47	VAL
1	A	75	THR
1	A	99	LEU
1	A	132	LEU
1	A	135	THR
1	A	141	ILE
1	A	145	ILE
1	A	152	GLU
1	A	156	VAL
1	A	186	ARG
1	A	196	LEU
1	A	226	GLU
1	B	34	ARG
1	B	47	VAL
1	B	73	PRO
1	B	132	LEU
1	B	135	THR
1	B	141	ILE
1	B	145	ILE
1	B	152	GLU
1	B	156	VAL
1	B	186	ARG
1	B	196	LEU
1	B	226	GLU
1	C	34	ARG
1	C	43	VAL
1	C	75	THR
1	C	132	LEU
1	C	135	THR

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Mol	Chain	Res	Type
1	C	141	ILE
1	C	145	ILE
1	C	156	VAL
1	C	170	LEU
1	C	186	ARG
1	C	196	LEU
1	C	226	GLU
1	D	34	ARG
1	D	43	VAL
1	D	55	LEU
1	D	75	THR
1	D	104	GLN
1	D	132	LEU
1	D	135	THR
1	D	141	ILE
1	D	145	ILE
1	D	156	VAL
1	D	186	ARG
1	D	189	ARG
1	D	196	LEU
1	D	225	SER
1	D	226	GLU
1	E	34	ARG
1	E	47	VAL
1	E	61	ASP
1	E	73	PRO
1	E	75	THR
1	E	106	VAL
1	E	132	LEU
1	E	135	THR
1	E	141	ILE
1	E	145	ILE
1	E	156	VAL
1	E	186	ARG
1	E	189	ARG
1	E	196	LEU
1	E	214	SER
1	E	225	SER
1	E	226	GLU
1	F	34	ARG
1	F	43	VAL
1	F	47	VAL

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Mol	Chain	Res	Type
1	F	55	LEU
1	F	75	THR
1	F	132	LEU
1	F	135	THR
1	F	141	ILE
1	F	142	SER
1	F	145	ILE
1	F	150	VAL
1	F	152	GLU
1	F	156	VAL
1	F	186	ARG
1	F	189	ARG
1	F	196	LEU
1	F	226	GLU
1	G	34	ARG
1	G	47	VAL
1	G	55	LEU
1	G	75	THR
1	G	99	LEU
1	G	100	LEU
1	G	106	VAL
1	G	132	LEU
1	G	135	THR
1	G	141	ILE
1	G	145	ILE
1	G	152	GLU
1	G	156	VAL
1	G	186	ARG
1	G	196	LEU
1	G	226	GLU
1	H	34	ARG
1	H	55	LEU
1	H	61	ASP
1	H	75	THR
1	H	106	VAL
1	H	132	LEU
1	H	135	THR
1	H	141	ILE
1	H	145	ILE
1	H	156	VAL
1	H	186	ARG
1	H	196	LEU

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Mol	Chain	Res	Type
1	H	226	GLU
1	I	34	ARG
1	I	47	VAL
1	I	55	LEU
1	I	75	THR
1	I	104	GLN
1	I	132	LEU
1	I	135	THR
1	I	141	ILE
1	I	145	ILE
1	I	152	GLU
1	I	186	ARG
1	I	196	LEU
1	I	226	GLU
1	J	34	ARG
1	J	47	VAL
1	J	55	LEU
1	J	61	ASP
1	J	73	PRO
1	J	75	THR
1	J	106	VAL
1	J	132	LEU
1	J	135	THR
1	J	141	ILE
1	J	145	ILE
1	J	156	VAL
1	J	186	ARG
1	J	196	LEU
1	J	225	SER
1	J	226	GLU
1	J	237	THR
1	K	34	ARG
1	K	47	VAL
1	K	55	LEU
1	K	73	PRO
1	K	75	THR
1	K	104	GLN
1	K	132	LEU
1	K	135	THR
1	K	141	ILE
1	K	145	ILE
1	K	150	VAL

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Mol	Chain	Res	Type
1	K	156	VAL
1	K	186	ARG
1	K	196	LEU
1	K	225	SER
1	K	226	GLU
1	L	34	ARG
1	L	47	VAL
1	L	75	THR
1	L	132	LEU
1	L	135	THR
1	L	141	ILE
1	L	145	ILE
1	L	150	VAL
1	L	152	GLU
1	L	156	VAL
1	L	186	ARG
1	L	196	LEU
1	L	225	SER
1	M	34	ARG
1	M	43	VAL
1	M	132	LEU
1	M	135	THR
1	M	145	ILE
1	M	152	GLU
1	M	156	VAL
1	M	186	ARG
1	M	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	70	GLN
1	A	84	GLN
1	A	95	GLN
1	A	158	ASN
1	A	179	GLN
1	A	202	ASN
1	A	215	GLN
1	A	256	HIS
1	B	36	ASN
1	B	48	ASN

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	95	GLN
1	B	158	ASN
1	B	168	GLN
1	B	202	ASN
1	B	215	GLN
1	C	48	ASN
1	C	67	GLN
1	C	70	GLN
1	C	84	GLN
1	C	95	GLN
1	C	110	GLN
1	C	115	ASN
1	C	158	ASN
1	C	169	GLN
1	C	179	GLN
1	C	202	ASN
1	C	215	GLN
1	D	48	ASN
1	D	84	GLN
1	D	95	GLN
1	D	104	GLN
1	D	127	GLN
1	D	158	ASN
1	D	179	GLN
1	D	202	ASN
1	D	215	GLN
1	D	256	HIS
1	E	48	ASN
1	E	84	GLN
1	E	95	GLN
1	E	104	GLN
1	E	115	ASN
1	E	127	GLN
1	E	158	ASN
1	E	169	GLN
1	E	179	GLN
1	E	202	ASN
1	E	256	HIS
1	F	48	ASN
1	F	67	GLN
1	F	70	GLN

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Mol	Chain	Res	Type
1	F	84	GLN
1	F	95	GLN
1	F	104	GLN
1	F	110	GLN
1	F	127	GLN
1	F	158	ASN
1	F	179	GLN
1	F	202	ASN
1	F	256	HIS
1	G	48	ASN
1	G	67	GLN
1	G	70	GLN
1	G	84	GLN
1	G	95	GLN
1	G	110	GLN
1	G	115	ASN
1	G	158	ASN
1	G	168	GLN
1	G	169	GLN
1	G	179	GLN
1	G	202	ASN
1	H	48	ASN
1	H	84	GLN
1	H	95	GLN
1	H	109	GLN
1	H	115	ASN
1	H	158	ASN
1	H	169	GLN
1	H	179	GLN
1	H	215	GLN
1	H	247	ASN
1	H	256	HIS
1	I	36	ASN
1	I	48	ASN
1	I	67	GLN
1	I	70	GLN
1	I	84	GLN
1	I	95	GLN
1	I	109	GLN
1	I	115	ASN
1	I	158	ASN
1	I	169	GLN

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Mol	Chain	Res	Type
1	I	179	GLN
1	I	202	ASN
1	J	36	ASN
1	J	48	ASN
1	J	67	GLN
1	J	70	GLN
1	J	91	GLN
1	J	95	GLN
1	J	104	GLN
1	J	115	ASN
1	J	158	ASN
1	J	168	GLN
1	J	202	ASN
1	J	215	GLN
1	J	247	ASN
1	J	256	HIS
1	K	48	ASN
1	K	67	GLN
1	K	70	GLN
1	K	95	GLN
1	K	104	GLN
1	K	158	ASN
1	K	179	GLN
1	K	202	ASN
1	K	215	GLN
1	L	48	ASN
1	L	70	GLN
1	L	95	GLN
1	L	104	GLN
1	L	158	ASN
1	L	169	GLN
1	L	179	GLN
1	L	256	HIS
1	M	46	GLN
1	M	48	ASN
1	M	70	GLN
1	M	84	GLN
1	M	95	GLN
1	M	109	GLN
1	M	110	GLN
1	M	158	ASN
1	M	168	GLN

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Mol	Chain	Res	Type
1	M	169	GLN
1	M	179	GLN
1	M	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	361	-	5,5,5	0.23	0	5,5,5	0.49	0
3	3GR	I	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.96	1 (25%)
3	3GR	E	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.96	1 (25%)
2	GOL	B	361	-	5,5,5	4.79	1 (20%)	5,5,5	4.47	1 (20%)
2	GOL	M	361	-	5,5,5	4.79	1 (20%)	5,5,5	4.47	1 (20%)
2	GOL	J	361	-	5,5,5	4.79	1 (20%)	5,5,5	4.47	1 (20%)
3	3GR	D	361	-	4,5,5	6.15	2 (50%)	4,5,5	14.97	1 (25%)
3	3GR	G	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.96	1 (25%)
3	3GR	H	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.97	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	3GR	K	361	-	4,5,5	6.15	2 (50%)	4,5,5	14.97	1 (25%)
3	3GR	L	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.97	1 (25%)
3	3GR	F	361	-	4,5,5	6.15	2 (50%)	4,5,5	14.96	1 (25%)
3	3GR	C	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.98	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	361	-	-	0/4/4/4	-
3	3GR	I	361	-	-	1/3/4/4	-
3	3GR	E	361	-	-	1/3/4/4	-
2	GOL	B	361	-	-	0/4/4/4	-
2	GOL	M	361	-	-	0/4/4/4	-
2	GOL	J	361	-	-	0/4/4/4	-
3	3GR	D	361	-	-	1/3/4/4	-
3	3GR	G	361	-	-	1/3/4/4	-
3	3GR	H	361	-	-	1/3/4/4	-
3	3GR	K	361	-	-	1/3/4/4	-
3	3GR	L	361	-	-	1/3/4/4	-
3	3GR	F	361	-	-	1/3/4/4	-
3	3GR	C	361	-	-	1/3/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	361	3GR	O3-C3	-10.68	0.97	1.42
3	I	361	3GR	O3-C3	-10.67	0.97	1.42
3	H	361	3GR	O3-C3	-10.67	0.97	1.42
3	L	361	3GR	O3-C3	-10.67	0.97	1.42
2	M	361	GOL	O3-C3	-10.66	0.97	1.42
3	E	361	3GR	O3-C3	-10.66	0.97	1.42
3	C	361	3GR	O3-C3	-10.66	0.97	1.42
3	D	361	3GR	O3-C3	-10.66	0.97	1.42
2	B	361	GOL	O3-C3	-10.66	0.97	1.42
3	K	361	3GR	O3-C3	-10.66	0.97	1.42
2	J	361	GOL	O3-C3	-10.65	0.97	1.42
3	F	361	3GR	O3-C3	-10.65	0.97	1.42
3	C	361	3GR	O1-C1	6.06	1.43	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	361	3GR	O1-C1	6.06	1.43	1.20
3	L	361	3GR	O1-C1	6.06	1.43	1.20
3	H	361	3GR	O1-C1	6.06	1.43	1.20
3	I	361	3GR	O1-C1	6.06	1.43	1.20
3	G	361	3GR	O1-C1	6.05	1.42	1.20
3	F	361	3GR	O1-C1	6.04	1.42	1.20
3	D	361	3GR	O1-C1	6.04	1.42	1.20
3	K	361	3GR	O1-C1	6.03	1.42	1.20

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	361	3GR	O3-C3-C2	29.94	155.34	112.39
3	K	361	3GR	O3-C3-C2	29.93	155.32	112.39
3	D	361	3GR	O3-C3-C2	29.92	155.32	112.39
3	H	361	3GR	O3-C3-C2	29.92	155.32	112.39
3	L	361	3GR	O3-C3-C2	29.92	155.31	112.39
3	G	361	3GR	O3-C3-C2	29.90	155.29	112.39
3	E	361	3GR	O3-C3-C2	29.90	155.29	112.39
3	F	361	3GR	O3-C3-C2	29.90	155.28	112.39
3	I	361	3GR	O3-C3-C2	29.89	155.28	112.39
2	M	361	GOL	O3-C3-C2	9.99	155.36	110.38
2	J	361	GOL	O3-C3-C2	9.99	155.34	110.38
2	B	361	GOL	O3-C3-C2	9.98	155.32	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	361	3GR	O2-C2-C3-O3
3	D	361	3GR	O2-C2-C3-O3
3	E	361	3GR	O2-C2-C3-O3
3	F	361	3GR	O2-C2-C3-O3
3	G	361	3GR	O2-C2-C3-O3
3	H	361	3GR	O2-C2-C3-O3
3	I	361	3GR	O2-C2-C3-O3
3	K	361	3GR	O2-C2-C3-O3
3	L	361	3GR	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	GOL	5	0
3	I	361	3GR	4	0
3	E	361	3GR	2	0
2	B	361	GOL	3	0
2	M	361	GOL	3	0
2	J	361	GOL	6	0
3	G	361	3GR	1	0
3	H	361	3GR	2	0
3	K	361	3GR	3	0
3	L	361	3GR	1	0
3	F	361	3GR	4	0
3	C	361	3GR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	29:THR	C	30:GLU	N	1.00

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	231/360 (64%)	1.40	64 (27%)	1 1	29, 93, 132, 143	2 (0%)
1	B	231/360 (64%)	1.10	46 (19%)	3 2	22, 80, 110, 123	2 (0%)
1	C	231/360 (64%)	0.96	36 (15%)	5 3	22, 77, 111, 116	2 (0%)
1	D	231/360 (64%)	0.99	45 (19%)	3 2	16, 82, 109, 123	2 (0%)
1	E	231/360 (64%)	0.59	18 (7%)	19 10	21, 61, 95, 111	2 (0%)
1	F	231/360 (64%)	1.25	48 (20%)	2 2	31, 80, 106, 111	2 (0%)
1	G	231/360 (64%)	1.39	62 (26%)	1 1	31, 86, 118, 126	2 (0%)
1	H	231/360 (64%)	0.88	33 (14%)	6 3	24, 64, 98, 109	2 (0%)
1	I	231/360 (64%)	0.79	35 (15%)	5 3	17, 62, 96, 109	2 (0%)
1	J	231/360 (64%)	0.33	11 (4%)	35 19	8, 48, 84, 100	2 (0%)
1	K	231/360 (64%)	0.73	30 (12%)	7 4	11, 59, 92, 107	2 (0%)
1	L	231/360 (64%)	0.59	22 (9%)	14 7	14, 63, 102, 115	2 (0%)
1	M	231/360 (64%)	1.48	63 (27%)	1 1	25, 93, 117, 130	2 (0%)
All	All	3003/4680 (64%)	0.96	513 (17%)	4 3	8, 75, 114, 143	26 (0%)

All (513) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	82	SER	10.2
1	C	82	SER	10.2
1	A	82	SER	9.9
1	B	82	SER	8.9
1	D	82	SER	8.9
1	B	74	ALA	8.5
1	G	82	SER	8.1
1	L	82	SER	8.0
1	M	227	VAL	8.0

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Mol	Chain	Res	Type	RSRZ
1	H	82	SER	7.5
1	I	82	SER	7.5
1	C	74	ALA	7.4
1	J	82	SER	7.0
1	K	82	SER	6.9
1	E	82	SER	6.9
1	I	74	ALA	6.4
1	M	225	SER	6.4
1	F	82	SER	6.3
1	H	74	ALA	6.3
1	L	74	ALA	6.1
1	A	74	ALA	5.9
1	M	74	ALA	5.5
1	A	259	LEU	5.4
1	G	74	ALA	5.4
1	A	225	SER	5.3
1	C	29	THR	5.3
1	D	113	ASP	5.3
1	K	230	ASP	5.3
1	E	231	GLU	5.3
1	C	231	GLU	5.2
1	M	226	GLU	5.0
1	J	231	GLU	4.9
1	K	74	ALA	4.8
1	M	202	ASN	4.8
1	M	29	THR	4.8
1	A	193	SER	4.8
1	F	81	GLN	4.7
1	B	195	GLN	4.6
1	E	74	ALA	4.4
1	M	109	GLN	4.4
1	E	230	ASP	4.4
1	F	74	ALA	4.4
1	D	105	ALA	4.4
1	F	29	THR	4.4
1	G	212	ASP	4.3
1	A	29	THR	4.3
1	J	74	ALA	4.2
1	G	234	GLY	4.2
1	A	32	PRO	4.2
1	D	74	ALA	4.2
1	I	231	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	193	SER	4.1
1	A	231	GLU	4.1
1	M	223	GLU	4.0
1	D	114	ALA	4.0
1	G	231	GLU	4.0
1	F	192	ALA	3.9
1	A	185	LEU	3.9
1	M	99	LEU	3.9
1	F	231	GLU	3.9
1	I	29	THR	3.9
1	H	234	GLY	3.9
1	G	192	ALA	3.9
1	G	198	ARG	3.9
1	M	224	PHE	3.9
1	K	29	THR	3.8
1	M	30	GLU	3.8
1	G	197	GLU	3.8
1	M	228	SER	3.8
1	D	108	LYS	3.8
1	B	190	GLU	3.8
1	M	108	LYS	3.8
1	B	219	GLU	3.8
1	B	225	SER	3.7
1	F	210	LEU	3.7
1	G	259	LEU	3.7
1	K	231	GLU	3.7
1	K	212	ASP	3.7
1	E	104	GLN	3.6
1	F	92	GLU	3.6
1	K	104	GLN	3.6
1	L	234	GLY	3.6
1	G	85	ALA	3.6
1	I	259	LEU	3.6
1	D	231	GLU	3.6
1	C	225	SER	3.6
1	J	230	ASP	3.6
1	I	81	GLN	3.5
1	M	81	GLN	3.5
1	C	259	LEU	3.5
1	F	211	GLU	3.5
1	B	36	ASN	3.5
1	A	254	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	29	THR	3.5
1	B	29	THR	3.5
1	G	92	GLU	3.5
1	B	179	GLN	3.4
1	I	198	ARG	3.4
1	F	230	ASP	3.4
1	G	211	GLU	3.4
1	F	171	ASP	3.4
1	A	217	PRO	3.4
1	J	212	ASP	3.4
1	M	199	ALA	3.4
1	B	198	ARG	3.4
1	I	221	ARG	3.4
1	M	198	ARG	3.4
1	D	246	ASN	3.3
1	M	259	LEU	3.3
1	H	180	PRO	3.3
1	M	179	GLN	3.3
1	F	198	ARG	3.3
1	C	233	THR	3.3
1	I	225	SER	3.3
1	H	113	ASP	3.3
1	B	246	ASN	3.3
1	H	129	ARG	3.3
1	D	192	ALA	3.3
1	D	232	GLY	3.3
1	A	192	ALA	3.2
1	M	195	GLN	3.2
1	B	213	GLY	3.2
1	G	147	ARG	3.2
1	G	172	PRO	3.2
1	G	217	PRO	3.2
1	D	102	ALA	3.2
1	K	198	ARG	3.2
1	C	179	GLN	3.2
1	D	225	SER	3.2
1	G	258	GLN	3.2
1	I	230	ASP	3.2
1	H	112	ALA	3.2
1	B	254	PHE	3.2
1	A	93	GLN	3.2
1	C	213	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	32	PRO	3.1
1	C	95	GLN	3.1
1	L	102	ALA	3.1
1	K	259	LEU	3.1
1	G	219	GLU	3.1
1	F	233	THR	3.1
1	C	230	ASP	3.1
1	H	231	GLU	3.1
1	A	233	THR	3.1
1	F	232	GLY	3.1
1	A	189	ARG	3.1
1	D	230	ASP	3.1
1	D	104	GLN	3.1
1	F	259	LEU	3.1
1	M	189	ARG	3.1
1	G	181	SER	3.1
1	I	30	GLU	3.1
1	H	230	ASP	3.1
1	A	172	PRO	3.1
1	M	32	PRO	3.0
1	F	201	ASP	3.0
1	F	179	GLN	3.0
1	E	95	GLN	3.0
1	B	178	THR	3.0
1	G	210	LEU	3.0
1	M	95	GLN	3.0
1	D	259	LEU	3.0
1	D	181	SER	3.0
1	F	95	GLN	3.0
1	B	232	GLY	2.9
1	E	113	ASP	2.9
1	K	201	ASP	2.9
1	A	81	GLN	2.9
1	L	29	THR	2.9
1	A	218	LEU	2.9
1	I	96	ARG	2.9
1	A	180	PRO	2.9
1	G	223	GLU	2.9
1	A	242	PHE	2.9
1	D	193	SER	2.9
1	E	181	SER	2.9
1	D	213	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	33	GLY	2.9
1	G	84	GLN	2.9
1	L	104	GLN	2.9
1	I	201	ASP	2.9
1	A	182	THR	2.9
1	D	180	PRO	2.9
1	G	221	ARG	2.9
1	M	110	GLN	2.8
1	G	201	ASP	2.8
1	A	219	GLU	2.8
1	A	248	GLU	2.8
1	A	234	GLY	2.8
1	M	122	LYS	2.8
1	A	179	GLN	2.8
1	M	201	ASP	2.8
1	A	223	GLU	2.8
1	K	221	ARG	2.8
1	A	247	ASN	2.8
1	D	111	TYR	2.8
1	H	81	GLN	2.8
1	A	198	ARG	2.8
1	L	231	GLU	2.8
1	I	179	GLN	2.8
1	B	32	PRO	2.8
1	G	152	GLU	2.8
1	I	233	THR	2.8
1	G	254	PHE	2.8
1	J	201	ASP	2.8
1	A	232	GLY	2.8
1	B	247	ASN	2.8
1	H	221	ARG	2.8
1	D	120	GLN	2.8
1	A	243	PRO	2.8
1	D	32	PRO	2.8
1	B	193	SER	2.8
1	I	171	ASP	2.7
1	A	229	VAL	2.7
1	H	120	GLN	2.7
1	L	120	GLN	2.7
1	F	180	PRO	2.7
1	G	245	PRO	2.7
1	M	92	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	213	GLY	2.7
1	F	221	ARG	2.7
1	M	96	ARG	2.7
1	F	53	LYS	2.7
1	I	195	GLN	2.7
1	F	197	GLU	2.7
1	B	233	THR	2.7
1	M	234	GLY	2.7
1	B	205	LYS	2.7
1	L	103	ASP	2.7
1	H	247	ASN	2.7
1	B	217	PRO	2.7
1	I	180	PRO	2.7
1	B	197	GLU	2.7
1	M	235	SER	2.7
1	D	212	ASP	2.7
1	M	97	TYR	2.7
1	M	134	TYR	2.7
1	B	259	LEU	2.7
1	C	99	LEU	2.7
1	F	96	ARG	2.7
1	K	39	ARG	2.7
1	F	63	LYS	2.7
1	M	232	GLY	2.7
1	D	233	THR	2.7
1	M	233	THR	2.7
1	H	259	LEU	2.7
1	A	30	GLU	2.6
1	B	234	GLY	2.6
1	B	235	SER	2.6
1	I	196	LEU	2.6
1	D	109	GLN	2.6
1	F	213	GLY	2.6
1	H	232	GLY	2.6
1	J	197	GLU	2.6
1	A	241	VAL	2.6
1	B	112	ALA	2.6
1	H	228	SER	2.6
1	A	216	TYR	2.6
1	M	111	TYR	2.6
1	A	53	LYS	2.6
1	G	58	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	218	LEU	2.6
1	D	112	ALA	2.6
1	M	254	PHE	2.6
1	M	230	ASP	2.6
1	B	194	GLY	2.6
1	K	233	THR	2.6
1	M	178	THR	2.6
1	B	108	LYS	2.6
1	F	235	SER	2.6
1	G	243	PRO	2.6
1	I	235	SER	2.6
1	A	169	GLN	2.6
1	F	212	ASP	2.6
1	D	99	LEU	2.6
1	D	116	ALA	2.6
1	F	39	ARG	2.6
1	F	102	ALA	2.6
1	M	94	ALA	2.6
1	F	181	SER	2.5
1	F	200	GLY	2.5
1	I	212	ASP	2.5
1	K	180	PRO	2.5
1	A	89	SER	2.5
1	C	228	SER	2.5
1	C	234	GLY	2.5
1	G	214	SER	2.5
1	K	234	GLY	2.5
1	M	104	GLN	2.5
1	L	230	ASP	2.5
1	M	36	ASN	2.5
1	M	102	ALA	2.5
1	D	29	THR	2.5
1	A	63	LYS	2.5
1	I	232	GLY	2.5
1	K	200	GLY	2.5
1	K	181	SER	2.5
1	G	149	ALA	2.5
1	M	231	GLU	2.5
1	D	171	ASP	2.5
1	A	59	GLY	2.5
1	G	204	ALA	2.5
1	I	254	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	221	ARG	2.5
1	C	32	PRO	2.5
1	G	195	GLN	2.5
1	F	114	ALA	2.4
1	K	192	ALA	2.4
1	L	105	ALA	2.4
1	A	96	ARG	2.4
1	F	36	ASN	2.4
1	G	171	ASP	2.4
1	M	239	ARG	2.4
1	L	200	GLY	2.4
1	C	190	GLU	2.4
1	D	197	GLU	2.4
1	F	152	GLU	2.4
1	G	248	GLU	2.4
1	A	196	LEU	2.4
1	B	171	ASP	2.4
1	C	201	ASP	2.4
1	M	171	ASP	2.4
1	L	232	GLY	2.4
1	A	209	LYS	2.4
1	D	242	PHE	2.4
1	M	190	GLU	2.4
1	M	181	SER	2.4
1	A	90	THR	2.4
1	C	246	ASN	2.4
1	H	233	THR	2.4
1	K	246	ASN	2.4
1	K	106	VAL	2.4
1	H	102	ALA	2.4
1	M	84	GLN	2.4
1	A	184	LEU	2.4
1	A	226	GLU	2.4
1	H	77	GLU	2.4
1	E	29	THR	2.4
1	F	234	GLY	2.4
1	H	171	ASP	2.4
1	B	104	GLN	2.4
1	C	81	GLN	2.4
1	H	109	GLN	2.4
1	B	207	SER	2.4
1	F	129	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	254	PHE	2.3
1	F	84	GLN	2.3
1	M	196	LEU	2.3
1	C	211	GLU	2.3
1	M	197	GLU	2.3
1	M	89	SER	2.3
1	A	221	ARG	2.3
1	I	213	GLY	2.3
1	D	93	GLN	2.3
1	H	254	PHE	2.3
1	M	93	GLN	2.3
1	C	227	VAL	2.3
1	F	172	PRO	2.3
1	C	207	SER	2.3
1	F	121	SER	2.3
1	G	247	ASN	2.3
1	K	179	GLN	2.3
1	I	92	GLU	2.3
1	G	220	GLY	2.3
1	I	200	GLY	2.3
1	B	257	ALA	2.3
1	D	117	ALA	2.3
1	G	199	ALA	2.3
1	H	181	SER	2.3
1	H	207	SER	2.3
1	J	233	THR	2.3
1	B	256	HIS	2.3
1	A	176	ASP	2.3
1	B	239	ARG	2.3
1	E	116	ALA	2.3
1	M	41	ALA	2.3
1	F	182	THR	2.3
1	M	135	THR	2.3
1	C	202	ASN	2.3
1	A	188	ARG	2.3
1	A	58	GLU	2.2
1	B	172	PRO	2.2
1	I	172	PRO	2.2
1	H	257	ALA	2.2
1	M	183	ALA	2.2
1	A	191	LEU	2.2
1	G	151	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	39	ARG	2.2
1	A	227	VAL	2.2
1	D	195	GLN	2.2
1	M	258	GLN	2.2
1	K	232	GLY	2.2
1	I	178	THR	2.2
1	J	235	SER	2.2
1	M	120	GLN	2.2
1	K	202	ASN	2.2
1	B	176	ASP	2.2
1	B	201	ASP	2.2
1	I	217	PRO	2.2
1	A	38	PHE	2.2
1	B	228	SER	2.2
1	A	36	ASN	2.2
1	B	30	GLU	2.2
1	F	202	ASN	2.2
1	G	77	GLU	2.2
1	G	185	LEU	2.2
1	H	211	GLU	2.2
1	A	245	PRO	2.2
1	E	232	GLY	2.2
1	C	181	SER	2.2
1	E	179	GLN	2.2
1	D	115	ASN	2.2
1	I	197	GLU	2.2
1	G	59	GLY	2.2
1	E	198	ARG	2.2
1	G	129	ARG	2.2
1	H	198	ARG	2.2
1	F	113	ASP	2.2
1	C	178	THR	2.1
1	A	120	GLN	2.1
1	C	218	LEU	2.1
1	J	179	GLN	2.1
1	L	259	LEU	2.1
1	F	225	SER	2.1
1	B	231	GLU	2.1
1	C	96	ARG	2.1
1	A	256	HIS	2.1
1	G	233	THR	2.1
1	A	99	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	191	LEU	2.1
1	K	195	GLN	2.1
1	B	181	SER	2.1
1	C	197	GLU	2.1
1	D	107	SER	2.1
1	E	197	GLU	2.1
1	G	30	GLU	2.1
1	I	223	GLU	2.1
1	K	32	PRO	2.1
1	A	86	ASN	2.1
1	I	246	ASN	2.1
1	F	256	HIS	2.1
1	G	145	ILE	2.1
1	I	182	THR	2.1
1	L	233	THR	2.1
1	D	97	TYR	2.1
1	C	221	ARG	2.1
1	H	39	ARG	2.1
1	B	110	GLN	2.1
1	F	195	GLN	2.1
1	H	195	GLN	2.1
1	B	200	GLY	2.1
1	M	193	SER	2.1
1	A	171	ASP	2.1
1	G	57	LYS	2.1
1	D	119	LEU	2.1
1	E	103	ASP	2.1
1	H	103	ASP	2.1
1	L	171	ASP	2.1
1	L	196	LEU	2.1
1	A	135	THR	2.1
1	B	189	ARG	2.1
1	D	90	THR	2.1
1	G	189	ARG	2.1
1	E	105	ALA	2.1
1	F	85	ALA	2.1
1	L	195	GLN	2.1
1	E	223	GLU	2.1
1	L	77	GLU	2.1
1	L	197	GLU	2.1
1	F	142	SER	2.1
1	G	225	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	202	ASN	2.1
1	H	196	LEU	2.1
1	K	204	ALA	2.1
1	A	195	GLN	2.1
1	A	258	GLN	2.1
1	C	84	GLN	2.1
1	F	104	GLN	2.1
1	G	232	GLY	2.1
1	C	77	GLU	2.1
1	D	30	GLU	2.1
1	G	125	VAL	2.0
1	H	53	LYS	2.0
1	I	209	LYS	2.0
1	M	229	VAL	2.0
1	G	86	ASN	2.0
1	A	178	THR	2.0
1	E	233	THR	2.0
1	L	112	ALA	2.0
1	B	258	GLN	2.0
1	C	93	GLN	2.0
1	C	232	GLY	2.0
1	H	215	GLN	2.0
1	B	180	PRO	2.0
1	C	172	PRO	2.0
1	K	30	GLU	2.0
1	A	186	ARG	2.0
1	J	207	SER	2.0
1	G	253	MET	2.0
1	D	83	ALA	2.0
1	D	182	THR	2.0
1	G	83	ALA	2.0
1	G	113	ASP	2.0
1	D	194	GLY	2.0
1	D	254	PHE	2.0
1	K	213	GLY	2.0
1	K	254	PHE	2.0
1	G	95	GLN	2.0
1	L	95	GLN	2.0
1	M	98	LYS	2.0
1	C	248	GLU	2.0
1	G	222	LEU	2.0
1	M	87	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	361	6/6	0.42	0.40	97,98,99,102	0
3	3GR	F	361	6/6	0.48	0.41	99,100,101,103	0
2	GOL	B	361	6/6	0.53	0.45	95,96,96,96	0
3	3GR	E	361	6/6	0.58	0.51	93,95,98,102	0
3	3GR	G	361	6/6	0.59	0.41	103,104,105,106	0
3	3GR	H	361	6/6	0.60	0.41	87,88,89,90	0
2	GOL	M	361	6/6	0.67	0.33	99,100,101,101	0
3	3GR	D	361	6/6	0.67	0.52	93,93,94,95	0
3	3GR	C	361	6/6	0.68	0.46	100,100,101,102	0
3	3GR	K	361	6/6	0.71	0.43	79,80,83,84	0
3	3GR	I	361	6/6	0.76	0.35	87,87,88,88	0
2	GOL	J	361	6/6	0.76	0.39	92,94,94,96	0
3	3GR	L	361	6/6	0.77	0.36	81,82,83,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.