



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:40 AM EDT

PDB ID : 2GFP / pdb_00002gfp
Title : Structure of the Multidrug Transporter EmrD from Escherichia coli
Authors : Yin, Y.; He, X.; Szewczyk, P.; Nguyen, T.; Chang, G.
Deposited on : 2006-03-22
Resolution : 3.50 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
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

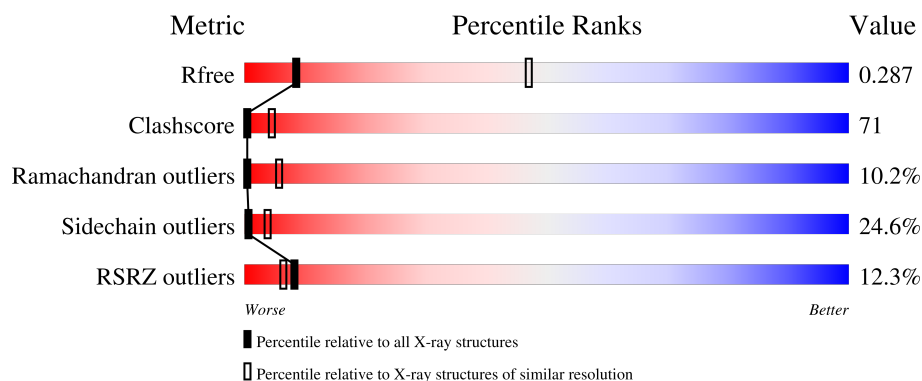
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	375	11% 22% 47% 25% 6%
1	B	375	14% 22% 48% 24% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5600 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.

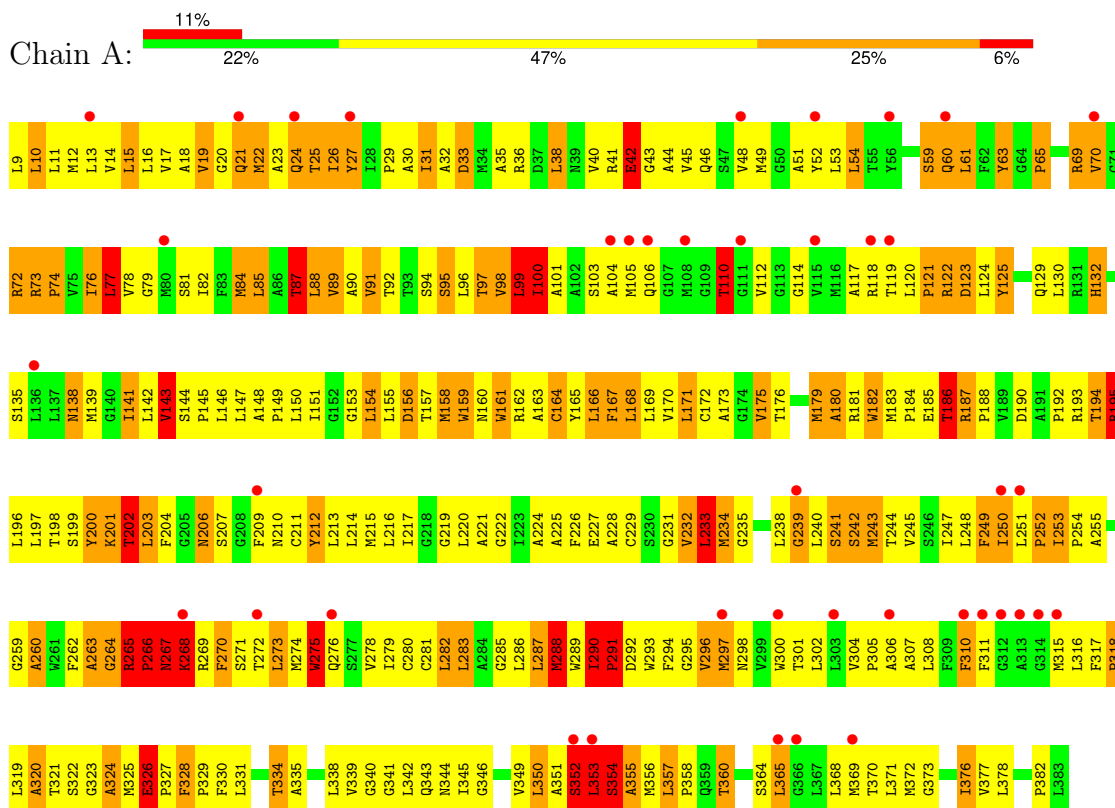
- Molecule 1 is a protein called Multidrug resistance protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2800	1842	455	472	31			
1	B	375	Total	C	N	O	S	0	0	0
			2800	1842	455	472	31			

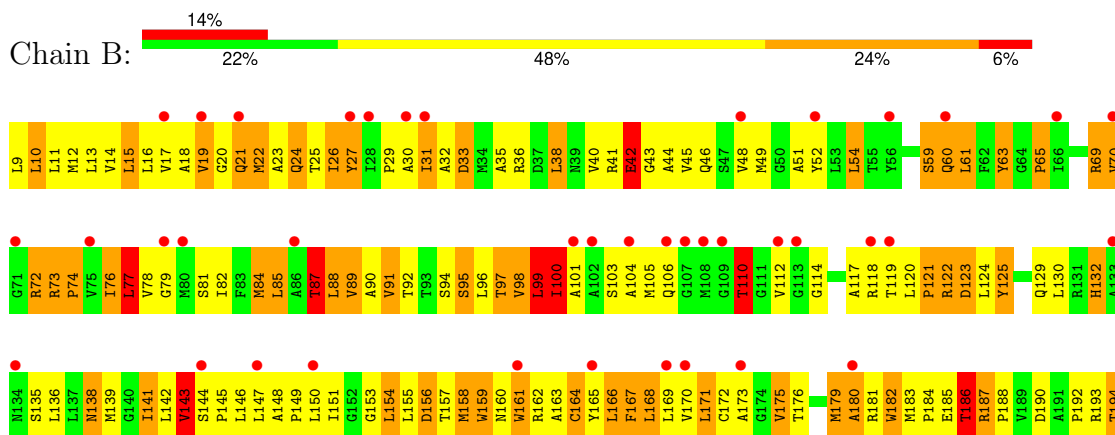
3 Residue-property plots

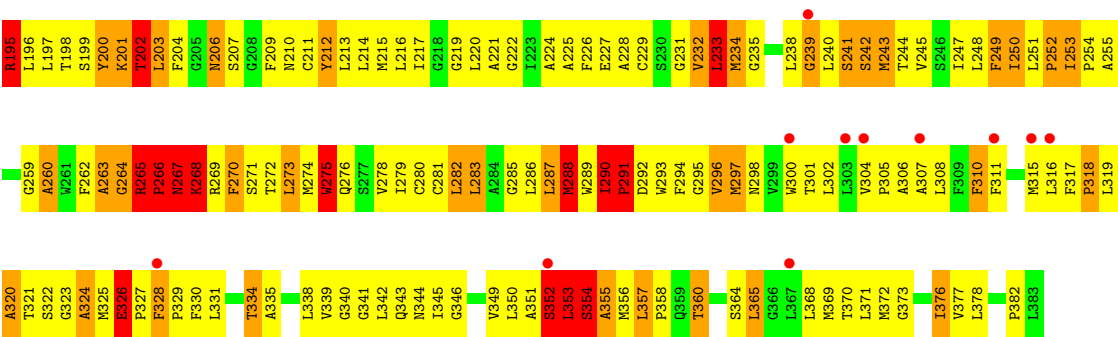
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Multidrug resistance protein D



• Molecule 1: Multidrug resistance protein D





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.50Å 124.50Å 109.40Å 90.00° 110.20° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.50) 61.7 (50.00-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.270 , 0.350 0.229 , 0.287	Depositor DCC
R_{free} test set	1321 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5600	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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

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	0.51	0/2864	1.35	57/3900 (1.5%)
1	B	0.51	0/2864	1.35	57/3900 (1.5%)
All	All	0.51	0/5728	1.35	114/7800 (1.5%)

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	1	2
1	B	1	2
All	All	2	4

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	353	LEU	CA-C-N	13.94	142.81	122.74
1	B	353	LEU	C-N-CA	13.94	142.81	122.74
1	A	353	LEU	CA-C-N	13.86	142.70	122.74
1	A	353	LEU	C-N-CA	13.86	142.70	122.74
1	B	354	SER	N-CA-C	12.33	127.63	112.58
1	A	354	SER	N-CA-C	12.32	127.62	112.58
1	A	100	ILE	N-CA-C	-11.39	96.85	111.09
1	B	100	ILE	N-CA-C	-11.35	96.90	111.09
1	B	195	ARG	N-CA-C	9.97	121.83	108.38
1	A	195	ARG	N-CA-C	9.96	121.83	108.38
1	A	241	SER	N-CA-C	-9.60	99.88	111.69
1	B	241	SER	N-CA-C	-9.60	99.88	111.69
1	B	320	ALA	N-CA-C	-9.57	99.96	112.68
1	A	320	ALA	N-CA-C	-9.52	100.02	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	LEU	N-CA-C	-8.89	102.56	113.50
1	A	99	LEU	N-CA-C	-8.89	102.57	113.50
1	A	352	SER	N-CA-C	8.32	128.53	110.80
1	B	352	SER	N-CA-C	8.29	128.47	110.80
1	A	285	GLY	N-CA-C	8.10	117.58	110.21
1	B	285	GLY	N-CA-C	8.03	117.51	110.21
1	B	321	THR	N-CA-C	-8.02	101.62	111.40
1	A	321	THR	N-CA-C	-7.98	101.66	111.40
1	B	233	LEU	N-CA-C	7.64	127.07	110.80
1	A	233	LEU	N-CA-C	7.61	127.01	110.80
1	B	265	ARG	CA-C-N	7.41	129.10	119.84
1	B	265	ARG	C-N-CA	7.41	129.10	119.84
1	A	265	ARG	CA-C-N	7.37	129.06	119.84
1	A	265	ARG	C-N-CA	7.37	129.06	119.84
1	B	239	GLY	N-CA-C	-7.09	104.22	112.73
1	A	239	GLY	N-CA-C	-7.07	104.24	112.73
1	B	378	LEU	N-CA-C	6.91	118.89	111.36
1	A	378	LEU	N-CA-C	6.89	118.88	111.36
1	B	253	ILE	CA-C-N	-6.85	111.93	119.19
1	B	253	ILE	C-N-CA	-6.85	111.93	119.19
1	A	171	LEU	N-CA-C	-6.84	103.75	111.14
1	B	171	LEU	N-CA-C	-6.84	103.76	111.14
1	A	253	ILE	CA-C-N	-6.82	111.96	119.19
1	A	253	ILE	C-N-CA	-6.82	111.96	119.19
1	A	318	PRO	N-CA-C	-6.78	105.23	113.98
1	A	43	GLY	N-CA-C	-6.73	104.15	112.77
1	B	324	ALA	N-CA-C	-6.71	103.06	111.11
1	A	324	ALA	N-CA-C	-6.70	103.07	111.11
1	B	43	GLY	N-CA-C	-6.69	104.21	112.77
1	B	318	PRO	N-CA-C	-6.59	105.27	113.84
1	A	232	VAL	N-CA-C	-6.58	95.65	109.34
1	B	232	VAL	N-CA-C	-6.56	95.69	109.34
1	B	186	THR	N-CA-C	6.56	124.77	110.80
1	A	186	THR	N-CA-C	6.56	124.76	110.80
1	B	263	ALA	N-CA-C	-6.54	103.42	111.33
1	A	263	ALA	N-CA-C	-6.51	103.45	111.33
1	A	355	ALA	N-CA-C	6.48	124.60	110.80
1	B	355	ALA	N-CA-C	6.47	124.58	110.80
1	A	353	LEU	O-C-N	6.42	131.13	122.59
1	B	353	LEU	O-C-N	6.39	131.09	122.59
1	A	77	LEU	N-CA-C	6.37	118.02	111.14
1	B	77	LEU	N-CA-C	6.34	117.99	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	SER	N-CA-C	-6.34	100.98	111.37
1	A	315	MET	N-CA-C	6.33	120.10	112.38
1	B	315	MET	N-CA-C	6.31	120.08	112.38
1	A	95	SER	N-CA-C	-6.29	101.05	111.37
1	A	264	GLY	N-CA-C	-6.22	98.43	113.18
1	B	264	GLY	N-CA-C	-6.22	98.43	113.18
1	A	202	THR	N-CA-C	-6.22	104.80	112.38
1	B	88	LEU	N-CA-C	6.16	118.78	111.33
1	B	202	THR	N-CA-C	-6.15	104.87	112.38
1	A	88	LEU	N-CA-C	6.13	118.74	111.33
1	B	249	PHE	N-CA-C	-6.11	104.62	111.28
1	A	249	PHE	N-CA-C	-6.08	104.66	111.28
1	B	260	ALA	N-CA-C	-6.07	104.59	111.14
1	A	260	ALA	N-CA-C	-6.06	104.59	111.14
1	B	270	PHE	N-CA-C	-6.04	104.02	111.33
1	A	270	PHE	N-CA-C	-6.00	104.07	111.33
1	B	221	ALA	N-CA-C	-5.93	104.90	111.36
1	B	198	THR	N-CA-C	-5.92	104.77	112.23
1	A	198	THR	N-CA-C	-5.92	104.78	112.23
1	A	221	ALA	N-CA-C	-5.89	104.93	111.36
1	A	183	MET	CA-C-N	5.58	126.81	119.84
1	A	183	MET	C-N-CA	5.58	126.81	119.84
1	B	183	MET	CA-C-N	5.54	126.76	119.84
1	B	183	MET	C-N-CA	5.54	126.76	119.84
1	B	31	ILE	N-CA-C	-5.50	104.97	110.30
1	A	110	THR	N-CA-C	-5.49	105.40	111.71
1	B	110	THR	N-CA-C	-5.47	105.42	111.71
1	A	31	ILE	N-CA-C	-5.47	105.00	110.30
1	A	242	SER	N-CA-C	-5.46	105.23	111.07
1	A	233	LEU	CB-CA-C	5.43	121.22	110.42
1	B	242	SER	N-CA-C	-5.41	105.28	111.07
1	A	123	ASP	N-CA-C	-5.40	105.39	111.28
1	B	123	ASP	N-CA-C	-5.40	105.39	111.28
1	B	233	LEU	CB-CA-C	5.40	121.17	110.42
1	B	85	LEU	N-CA-C	-5.39	105.48	111.36
1	A	85	LEU	N-CA-C	-5.39	105.49	111.36
1	A	54	LEU	N-CA-C	-5.35	105.35	111.07
1	B	54	LEU	N-CA-C	-5.33	105.37	111.07
1	B	288	MET	N-CA-C	5.29	122.06	110.80
1	A	288	MET	N-CA-C	5.28	122.04	110.80
1	B	326	GLU	CA-C-N	-5.21	113.56	118.97
1	B	326	GLU	C-N-CA	-5.21	113.56	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ILE	N-CA-C	5.21	120.12	108.88
1	A	290	ILE	N-CA-C	5.20	120.10	108.88
1	A	275	TRP	N-CA-C	5.18	116.62	110.97
1	B	275	TRP	N-CA-C	5.17	116.60	110.97
1	A	42	GLU	N-CA-C	5.16	121.80	110.80
1	B	42	GLU	N-CA-C	5.15	121.76	110.80
1	B	357	LEU	CA-C-N	-5.12	113.65	119.28
1	B	357	LEU	C-N-CA	-5.12	113.65	119.28
1	A	357	LEU	CA-C-N	-5.11	113.66	119.28
1	A	357	LEU	C-N-CA	-5.11	113.66	119.28
1	A	326	GLU	CA-C-N	-5.10	113.67	118.97
1	A	326	GLU	C-N-CA	-5.10	113.67	118.97
1	A	63	TYR	N-CA-C	-5.09	106.33	112.54
1	B	63	TYR	N-CA-C	-5.07	106.35	112.54
1	A	316	LEU	N-CA-C	5.04	119.43	113.28
1	B	316	LEU	N-CA-C	5.02	119.41	113.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	LEU	CA
1	B	233	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	LEU	Mainchain
1	A	354	SER	Mainchain
1	B	353	LEU	Mainchain
1	B	354	SER	Mainchain

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	2800	0	2932	415	0
1	B	2800	0	2932	416	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5600	0	5864	817	0

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 71.

All (817) 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:A:200:TYR:HE1	1:B:204:PHE:CE1	1.38	1.40
1:A:200:TYR:CE1	1:B:204:PHE:CE1	2.29	1.21
1:A:263:ALA:HA	1:A:268:LYS:HB2	1.15	1.10
1:B:20:GLY:HA2	1:B:110:THR:HB	1.32	1.09
1:A:20:GLY:HA2	1:A:110:THR:HB	1.32	1.08
1:B:263:ALA:HA	1:B:268:LYS:HB2	1.15	1.07
1:A:204:PHE:CE1	1:B:200:TYR:HE1	1.73	1.06
1:B:273:LEU:HG	1:B:370:THR:HA	1.40	1.02
1:A:273:LEU:HG	1:A:370:THR:HA	1.39	1.01
1:B:248:LEU:O	1:B:252:PRO:HD2	1.65	0.97
1:A:248:LEU:O	1:A:252:PRO:HD2	1.65	0.95
1:B:91:VAL:HG12	1:B:99:LEU:HD12	1.50	0.92
1:B:73:ARG:HG3	1:B:74:PRO:HD3	1.52	0.91
1:A:91:VAL:HG12	1:A:99:LEU:HD12	1.50	0.90
1:B:117:ALA:O	1:B:121:PRO:HD2	1.72	0.90
1:A:73:ARG:HG3	1:A:74:PRO:HD3	1.52	0.89
1:B:301:THR:O	1:B:305:PRO:HD2	1.73	0.89
1:A:204:PHE:CE1	1:B:200:TYR:CE1	2.61	0.89
1:A:117:ALA:O	1:A:121:PRO:HD2	1.72	0.89
1:A:357:LEU:HB2	1:A:358:PRO:HD3	1.56	0.88
1:A:279:ILE:HD12	1:A:295:GLY:HA2	1.56	0.88
1:A:301:THR:O	1:A:305:PRO:HD2	1.73	0.87
1:A:141:ILE:O	1:A:145:PRO:HD2	1.75	0.87
1:B:262:PHE:HA	1:B:265:ARG:HB2	1.54	0.87
1:B:357:LEU:HB2	1:B:358:PRO:HD3	1.56	0.87
1:B:141:ILE:O	1:B:145:PRO:HD2	1.75	0.87
1:A:25:THR:O	1:A:29:PRO:HD2	1.75	0.87
1:A:262:PHE:HA	1:A:265:ARG:HB2	1.54	0.87
1:B:25:THR:O	1:B:29:PRO:HD2	1.75	0.86
1:A:84:MET:O	1:A:87:THR:HB	1.75	0.86
1:B:279:ILE:HD12	1:B:295:GLY:HA2	1.56	0.86
1:A:200:TYR:HE1	1:B:204:PHE:CD1	1.94	0.86
1:A:148:ALA:HB3	1:A:149:PRO:HD3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ILE:HG13	1:B:48:VAL:HG11	1.58	0.85
1:B:32:ALA:HB1	1:B:233:LEU:HB3	1.58	0.85
1:A:32:ALA:HB1	1:A:233:LEU:HB3	1.58	0.85
1:B:148:ALA:HB3	1:B:149:PRO:HD3	1.59	0.84
1:B:84:MET:O	1:B:87:THR:HB	1.75	0.84
1:B:319:LEU:HA	1:B:322:SER:HB2	1.60	0.84
1:B:84:MET:HG3	1:B:162:ARG:HH12	1.43	0.84
1:A:319:LEU:HA	1:A:322:SER:HB2	1.60	0.84
1:A:84:MET:HG3	1:A:162:ARG:HH12	1.43	0.83
1:A:201:LYS:HE3	1:B:200:TYR:OH	1.78	0.83
1:B:263:ALA:HA	1:B:268:LYS:CB	2.06	0.83
1:B:157:THR:HB	1:B:160:ASN:HB2	1.61	0.82
1:A:31:ILE:HG13	1:A:48:VAL:HG11	1.58	0.82
1:B:290:ILE:HG13	1:B:291:PRO:HD3	1.60	0.82
1:A:290:ILE:HG13	1:A:291:PRO:HD3	1.59	0.82
1:A:157:THR:HB	1:A:160:ASN:HB2	1.60	0.82
1:A:42:GLU:OE1	1:A:45:VAL:HB	1.80	0.81
1:B:328:PHE:HB2	1:B:329:PRO:HD3	1.62	0.81
1:B:42:GLU:OE1	1:B:45:VAL:HB	1.80	0.81
1:B:272:THR:HG22	1:B:302:LEU:HD22	1.62	0.81
1:A:272:THR:HG22	1:A:302:LEU:HD22	1.62	0.81
1:A:32:ALA:HA	1:A:233:LEU:HD13	1.64	0.80
1:A:200:TYR:CE1	1:B:204:PHE:CD1	2.68	0.80
1:A:328:PHE:HB2	1:A:329:PRO:HD3	1.62	0.80
1:B:32:ALA:HA	1:B:233:LEU:HD13	1.64	0.80
1:B:95:SER:O	1:B:100:ILE:HG23	1.82	0.80
1:A:88:LEU:HA	1:A:91:VAL:HG22	1.64	0.79
1:A:95:SER:O	1:A:100:ILE:HG23	1.82	0.79
1:A:262:PHE:CE1	1:A:271:SER:HB2	2.18	0.79
1:A:250:ILE:O	1:A:254:PRO:HD2	1.83	0.78
1:A:326:GLU:HG3	1:A:327:PRO:HD2	1.65	0.78
1:B:262:PHE:CE1	1:B:271:SER:HB2	2.18	0.78
1:A:203:LEU:O	1:A:207:SER:HB2	1.84	0.78
1:B:250:ILE:O	1:B:254:PRO:HD2	1.83	0.78
1:A:22:MET:HG2	1:A:164:CYS:SG	2.24	0.78
1:A:31:ILE:HD11	1:A:104:ALA:HB2	1.65	0.78
1:B:31:ILE:HD11	1:B:104:ALA:HB2	1.65	0.78
1:B:207:SER:HA	1:B:210:ASN:HB3	1.65	0.78
1:B:88:LEU:HA	1:B:91:VAL:HG22	1.63	0.77
1:B:203:LEU:O	1:B:207:SER:HB2	1.83	0.77
1:B:326:GLU:HG3	1:B:327:PRO:HD2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:MET:HG2	1:B:164:CYS:SG	2.24	0.76
1:B:19:VAL:HG23	1:B:165:TYR:HA	1.68	0.76
1:A:216:LEU:HD23	1:A:369:MET:HE3	1.67	0.76
1:A:19:VAL:HG23	1:A:165:TYR:HA	1.68	0.76
1:A:207:SER:HA	1:A:210:ASN:HB3	1.65	0.75
1:A:32:ALA:C	1:A:233:LEU:HB3	2.12	0.75
1:A:352:SER:O	1:A:353:LEU:HD12	1.86	0.75
1:B:216:LEU:HD23	1:B:369:MET:HE3	1.67	0.75
1:A:46:GLN:HG3	1:A:225:ALA:HB1	1.69	0.75
1:A:263:ALA:HA	1:A:268:LYS:CB	2.06	0.75
1:B:352:SER:O	1:B:353:LEU:HD12	1.86	0.75
1:B:46:GLN:HG3	1:B:225:ALA:HB1	1.69	0.75
1:B:32:ALA:C	1:B:233:LEU:HB3	2.12	0.74
1:A:269:ARG:HH11	1:A:372:MET:HB3	1.52	0.74
1:B:269:ARG:HH11	1:B:372:MET:HB3	1.52	0.74
1:A:16:LEU:HB2	1:A:172:CYS:SG	2.28	0.73
1:B:21:GLN:HB2	1:B:143:VAL:HG13	1.70	0.73
1:B:97:THR:O	1:B:99:LEU:N	2.22	0.73
1:A:97:THR:O	1:A:99:LEU:N	2.22	0.73
1:B:16:LEU:HB2	1:B:172:CYS:SG	2.28	0.73
1:A:202:THR:HG22	1:A:206:ASN:HB3	1.70	0.73
1:B:145:PRO:O	1:B:149:PRO:HD2	1.89	0.73
1:B:217:ILE:HD11	1:B:331:LEU:O	1.89	0.73
1:B:267:ASN:O	1:B:269:ARG:N	2.22	0.73
1:A:32:ALA:HB1	1:A:233:LEU:CB	2.19	0.72
1:A:145:PRO:O	1:A:149:PRO:HD2	1.89	0.72
1:A:267:ASN:O	1:A:269:ARG:N	2.22	0.72
1:B:32:ALA:HB1	1:B:233:LEU:CB	2.19	0.72
1:A:326:GLU:O	1:A:330:PHE:HB2	1.89	0.72
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.71	0.72
1:A:323:GLY:O	1:A:327:PRO:HD2	1.89	0.72
1:B:202:THR:HG22	1:B:206:ASN:HB3	1.70	0.72
1:A:21:GLN:HB2	1:A:143:VAL:HG13	1.69	0.71
1:A:94:SER:O	1:A:99:LEU:HB2	1.89	0.71
1:A:217:ILE:HD11	1:A:331:LEU:O	1.89	0.71
1:B:326:GLU:O	1:B:330:PHE:HB2	1.89	0.71
1:A:240:LEU:HA	1:A:243:MET:HB3	1.72	0.71
1:B:94:SER:O	1:B:99:LEU:HB2	1.89	0.71
1:B:72:ARG:O	1:B:76:ILE:HB	1.91	0.71
1:B:323:GLY:O	1:B:327:PRO:HD2	1.89	0.71
1:A:72:ARG:O	1:A:76:ILE:HB	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HG21	1:A:161:TRP:HE1	1.56	0.70
1:B:59:SER:O	1:B:63:TYR:HB3	1.92	0.70
1:B:265:ARG:HG2	1:B:266:PRO:HD2	1.73	0.70
1:B:196:LEU:HA	1:B:199:SER:HB2	1.73	0.70
1:A:196:LEU:HA	1:A:199:SER:HB2	1.74	0.70
1:B:251:LEU:HB3	1:B:252:PRO:HD3	1.71	0.70
1:B:294:PHE:HD2	1:B:297:MET:SD	2.15	0.70
1:A:200:TYR:OH	1:B:201:LYS:HE3	1.91	0.70
1:A:59:SER:O	1:A:63:TYR:HB3	1.91	0.70
1:A:212:TYR:HB2	1:A:269:ARG:NH2	2.07	0.70
1:A:288:MET:O	1:A:291:PRO:HD2	1.93	0.69
1:A:294:PHE:HD2	1:A:297:MET:SD	2.15	0.69
1:B:212:TYR:HB2	1:B:269:ARG:NH2	2.07	0.69
1:A:159:TRP:HA	1:A:162:ARG:CG	2.22	0.69
1:B:35:ALA:HA	1:B:38:LEU:HG	1.73	0.69
1:B:159:TRP:HA	1:B:162:ARG:CG	2.22	0.69
1:B:240:LEU:HA	1:B:243:MET:HB3	1.73	0.69
1:B:288:MET:O	1:B:291:PRO:HD2	1.92	0.69
1:B:87:THR:HG21	1:B:161:TRP:HE1	1.56	0.69
1:A:91:VAL:O	1:A:95:SER:HB2	1.93	0.69
1:A:262:PHE:HE1	1:A:271:SER:HB2	1.56	0.68
1:A:327:PRO:O	1:A:331:LEU:HB2	1.92	0.68
1:B:69:ARG:HG2	1:B:186:THR:H	1.57	0.68
1:B:262:PHE:HE1	1:B:271:SER:HB2	1.56	0.68
1:B:327:PRO:O	1:B:331:LEU:HB2	1.92	0.68
1:A:69:ARG:HG2	1:A:186:THR:H	1.57	0.68
1:A:265:ARG:HG2	1:A:266:PRO:HD2	1.73	0.68
1:A:35:ALA:HA	1:A:38:LEU:HG	1.73	0.68
1:B:32:ALA:CB	1:B:233:LEU:HB3	2.24	0.68
1:B:91:VAL:O	1:B:95:SER:HB2	1.94	0.67
1:B:368:LEU:HG	1:B:372:MET:HE2	1.76	0.67
1:B:327:PRO:HA	1:B:331:LEU:HD13	1.75	0.67
1:A:36:ARG:HD2	1:A:233:LEU:HB2	1.75	0.67
1:B:267:ASN:C	1:B:269:ARG:H	2.02	0.67
1:A:294:PHE:CD2	1:A:297:MET:SD	2.88	0.67
1:A:25:THR:HB	1:A:242:SER:OG	1.95	0.67
1:A:234:MET:O	1:A:238:LEU:HB2	1.95	0.67
1:A:267:ASN:C	1:A:269:ARG:H	2.02	0.67
1:A:148:ALA:HB2	1:A:243:MET:HB2	1.77	0.67
1:A:195:ARG:HG3	1:A:197:LEU:H	1.59	0.67
1:B:252:PRO:HB3	1:B:301:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PRO:HA	1:A:331:LEU:HD13	1.75	0.67
1:B:98:VAL:O	1:B:101:ALA:HB3	1.94	0.67
1:A:245:VAL:HG22	1:A:249:PHE:CE2	2.30	0.67
1:B:148:ALA:HB2	1:B:243:MET:HB2	1.77	0.67
1:A:32:ALA:CB	1:A:233:LEU:HB3	2.24	0.67
1:B:275:TRP:HA	1:B:275:TRP:CE3	2.29	0.67
1:B:294:PHE:CD2	1:B:297:MET:SD	2.88	0.67
1:A:275:TRP:CE3	1:A:275:TRP:HA	2.29	0.67
1:B:227:GLU:HB2	1:B:296:VAL:HG22	1.77	0.67
1:A:227:GLU:HB2	1:A:296:VAL:HG22	1.78	0.66
1:B:19:VAL:HG22	1:B:110:THR:HG21	1.77	0.66
1:B:195:ARG:HG3	1:B:197:LEU:H	1.59	0.66
1:A:356:MET:O	1:A:360:THR:HB	1.96	0.66
1:B:36:ARG:HD2	1:B:233:LEU:HB2	1.75	0.66
1:A:252:PRO:HB3	1:A:301:THR:HG23	1.75	0.66
1:A:98:VAL:O	1:A:101:ALA:HB3	1.95	0.66
1:B:234:MET:O	1:B:238:LEU:HB2	1.95	0.66
1:B:143:VAL:O	1:B:147:LEU:HD23	1.96	0.66
1:B:245:VAL:HG22	1:B:249:PHE:CE2	2.30	0.66
1:B:273:LEU:CG	1:B:370:THR:HA	2.23	0.66
1:A:368:LEU:HG	1:A:372:MET:HE2	1.76	0.66
1:B:32:ALA:HB1	1:B:233:LEU:HD22	1.76	0.66
1:B:209:PHE:O	1:B:212:TYR:HB3	1.96	0.66
1:A:32:ALA:HB1	1:A:233:LEU:HD22	1.76	0.65
1:A:345:ILE:O	1:A:349:VAL:HB	1.97	0.65
1:A:65:PRO:HB3	1:A:190:ASP:HB3	1.78	0.65
1:B:77:LEU:HB2	1:B:169:LEU:HD21	1.79	0.65
1:A:87:THR:O	1:A:91:VAL:HG13	1.97	0.65
1:A:201:LYS:CE	1:B:200:TYR:OH	2.44	0.65
1:B:49:MET:SD	1:B:228:ALA:HB3	2.37	0.65
1:B:307:ALA:O	1:B:311:PHE:HB2	1.97	0.65
1:B:356:MET:O	1:B:360:THR:HB	1.95	0.65
1:A:209:PHE:O	1:A:212:TYR:HB3	1.96	0.65
1:A:211:CYS:SG	1:A:372:MET:SD	2.93	0.65
1:A:212:TYR:HB2	1:A:269:ARG:CZ	2.27	0.65
1:B:212:TYR:HB2	1:B:269:ARG:CZ	2.27	0.65
1:A:19:VAL:HG22	1:A:110:THR:HG21	1.77	0.64
1:B:345:ILE:O	1:B:349:VAL:HB	1.97	0.64
1:A:84:MET:HE2	1:A:162:ARG:NH1	2.11	0.64
1:A:307:ALA:O	1:A:311:PHE:HB2	1.97	0.64
1:A:49:MET:SD	1:A:228:ALA:HB3	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:O	1:A:147:LEU:HD23	1.96	0.64
1:B:65:PRO:HB3	1:B:190:ASP:HB3	1.78	0.64
1:B:216:LEU:O	1:B:220:LEU:HB2	1.97	0.64
1:A:77:LEU:HB2	1:A:169:LEU:HD21	1.79	0.64
1:B:87:THR:O	1:B:91:VAL:HG13	1.97	0.64
1:A:216:LEU:O	1:A:220:LEU:HB2	1.97	0.64
1:B:84:MET:HE2	1:B:162:ARG:NH1	2.11	0.64
1:B:25:THR:HB	1:B:242:SER:OG	1.98	0.64
1:A:269:ARG:NE	1:A:376:ILE:HG21	2.13	0.64
1:B:269:ARG:NE	1:B:376:ILE:HG21	2.13	0.63
1:B:286:LEU:HD22	1:B:287:LEU:HD22	1.79	0.63
1:A:46:GLN:CG	1:A:225:ALA:HB1	2.28	0.63
1:A:286:LEU:HD22	1:A:287:LEU:HD22	1.79	0.63
1:B:46:GLN:CG	1:B:225:ALA:HB1	2.28	0.63
1:B:243:MET:SD	1:B:244:THR:N	2.72	0.63
1:B:211:CYS:SG	1:B:372:MET:SD	2.93	0.62
1:A:243:MET:SD	1:A:244:THR:N	2.72	0.62
1:B:267:ASN:C	1:B:269:ARG:N	2.57	0.62
1:A:192:PRO:O	1:A:193:ARG:HG3	2.00	0.62
1:B:192:PRO:O	1:B:193:ARG:HG3	2.00	0.62
1:B:213:LEU:HD21	1:B:306:ALA:HB1	1.81	0.62
1:A:268:LYS:HZ2	1:A:306:ALA:N	1.97	0.62
1:B:269:ARG:NH2	1:B:376:ILE:HG13	2.14	0.62
1:A:267:ASN:C	1:A:269:ARG:N	2.57	0.62
1:B:185:GLU:O	1:B:186:THR:HG22	2.00	0.62
1:B:268:LYS:HZ2	1:B:306:ALA:N	1.97	0.62
1:A:12:MET:HB3	1:A:176:THR:HG22	1.82	0.61
1:A:32:ALA:O	1:A:36:ARG:HB2	1.99	0.61
1:A:269:ARG:NH2	1:A:376:ILE:HG13	2.14	0.61
1:B:32:ALA:O	1:B:36:ARG:HB2	1.99	0.61
1:B:139:MET:O	1:B:143:VAL:HG23	2.01	0.61
1:B:269:ARG:HB3	1:B:373:GLY:HA2	1.81	0.61
1:A:38:LEU:HD23	1:A:100:ILE:HG21	1.82	0.61
1:A:81:SER:O	1:A:84:MET:HG2	2.00	0.61
1:A:213:LEU:HD21	1:A:306:ALA:HB1	1.81	0.61
1:A:269:ARG:HB3	1:A:373:GLY:HA2	1.81	0.61
1:A:139:MET:O	1:A:143:VAL:HG23	2.01	0.61
1:B:212:TYR:OH	1:B:268:LYS:HE2	2.01	0.61
1:B:342:LEU:O	1:B:345:ILE:HG22	2.01	0.61
1:B:12:MET:HB3	1:B:176:THR:HG22	1.82	0.61
1:B:38:LEU:HD23	1:B:100:ILE:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:SER:O	1:B:84:MET:HG2	2.01	0.61
1:A:73:ARG:HA	1:A:77:LEU:CD1	2.31	0.61
1:A:300:TRP:CH2	1:A:304:VAL:HG21	2.36	0.61
1:A:342:LEU:O	1:A:345:ILE:HG22	2.01	0.61
1:B:73:ARG:HA	1:B:77:LEU:CD1	2.31	0.61
1:B:300:TRP:CH2	1:B:304:VAL:HG21	2.36	0.60
1:A:159:TRP:HA	1:A:162:ARG:HG3	1.83	0.60
1:B:373:GLY:O	1:B:377:VAL:HG23	2.02	0.60
1:A:212:TYR:OH	1:A:268:LYS:HE2	2.01	0.60
1:A:185:GLU:O	1:A:186:THR:HG22	2.00	0.60
1:A:273:LEU:CG	1:A:370:THR:HA	2.23	0.60
1:B:73:ARG:O	1:B:77:LEU:HD22	2.01	0.60
1:A:357:LEU:O	1:A:360:THR:HG22	2.01	0.60
1:A:373:GLY:O	1:A:377:VAL:HG23	2.02	0.60
1:B:159:TRP:HA	1:B:162:ARG:HG3	1.82	0.60
1:B:357:LEU:O	1:B:360:THR:HG22	2.01	0.60
1:A:11:LEU:O	1:A:14:VAL:HG22	2.01	0.60
1:B:262:PHE:HZ	1:B:270:PHE:HD2	1.50	0.60
1:A:17:VAL:HB	1:A:139:MET:HG2	1.84	0.60
1:B:324:ALA:O	1:B:329:PRO:HD2	2.02	0.60
1:A:282:LEU:HB3	1:A:291:PRO:HA	1.83	0.60
1:B:17:VAL:HB	1:B:139:MET:HG2	1.84	0.60
1:B:17:VAL:HG21	1:B:138:ASN:HD21	1.67	0.60
1:B:11:LEU:O	1:B:14:VAL:HG22	2.01	0.59
1:A:231:GLY:HA3	1:A:238:LEU:HD21	1.83	0.59
1:A:262:PHE:HZ	1:A:270:PHE:HD2	1.50	0.59
1:A:280:CYS:O	1:A:283:LEU:HB3	2.03	0.59
1:B:24:GLN:HA	1:B:27:TYR:CE2	2.37	0.59
1:B:298:ASN:HD21	1:B:302:LEU:HD21	1.67	0.59
1:A:24:GLN:HA	1:A:27:TYR:CE2	2.37	0.59
1:A:163:ALA:O	1:A:167:PHE:HB3	2.03	0.59
1:A:200:TYR:HE1	1:B:204:PHE:CZ	2.12	0.59
1:A:298:ASN:HD21	1:A:302:LEU:HD21	1.67	0.59
1:A:324:ALA:O	1:A:329:PRO:HD2	2.02	0.59
1:B:231:GLY:HA3	1:B:238:LEU:HD21	1.84	0.59
1:A:73:ARG:O	1:A:77:LEU:HD22	2.01	0.59
1:B:49:MET:SD	1:B:225:ALA:HA	2.43	0.59
1:B:280:CYS:O	1:B:283:LEU:HB3	2.03	0.59
1:B:282:LEU:HB3	1:B:291:PRO:HA	1.83	0.59
1:A:186:THR:O	1:A:190:ASP:HB2	2.02	0.58
1:A:276:GLN:NE2	1:A:365:LEU:HD13	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:NH1	1:B:372:MET:HB3	2.17	0.58
1:B:186:THR:O	1:B:190:ASP:HB2	2.02	0.58
1:A:94:SER:C	1:A:99:LEU:HB2	2.29	0.58
1:B:94:SER:C	1:B:99:LEU:HB2	2.29	0.58
1:A:17:VAL:HG21	1:A:138:ASN:HD21	1.67	0.58
1:A:32:ALA:CB	1:A:233:LEU:HD22	2.33	0.58
1:A:40:VAL:HG23	1:A:44:ALA:HB2	1.86	0.58
1:A:204:PHE:CD1	1:B:200:TYR:HE1	2.18	0.58
1:A:266:PRO:O	1:A:267:ASN:O	2.22	0.58
1:A:269:ARG:NH1	1:A:372:MET:HB3	2.17	0.58
1:A:319:LEU:O	1:A:323:GLY:HA3	2.04	0.58
1:B:194:THR:HG22	1:B:195:ARG:H	1.69	0.58
1:A:49:MET:SD	1:A:225:ALA:HA	2.43	0.58
1:B:40:VAL:HG23	1:B:44:ALA:HB2	1.86	0.58
1:B:276:GLN:NE2	1:B:365:LEU:HD13	2.19	0.58
1:B:41:ARG:HH21	1:B:42:GLU:HB2	1.69	0.58
1:B:32:ALA:CB	1:B:233:LEU:HD22	2.34	0.57
1:B:163:ALA:O	1:B:167:PHE:HB3	2.03	0.57
1:B:293:TRP:N	1:B:293:TRP:CD1	2.72	0.57
1:A:41:ARG:HH21	1:A:42:GLU:HB2	1.69	0.57
1:A:194:THR:HG22	1:A:195:ARG:H	1.69	0.57
1:B:266:PRO:O	1:B:267:ASN:O	2.22	0.57
1:A:260:ALA:HB2	1:A:308:LEU:HD23	1.85	0.57
1:B:32:ALA:CA	1:B:233:LEU:HB3	2.35	0.57
1:B:214:LEU:HD22	1:B:334:THR:OG1	2.03	0.57
1:A:293:TRP:N	1:A:293:TRP:CD1	2.72	0.57
1:A:214:LEU:HD22	1:A:334:THR:OG1	2.03	0.57
1:B:319:LEU:O	1:B:323:GLY:HA3	2.04	0.57
1:B:260:ALA:HB2	1:B:308:LEU:HD23	1.85	0.57
1:B:251:LEU:HB3	1:B:252:PRO:CD	2.35	0.56
1:B:87:THR:CG2	1:B:88:LEU:N	2.68	0.56
1:B:269:ARG:HD2	1:B:373:GLY:HA2	1.88	0.56
1:A:351:ALA:HB3	1:A:354:SER:OG	2.06	0.56
1:A:207:SER:HA	1:A:210:ASN:CB	2.34	0.56
1:B:85:LEU:HA	1:B:162:ARG:NH2	2.20	0.56
1:A:32:ALA:CA	1:A:233:LEU:HB3	2.35	0.56
1:B:233:LEU:HD23	1:B:238:LEU:HD21	1.88	0.56
1:A:96:LEU:O	1:A:100:ILE:HD12	2.06	0.56
1:B:27:TYR:HA	1:B:30:ALA:HB3	1.88	0.56
1:A:49:MET:O	1:A:52:TYR:HB3	2.06	0.56
1:A:269:ARG:HD2	1:A:373:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HB2	1:B:358:PRO:CD	2.32	0.56
1:B:84:MET:SD	1:B:165:TYR:CD1	2.99	0.56
1:B:207:SER:HA	1:B:210:ASN:CB	2.34	0.56
1:A:85:LEU:HA	1:A:162:ARG:NH2	2.20	0.56
1:A:232:VAL:HG13	1:A:232:VAL:O	2.06	0.56
1:A:91:VAL:HG11	1:A:103:SER:OG	2.06	0.55
1:B:98:VAL:HG22	1:B:101:ALA:HB3	1.88	0.55
1:B:242:SER:O	1:B:245:VAL:HG12	2.06	0.55
1:A:181:ARG:O	1:A:182:TRP:HB2	2.05	0.55
1:A:242:SER:O	1:A:245:VAL:HG12	2.06	0.55
1:B:290:ILE:O	1:B:294:PHE:HB3	2.06	0.55
1:B:328:PHE:HB2	1:B:329:PRO:CD	2.35	0.55
1:B:351:ALA:HB3	1:B:354:SER:OG	2.06	0.55
1:A:84:MET:SD	1:A:165:TYR:CD1	2.99	0.55
1:A:87:THR:CG2	1:A:88:LEU:N	2.68	0.55
1:A:357:LEU:HB2	1:A:358:PRO:CD	2.32	0.55
1:A:27:TYR:HA	1:A:30:ALA:HB3	1.88	0.55
1:A:204:PHE:CD1	1:B:200:TYR:CE1	2.95	0.55
1:A:335:ALA:O	1:A:339:VAL:HG23	2.07	0.55
1:B:91:VAL:HG11	1:B:103:SER:OG	2.06	0.55
1:B:94:SER:HB3	1:B:99:LEU:HD23	1.89	0.55
1:B:148:ALA:HB3	1:B:149:PRO:CD	2.35	0.55
1:B:181:ARG:O	1:B:182:TRP:HB2	2.06	0.55
1:A:10:LEU:H	1:A:10:LEU:HD23	1.72	0.55
1:A:233:LEU:HD23	1:A:238:LEU:HD21	1.88	0.55
1:B:96:LEU:O	1:B:100:ILE:HD12	2.06	0.55
1:A:42:GLU:OE2	1:A:233:LEU:HD11	2.07	0.55
1:A:290:ILE:O	1:A:294:PHE:HB3	2.06	0.55
1:B:114:GLY:O	1:B:117:ALA:HB3	2.07	0.55
1:B:232:VAL:HG13	1:B:232:VAL:O	2.06	0.55
1:A:98:VAL:HG22	1:A:101:ALA:HB3	1.88	0.54
1:A:251:LEU:HB3	1:A:252:PRO:CD	2.35	0.54
1:A:84:MET:C	1:A:87:THR:HB	2.32	0.54
1:A:119:THR:O	1:A:122:ARG:HB2	2.07	0.54
1:B:49:MET:O	1:B:52:TYR:HB3	2.06	0.54
1:A:148:ALA:HB3	1:A:149:PRO:CD	2.35	0.54
1:B:335:ALA:O	1:B:339:VAL:HG23	2.06	0.54
1:B:32:ALA:HB1	1:B:233:LEU:CD2	2.37	0.54
1:B:119:THR:O	1:B:122:ARG:HB2	2.07	0.54
1:B:42:GLU:OE2	1:B:233:LEU:HD11	2.07	0.54
1:A:298:ASN:O	1:A:302:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:C	1:B:87:THR:HB	2.32	0.54
1:B:195:ARG:NH1	1:B:196:LEU:HB2	2.23	0.54
1:A:94:SER:HB3	1:A:99:LEU:HD23	1.89	0.54
1:B:10:LEU:HD23	1:B:10:LEU:H	1.72	0.54
1:B:239:GLY:O	1:B:242:SER:HB3	2.08	0.54
1:A:32:ALA:HB1	1:A:233:LEU:CD2	2.37	0.54
1:A:195:ARG:NH1	1:A:196:LEU:HB2	2.23	0.54
1:B:298:ASN:O	1:B:302:LEU:HG	2.08	0.54
1:A:339:VAL:O	1:A:342:LEU:HB2	2.08	0.54
1:B:94:SER:HA	1:B:97:THR:HB	1.90	0.54
1:A:59:SER:C	1:A:63:TYR:HB3	2.32	0.54
1:A:94:SER:O	1:A:95:SER:C	2.51	0.54
1:A:148:ALA:CB	1:A:149:PRO:HD3	2.35	0.54
1:A:239:GLY:O	1:A:242:SER:HB3	2.08	0.54
1:A:317:PHE:C	1:A:319:LEU:N	2.66	0.54
1:B:148:ALA:CB	1:B:149:PRO:HD3	2.35	0.53
1:B:267:ASN:OD1	1:B:376:ILE:HG23	2.07	0.53
1:A:267:ASN:OD1	1:A:376:ILE:HG23	2.07	0.53
1:B:22:MET:O	1:B:26:ILE:HB	2.09	0.53
1:B:59:SER:C	1:B:63:TYR:HB3	2.32	0.53
1:B:87:THR:HG22	1:B:88:LEU:H	1.73	0.53
1:B:275:TRP:HA	1:B:275:TRP:HE3	1.71	0.53
1:A:114:GLY:O	1:A:117:ALA:HB3	2.07	0.53
1:B:94:SER:O	1:B:95:SER:C	2.51	0.53
1:B:339:VAL:O	1:B:342:LEU:HB2	2.08	0.53
1:A:225:ALA:O	1:A:229:CYS:HB2	2.09	0.53
1:B:82:ILE:HA	1:B:85:LEU:HD13	1.91	0.53
1:B:279:ILE:HD13	1:B:294:PHE:CE1	2.44	0.53
1:A:87:THR:HG22	1:A:88:LEU:H	1.73	0.53
1:B:149:PRO:O	1:B:153:GLY:HA3	2.09	0.53
1:A:149:PRO:O	1:A:153:GLY:HA3	2.09	0.53
1:A:247:ILE:O	1:A:250:ILE:HG22	2.08	0.53
1:B:247:ILE:O	1:B:250:ILE:HG22	2.08	0.53
1:A:279:ILE:HD13	1:A:294:PHE:CE1	2.44	0.53
1:A:274:MET:O	1:A:278:VAL:HG23	2.09	0.53
1:A:129:GLN:O	1:A:129:GLN:HG2	2.09	0.52
1:B:49:MET:SD	1:B:224:ALA:O	2.68	0.52
1:A:16:LEU:O	1:A:19:VAL:HG13	2.09	0.52
1:A:187:ARG:CZ	1:A:188:PRO:HA	2.39	0.52
1:A:94:SER:HA	1:A:97:THR:HB	1.90	0.52
1:A:95:SER:C	1:A:100:ILE:HG23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLU:HG2	1:B:186:THR:N	2.25	0.52
1:B:225:ALA:O	1:B:229:CYS:HB2	2.09	0.52
1:A:122:ARG:O	1:A:125:TYR:HB3	2.10	0.52
1:A:217:ILE:HD11	1:A:331:LEU:C	2.34	0.52
1:A:222:GLY:O	1:A:225:ALA:HB3	2.10	0.52
1:B:274:MET:O	1:B:278:VAL:HG23	2.09	0.52
1:A:49:MET:SD	1:A:224:ALA:O	2.68	0.52
1:B:95:SER:C	1:B:100:ILE:HG23	2.34	0.52
1:B:129:GLN:O	1:B:129:GLN:HG2	2.09	0.52
1:B:150:LEU:HD23	1:B:157:THR:HG21	1.91	0.52
1:A:22:MET:O	1:A:26:ILE:HB	2.09	0.52
1:A:171:LEU:O	1:A:175:VAL:HG23	2.09	0.52
1:A:268:LYS:O	1:A:271:SER:HB3	2.10	0.52
1:A:318:PRO:C	1:A:320:ALA:H	2.18	0.52
1:B:222:GLY:O	1:B:225:ALA:HB3	2.10	0.52
1:B:187:ARG:CZ	1:B:188:PRO:HA	2.39	0.52
1:A:185:GLU:HG2	1:A:186:THR:N	2.25	0.52
1:A:265:ARG:CG	1:A:266:PRO:HD2	2.40	0.52
1:B:122:ARG:O	1:B:125:TYR:HB3	2.10	0.52
1:B:217:ILE:HD11	1:B:331:LEU:C	2.34	0.52
1:A:82:ILE:HA	1:A:85:LEU:HD13	1.91	0.51
1:A:250:ILE:O	1:A:253:ILE:HG22	2.10	0.51
1:B:16:LEU:O	1:B:19:VAL:HG13	2.09	0.51
1:B:293:TRP:CD1	1:B:293:TRP:H	2.28	0.51
1:A:275:TRP:HA	1:A:275:TRP:HE3	1.71	0.51
1:B:171:LEU:O	1:B:175:VAL:HG23	2.09	0.51
1:B:278:VAL:O	1:B:281:CYS:SG	2.67	0.51
1:A:328:PHE:HB2	1:A:329:PRO:CD	2.35	0.51
1:B:306:ALA:O	1:B:310:PHE:HB2	2.11	0.51
1:A:29:PRO:HB3	1:A:238:LEU:C	2.36	0.51
1:A:179:MET:O	1:A:180:ALA:HB2	2.11	0.51
1:A:248:LEU:HG	1:A:297:MET:HB2	1.93	0.51
1:B:172:CYS:O	1:B:176:THR:HG23	2.11	0.51
1:A:187:ARG:HB3	1:A:188:PRO:HD3	1.93	0.51
1:B:29:PRO:O	1:B:32:ALA:HB3	2.11	0.51
1:B:250:ILE:O	1:B:253:ILE:HG22	2.10	0.51
1:B:279:ILE:HD11	1:B:298:ASN:HB3	1.92	0.51
1:A:279:ILE:HD11	1:A:298:ASN:HB3	1.92	0.51
1:B:179:MET:O	1:B:180:ALA:HB2	2.11	0.51
1:B:317:PHE:C	1:B:319:LEU:N	2.66	0.51
1:B:202:THR:O	1:B:206:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HB2	1:A:372:MET:HE1	1.92	0.51
1:B:318:PRO:C	1:B:320:ALA:H	2.18	0.51
1:A:59:SER:HA	1:A:63:TYR:HB3	1.93	0.51
1:B:268:LYS:O	1:B:271:SER:HB3	2.10	0.51
1:A:18:ALA:HB3	1:A:168:LEU:HG	1.93	0.50
1:A:125:TYR:HA	1:A:130:LEU:HB2	1.92	0.50
1:B:18:ALA:HB3	1:B:168:LEU:HG	1.93	0.50
1:B:215:MET:HB2	1:B:372:MET:HE1	1.92	0.50
1:A:172:CYS:O	1:A:176:THR:HG23	2.11	0.50
1:B:59:SER:HA	1:B:63:TYR:HB3	1.93	0.50
1:A:29:PRO:O	1:A:32:ALA:HB3	2.11	0.50
1:A:150:LEU:HD23	1:A:157:THR:HG21	1.91	0.50
1:A:293:TRP:CD1	1:A:293:TRP:H	2.28	0.50
1:B:125:TYR:HA	1:B:130:LEU:HB2	1.92	0.50
1:B:326:GLU:HG3	1:B:327:PRO:CD	2.40	0.50
1:A:306:ALA:O	1:A:310:PHE:HB2	2.11	0.50
1:B:20:GLY:CA	1:B:110:THR:HB	2.23	0.50
1:A:61:LEU:HD13	1:A:329:PRO:HD3	1.93	0.50
1:A:179:MET:HG2	1:A:180:ALA:N	2.27	0.50
1:B:87:THR:O	1:B:91:VAL:HG22	2.11	0.50
1:B:248:LEU:HG	1:B:297:MET:HB2	1.93	0.50
1:A:135:SER:O	1:A:138:ASN:HB3	2.12	0.50
1:B:61:LEU:HD13	1:B:329:PRO:HD3	1.93	0.50
1:B:187:ARG:HB3	1:B:188:PRO:HD3	1.93	0.50
1:B:29:PRO:HB3	1:B:238:LEU:O	2.11	0.50
1:A:279:ILE:HD11	1:A:298:ASN:CB	2.42	0.50
1:B:29:PRO:HB3	1:B:238:LEU:C	2.36	0.50
1:B:84:MET:HE2	1:B:162:ARG:HH11	1.74	0.50
1:A:202:THR:O	1:A:206:ASN:N	2.44	0.50
1:B:345:ILE:O	1:B:349:VAL:N	2.45	0.50
1:B:346:GLY:O	1:B:349:VAL:HG12	2.11	0.50
1:A:74:PRO:O	1:A:78:VAL:HB	2.11	0.49
1:A:345:ILE:O	1:A:349:VAL:N	2.45	0.49
1:B:179:MET:HG2	1:B:180:ALA:N	2.27	0.49
1:A:27:TYR:O	1:A:31:ILE:HG12	2.12	0.49
1:A:172:CYS:SG	1:A:176:THR:CG2	3.00	0.49
1:A:346:GLY:O	1:A:349:VAL:HG12	2.11	0.49
1:B:74:PRO:O	1:B:78:VAL:HB	2.11	0.49
1:B:172:CYS:SG	1:B:176:THR:CG2	3.00	0.49
1:B:253:ILE:HG23	1:B:254:PRO:HD3	1.94	0.49
1:A:32:ALA:CA	1:A:233:LEU:HD13	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TRP:CD1	1:A:161:TRP:C	2.90	0.49
1:B:368:LEU:O	1:B:371:LEU:HG	2.11	0.49
1:B:91:VAL:CG1	1:B:99:LEU:HD12	2.34	0.49
1:B:96:LEU:HG	1:B:97:THR:H	1.78	0.49
1:A:19:VAL:HG11	1:A:169:LEU:HB2	1.94	0.49
1:A:29:PRO:HB3	1:A:238:LEU:O	2.11	0.49
1:A:87:THR:O	1:A:91:VAL:HG22	2.11	0.49
1:B:265:ARG:CG	1:B:266:PRO:HD2	2.40	0.49
1:B:279:ILE:HD11	1:B:298:ASN:CB	2.42	0.49
1:A:96:LEU:HG	1:A:97:THR:H	1.78	0.49
1:B:135:SER:O	1:B:138:ASN:HB3	2.12	0.49
1:A:59:SER:HB3	1:A:112:VAL:HG13	1.95	0.49
1:A:84:MET:HE2	1:A:162:ARG:HH11	1.74	0.49
1:A:368:LEU:O	1:A:371:LEU:HG	2.12	0.49
1:B:360:THR:O	1:B:364:SER:HB2	2.12	0.49
1:A:26:ILE:HD11	1:A:151:ILE:HG13	1.95	0.49
1:B:19:VAL:HG11	1:B:169:LEU:HB2	1.94	0.49
1:B:27:TYR:O	1:B:31:ILE:HG12	2.12	0.49
1:A:253:ILE:HG23	1:A:254:PRO:HD3	1.94	0.49
1:A:360:THR:O	1:A:364:SER:HB2	2.12	0.49
1:B:161:TRP:CD1	1:B:161:TRP:C	2.90	0.49
1:A:90:ALA:O	1:A:94:SER:HB2	2.13	0.48
1:A:153:GLY:O	1:A:154:LEU:HD22	2.13	0.48
1:A:84:MET:O	1:A:87:THR:CB	2.56	0.48
1:B:339:VAL:HA	1:B:342:LEU:HD12	1.95	0.48
1:A:21:GLN:CB	1:A:143:VAL:HG22	2.43	0.48
1:B:19:VAL:CG2	1:B:165:TYR:HA	2.42	0.48
1:A:212:TYR:CE1	1:A:269:ARG:HG2	2.48	0.48
1:A:260:ALA:O	1:A:263:ALA:HB3	2.14	0.48
1:B:260:ALA:HB2	1:B:308:LEU:CD2	2.43	0.48
1:B:293:TRP:N	1:B:293:TRP:HD1	2.11	0.48
1:A:260:ALA:HB2	1:A:308:LEU:CD2	2.43	0.48
1:B:286:LEU:HB2	1:B:290:ILE:HD11	1.96	0.48
1:B:212:TYR:CE1	1:B:269:ARG:HG2	2.48	0.48
1:A:79:GLY:O	1:A:82:ILE:HG22	2.13	0.48
1:A:91:VAL:CG1	1:A:99:LEU:HD12	2.34	0.48
1:B:201:LYS:C	1:B:203:LEU:N	2.70	0.48
1:A:286:LEU:HB2	1:A:290:ILE:HD11	1.96	0.48
1:B:79:GLY:O	1:B:82:ILE:HG22	2.13	0.48
1:B:146:LEU:O	1:B:150:LEU:HB2	2.14	0.48
1:B:153:GLY:O	1:B:154:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:CG	1:A:74:PRO:HD3	2.36	0.48
1:A:87:THR:CG2	1:A:161:TRP:HE1	2.25	0.48
1:B:44:ALA:O	1:B:48:VAL:HG23	2.13	0.48
1:B:90:ALA:O	1:B:94:SER:HB2	2.13	0.48
1:B:21:GLN:CB	1:B:143:VAL:HG22	2.43	0.48
1:B:59:SER:HB3	1:B:112:VAL:HG13	1.95	0.48
1:B:73:ARG:HA	1:B:77:LEU:HD11	1.96	0.48
1:B:268:LYS:HZ2	1:B:305:PRO:C	2.21	0.48
1:A:36:ARG:HD2	1:A:233:LEU:CB	2.44	0.47
1:A:227:GLU:HA	1:A:292:ASP:HB2	1.96	0.47
1:B:159:TRP:CD1	1:B:159:TRP:C	2.92	0.47
1:B:164:CYS:O	1:B:168:LEU:HB2	2.15	0.47
1:A:44:ALA:O	1:A:48:VAL:HG23	2.13	0.47
1:A:268:LYS:HZ2	1:A:305:PRO:C	2.21	0.47
1:B:84:MET:O	1:B:87:THR:CB	2.56	0.47
1:B:245:VAL:HG22	1:B:249:PHE:CZ	2.49	0.47
1:A:322:SER:O	1:A:326:GLU:HG2	2.14	0.47
1:B:322:SER:O	1:B:326:GLU:HG2	2.14	0.47
1:A:293:TRP:N	1:A:293:TRP:HD1	2.11	0.47
1:B:265:ARG:C	1:B:267:ASN:N	2.72	0.47
1:A:84:MET:HE1	1:A:165:TYR:HB3	1.97	0.47
1:A:146:LEU:O	1:A:150:LEU:HB2	2.14	0.47
1:A:159:TRP:CD1	1:A:159:TRP:C	2.92	0.47
1:A:166:LEU:O	1:A:170:VAL:HG22	2.15	0.47
1:A:201:LYS:C	1:A:203:LEU:N	2.70	0.47
1:A:339:VAL:HA	1:A:342:LEU:HD12	1.95	0.47
1:B:15:LEU:HB3	1:B:172:CYS:HB2	1.97	0.47
1:B:26:ILE:HD11	1:B:151:ILE:HG13	1.95	0.47
1:B:186:THR:O	1:B:186:THR:HG23	2.14	0.47
1:B:260:ALA:O	1:B:263:ALA:HB3	2.14	0.47
1:A:32:ALA:O	1:A:233:LEU:HB3	2.15	0.47
1:A:186:THR:O	1:A:186:THR:HG23	2.14	0.47
1:A:278:VAL:O	1:A:281:CYS:SG	2.67	0.47
1:B:61:LEU:O	1:B:65:PRO:HD2	2.15	0.47
1:B:266:PRO:C	1:B:267:ASN:O	2.57	0.47
1:A:53:LEU:HA	1:A:53:LEU:HD23	1.78	0.47
1:B:59:SER:O	1:B:60:GLN:C	2.58	0.47
1:A:77:LEU:HB2	1:A:169:LEU:CD2	2.45	0.46
1:B:282:LEU:O	1:B:291:PRO:HG3	2.15	0.46
1:A:59:SER:O	1:A:60:GLN:C	2.58	0.46
1:B:32:ALA:O	1:B:233:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HB3	1:A:172:CYS:HB2	1.97	0.46
1:A:164:CYS:O	1:A:168:LEU:HB2	2.15	0.46
1:A:272:THR:HA	1:A:302:LEU:HD22	1.96	0.46
1:B:227:GLU:HA	1:B:292:ASP:HB2	1.96	0.46
1:A:9:LEU:HB2	1:A:10:LEU:HD23	1.98	0.46
1:A:173:ALA:HA	1:A:176:THR:OG1	2.15	0.46
1:B:278:VAL:HG13	1:B:281:CYS:SG	2.56	0.46
1:A:19:VAL:CG2	1:A:165:TYR:HA	2.42	0.46
1:A:158:MET:O	1:A:162:ARG:HG2	2.15	0.46
1:A:200:TYR:CE1	1:B:204:PHE:CZ	2.96	0.46
1:A:245:VAL:HG22	1:A:249:PHE:CZ	2.49	0.46
1:A:266:PRO:C	1:A:267:ASN:O	2.57	0.46
1:A:282:LEU:O	1:A:291:PRO:HG3	2.16	0.46
1:B:269:ARG:HA	1:B:272:THR:OG1	2.16	0.46
1:B:272:THR:HA	1:B:302:LEU:HD22	1.96	0.46
1:A:32:ALA:HB1	1:A:233:LEU:CG	2.45	0.46
1:A:61:LEU:HD22	1:A:329:PRO:HG3	1.98	0.46
1:A:159:TRP:HA	1:A:162:ARG:HG2	1.97	0.46
1:A:281:CYS:SG	1:A:282:LEU:HD22	2.56	0.46
1:B:18:ALA:HA	1:B:21:GLN:OE1	2.16	0.46
1:B:173:ALA:HA	1:B:176:THR:OG1	2.15	0.46
1:B:281:CYS:SG	1:B:282:LEU:HD22	2.56	0.46
1:A:294:PHE:O	1:A:297:MET:HB3	2.16	0.46
1:B:24:GLN:HA	1:B:27:TYR:CD2	2.51	0.46
1:B:158:MET:O	1:B:162:ARG:HG2	2.15	0.46
1:B:340:GLY:O	1:B:343:GLN:HB3	2.16	0.46
1:A:22:MET:HA	1:A:147:LEU:HD21	1.97	0.46
1:B:294:PHE:O	1:B:297:MET:HB3	2.16	0.46
1:A:24:GLN:HA	1:A:27:TYR:CD2	2.51	0.46
1:B:77:LEU:HB2	1:B:169:LEU:CD2	2.45	0.46
1:B:264:GLY:O	1:B:265:ARG:C	2.59	0.46
1:A:269:ARG:HA	1:A:272:THR:OG1	2.16	0.46
1:A:340:GLY:O	1:A:343:GLN:HB3	2.16	0.46
1:A:18:ALA:HA	1:A:21:GLN:OE1	2.16	0.45
1:A:61:LEU:O	1:A:65:PRO:HD2	2.15	0.45
1:A:73:ARG:HA	1:A:77:LEU:HD11	1.96	0.45
1:A:326:GLU:HG3	1:A:327:PRO:CD	2.40	0.45
1:B:26:ILE:HD12	1:B:26:ILE:HA	1.89	0.45
1:A:27:TYR:CD1	1:A:27:TYR:C	2.94	0.45
1:A:91:VAL:HA	1:A:99:LEU:HB3	1.98	0.45
1:A:99:LEU:C	1:A:101:ALA:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:HE1	1:B:165:TYR:HB3	1.97	0.45
1:B:166:LEU:O	1:B:170:VAL:HG22	2.15	0.45
1:A:243:MET:O	1:A:247:ILE:HG13	2.16	0.45
1:B:226:PHE:O	1:B:229:CYS:HB3	2.17	0.45
1:A:69:ARG:HG2	1:A:186:THR:HA	1.99	0.45
1:B:22:MET:HA	1:B:147:LEU:HD21	1.97	0.45
1:B:317:PHE:HB3	1:B:318:PRO:CD	2.46	0.45
1:B:238:LEU:O	1:B:241:SER:HB3	2.17	0.45
1:A:21:GLN:CG	1:A:143:VAL:HG22	2.47	0.45
1:A:125:TYR:CD1	1:A:130:LEU:O	2.70	0.45
1:A:278:VAL:HG13	1:A:281:CYS:SG	2.56	0.45
1:B:21:GLN:CG	1:B:143:VAL:HG22	2.47	0.45
1:B:69:ARG:HG2	1:B:186:THR:HA	1.99	0.45
1:B:91:VAL:HA	1:B:99:LEU:HB3	1.98	0.45
1:B:159:TRP:HA	1:B:162:ARG:HG2	1.97	0.45
1:B:354:SER:O	1:B:358:PRO:HD2	2.17	0.45
1:A:219:GLY:HA3	1:A:365:LEU:HG	1.99	0.45
1:A:317:PHE:C	1:A:319:LEU:H	2.25	0.45
1:B:32:ALA:HB1	1:B:233:LEU:CG	2.46	0.45
1:B:36:ARG:HD2	1:B:233:LEU:CB	2.44	0.45
1:B:87:THR:CG2	1:B:161:TRP:HE1	2.25	0.45
1:B:169:LEU:O	1:B:172:CYS:HB3	2.17	0.45
1:A:106:GLN:NE2	1:A:106:GLN:HA	2.32	0.45
1:B:9:LEU:HB2	1:B:10:LEU:HD23	1.98	0.45
1:B:27:TYR:CD1	1:B:27:TYR:C	2.94	0.45
1:B:61:LEU:HD22	1:B:329:PRO:HG3	1.98	0.45
1:A:264:GLY:O	1:A:265:ARG:C	2.59	0.44
1:A:317:PHE:HB3	1:A:318:PRO:CD	2.46	0.44
1:B:267:ASN:OD1	1:B:376:ILE:HD12	2.17	0.44
1:A:13:LEU:O	1:A:17:VAL:HG22	2.18	0.44
1:A:226:PHE:O	1:A:229:CYS:HB3	2.17	0.44
1:A:263:ALA:CA	1:A:268:LYS:HB2	2.11	0.44
1:A:265:ARG:C	1:A:267:ASN:N	2.72	0.44
1:A:354:SER:O	1:A:358:PRO:HD2	2.17	0.44
1:B:22:MET:HE2	1:B:146:LEU:HB2	1.99	0.44
1:B:165:TYR:CE1	1:B:169:LEU:HD13	2.53	0.44
1:B:263:ALA:CA	1:B:268:LYS:HB2	2.11	0.44
1:A:22:MET:O	1:A:147:LEU:HD11	2.17	0.44
1:A:238:LEU:O	1:A:241:SER:HB3	2.17	0.44
1:B:18:ALA:HB2	1:B:142:LEU:HD13	2.00	0.44
1:B:99:LEU:C	1:B:101:ALA:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:NE2	1:B:106:GLN:HA	2.32	0.44
1:A:165:TYR:CE1	1:A:169:LEU:HD13	2.53	0.44
1:A:169:LEU:O	1:A:172:CYS:HB3	2.17	0.44
1:A:262:PHE:HZ	1:A:270:PHE:CD2	2.31	0.44
1:B:32:ALA:CA	1:B:233:LEU:HD13	2.40	0.44
1:B:243:MET:O	1:B:247:ILE:HG13	2.16	0.44
1:A:18:ALA:HB2	1:A:142:LEU:HD13	2.00	0.44
1:A:319:LEU:C	1:A:323:GLY:H	2.26	0.44
1:A:210:ASN:O	1:A:214:LEU:HB2	2.18	0.44
1:B:125:TYR:CD1	1:B:130:LEU:O	2.70	0.44
1:A:22:MET:HE2	1:A:146:LEU:HB2	1.99	0.44
1:A:214:LEU:HD22	1:A:334:THR:HG1	1.83	0.44
1:A:298:ASN:ND2	1:A:302:LEU:HD21	2.33	0.44
1:B:310:PHE:HD2	1:B:310:PHE:HA	1.72	0.44
1:A:31:ILE:HD13	1:A:31:ILE:HA	1.84	0.44
1:A:48:VAL:O	1:A:51:ALA:HB3	2.18	0.44
1:A:267:ASN:OD1	1:A:376:ILE:HD12	2.17	0.44
1:A:373:GLY:O	1:A:376:ILE:HG22	2.18	0.44
1:B:94:SER:HB2	1:B:99:LEU:HG	2.00	0.44
1:B:155:LEU:HB3	1:B:156:ASP:H	1.67	0.44
1:A:42:GLU:OE1	1:A:42:GLU:O	2.36	0.43
1:B:373:GLY:O	1:B:376:ILE:HG22	2.18	0.43
1:B:13:LEU:O	1:B:17:VAL:HG22	2.18	0.43
1:B:73:ARG:HA	1:B:77:LEU:HD13	1.99	0.43
1:B:210:ASN:O	1:B:214:LEU:HB2	2.18	0.43
1:B:319:LEU:C	1:B:323:GLY:H	2.26	0.43
1:B:349:VAL:C	1:B:351:ALA:H	2.26	0.43
1:A:20:GLY:CA	1:A:110:THR:HB	2.23	0.43
1:A:59:SER:CA	1:A:63:TYR:HB3	2.48	0.43
1:A:250:ILE:O	1:A:254:PRO:CD	2.62	0.43
1:B:18:ALA:O	1:B:21:GLN:HG2	2.17	0.43
1:B:33:ASP:OD2	1:B:234:MET:HA	2.18	0.43
1:B:59:SER:CA	1:B:63:TYR:HB3	2.48	0.43
1:B:276:GLN:O	1:B:279:ILE:HB	2.18	0.43
1:A:18:ALA:O	1:A:21:GLN:HG2	2.17	0.43
1:A:94:SER:HB2	1:A:99:LEU:HG	2.00	0.43
1:A:276:GLN:O	1:A:279:ILE:HB	2.19	0.43
1:B:120:LEU:O	1:B:123:ASP:HB2	2.19	0.43
1:B:262:PHE:HZ	1:B:270:PHE:CD2	2.31	0.43
1:A:26:ILE:O	1:A:29:PRO:HG2	2.19	0.43
1:B:22:MET:O	1:B:147:LEU:HD11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ILE:O	1:B:29:PRO:HG2	2.19	0.43
1:B:219:GLY:HA3	1:B:365:LEU:HG	1.99	0.43
1:B:317:PHE:C	1:B:319:LEU:H	2.25	0.43
1:A:33:ASP:OD2	1:A:234:MET:HA	2.18	0.43
1:A:155:LEU:HB3	1:A:156:ASP:H	1.67	0.43
1:B:33:ASP:CG	1:B:234:MET:HA	2.44	0.43
1:A:349:VAL:C	1:A:351:ALA:H	2.26	0.43
1:B:48:VAL:O	1:B:51:ALA:HB3	2.18	0.43
1:B:61:LEU:O	1:B:65:PRO:CD	2.67	0.43
1:B:253:ILE:HG23	1:B:254:PRO:CD	2.49	0.43
1:B:317:PHE:HB3	1:B:318:PRO:HD2	2.01	0.43
1:A:212:TYR:O	1:A:216:LEU:HB2	2.19	0.43
1:A:253:ILE:HG23	1:A:254:PRO:CD	2.49	0.43
1:B:23:ALA:HB2	1:B:165:TYR:HD2	1.84	0.43
1:A:273:LEU:HD23	1:A:274:MET:N	2.34	0.43
1:B:84:MET:HE3	1:B:84:MET:HB2	1.95	0.43
1:B:42:GLU:OE1	1:B:42:GLU:O	2.36	0.43
1:B:273:LEU:HD23	1:B:274:MET:N	2.34	0.43
1:A:33:ASP:CG	1:A:234:MET:HA	2.44	0.42
1:A:46:GLN:HA	1:A:49:MET:HE3	2.01	0.42
1:A:92:THR:O	1:A:95:SER:CB	2.67	0.42
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.91	0.42
1:B:121:PRO:O	1:B:124:LEU:HB3	2.19	0.42
1:A:156:ASP:HB3	1:A:158:MET:HE3	2.00	0.42
1:A:317:PHE:HB3	1:A:318:PRO:HD2	2.01	0.42
1:A:172:CYS:SG	1:A:176:THR:HG21	2.59	0.42
1:B:21:GLN:OE1	1:B:142:LEU:HB2	2.19	0.42
1:B:141:ILE:HD13	1:B:141:ILE:HA	1.91	0.42
1:B:212:TYR:O	1:B:216:LEU:HB2	2.19	0.42
1:A:91:VAL:O	1:A:95:SER:CB	2.64	0.42
1:A:120:LEU:O	1:A:123:ASP:HB2	2.19	0.42
1:B:36:ARG:HD2	1:B:233:LEU:CG	2.50	0.42
1:B:91:VAL:O	1:B:95:SER:CB	2.64	0.42
1:B:156:ASP:HB3	1:B:158:MET:HE3	2.00	0.42
1:B:341:GLY:O	1:B:345:ILE:HB	2.20	0.42
1:A:240:LEU:HG	1:A:243:MET:HE3	2.02	0.42
1:A:253:ILE:HD13	1:A:304:VAL:HG11	2.01	0.42
1:A:341:GLY:O	1:A:345:ILE:HB	2.20	0.42
1:B:94:SER:O	1:B:97:THR:O	2.38	0.42
1:B:252:PRO:HA	1:B:255:ALA:HB3	2.01	0.42
1:B:253:ILE:HD13	1:B:304:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASN:ND2	1:B:302:LEU:HD21	2.33	0.42
1:A:23:ALA:HB2	1:A:165:TYR:HD2	1.84	0.42
1:A:94:SER:O	1:A:97:THR:O	2.38	0.42
1:B:89:VAL:HG23	1:B:90:ALA:H	1.84	0.42
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.93	0.42
1:B:240:LEU:HG	1:B:243:MET:HE3	2.02	0.42
1:B:259:GLY:HA2	1:B:262:PHE:HB3	2.02	0.42
1:A:187:ARG:N	1:A:188:PRO:CD	2.83	0.42
1:A:201:LYS:HD2	1:B:200:TYR:HE2	1.85	0.42
1:A:349:VAL:O	1:A:351:ALA:N	2.53	0.42
1:B:21:GLN:HE21	1:B:21:GLN:HB3	1.55	0.42
1:B:187:ARG:N	1:B:188:PRO:CD	2.83	0.42
1:B:325:MET:HA	1:B:329:PRO:HD2	2.02	0.42
1:A:201:LYS:C	1:A:203:LEU:H	2.28	0.42
1:A:252:PRO:HA	1:A:255:ALA:HB3	2.01	0.42
1:B:25:THR:OG1	1:B:147:LEU:HG	2.20	0.42
1:B:46:GLN:HA	1:B:49:MET:HE3	2.01	0.42
1:B:172:CYS:SG	1:B:176:THR:HG21	2.59	0.42
1:A:61:LEU:O	1:A:65:PRO:CD	2.67	0.42
1:B:84:MET:SD	1:B:165:TYR:HB3	2.60	0.42
1:A:25:THR:OG1	1:A:147:LEU:HG	2.19	0.41
1:B:97:THR:C	1:B:99:LEU:N	2.78	0.41
1:A:21:GLN:OE1	1:A:142:LEU:HB2	2.19	0.41
1:A:262:PHE:CZ	1:A:270:PHE:HD2	2.33	0.41
1:A:121:PRO:O	1:A:124:LEU:HB3	2.19	0.41
1:B:323:GLY:HA2	1:B:326:GLU:CG	2.51	0.41
1:A:97:THR:C	1:A:99:LEU:N	2.78	0.41
1:B:217:ILE:HG12	1:B:331:LEU:HB3	2.02	0.41
1:A:36:ARG:HD2	1:A:233:LEU:CG	2.50	0.41
1:A:89:VAL:HG23	1:A:90:ALA:H	1.84	0.41
1:A:172:CYS:O	1:A:176:THR:N	2.54	0.41
1:A:179:MET:O	1:A:180:ALA:CB	2.69	0.41
1:A:376:ILE:HD13	1:A:376:ILE:O	2.21	0.41
1:B:214:LEU:HD22	1:B:334:THR:HG1	1.83	0.41
1:B:349:VAL:O	1:B:351:ALA:N	2.53	0.41
1:A:9:LEU:HB2	1:A:10:LEU:H	1.65	0.41
1:A:323:GLY:HA2	1:A:326:GLU:CG	2.50	0.41
1:B:92:THR:O	1:B:95:SER:CB	2.67	0.41
1:B:265:ARG:O	1:B:267:ASN:N	2.54	0.41
1:A:259:GLY:HA2	1:A:262:PHE:HB3	2.02	0.41
1:A:281:CYS:SG	1:A:282:LEU:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:SER:O	1:A:368:LEU:HB2	2.20	0.41
1:B:248:LEU:HD13	1:B:248:LEU:HA	1.78	0.41
1:B:318:PRO:C	1:B:320:ALA:N	2.78	0.41
1:B:364:SER:O	1:B:368:LEU:HB2	2.20	0.41
1:A:14:VAL:HG23	1:A:15:LEU:HD13	2.03	0.41
1:A:97:THR:C	1:A:99:LEU:H	2.29	0.41
1:A:141:ILE:HD13	1:A:141:ILE:HA	1.91	0.41
1:A:165:TYR:CD1	1:A:165:TYR:C	2.99	0.41
1:A:217:ILE:HG12	1:A:331:LEU:HB3	2.02	0.41
1:A:233:LEU:HD23	1:A:238:LEU:CD2	2.51	0.41
1:B:14:VAL:HG23	1:B:15:LEU:HD13	2.03	0.41
1:B:21:GLN:HA	1:B:24:GLN:HB3	2.03	0.41
1:B:95:SER:O	1:B:96:LEU:C	2.63	0.41
1:B:97:THR:O	1:B:98:VAL:C	2.64	0.41
1:B:267:ASN:O	1:B:268:LYS:C	2.64	0.41
1:B:272:THR:HB	1:B:369:MET:HG2	2.03	0.41
1:A:274:MET:C	1:A:274:MET:SD	3.03	0.41
1:A:325:MET:HA	1:A:329:PRO:HD2	2.02	0.41
1:A:342:LEU:HA	1:A:345:ILE:CG2	2.51	0.41
1:A:345:ILE:CG2	1:A:346:GLY:N	2.84	0.41
1:B:172:CYS:O	1:B:176:THR:N	2.54	0.41
1:B:274:MET:SD	1:B:274:MET:C	3.03	0.41
1:A:350:LEU:O	1:A:350:LEU:HG	2.21	0.40
1:B:69:ARG:O	1:B:70:VAL:HB	2.21	0.40
1:B:165:TYR:CD1	1:B:165:TYR:C	2.99	0.40
1:A:84:MET:SD	1:A:165:TYR:HB3	2.60	0.40
1:B:15:LEU:O	1:B:19:VAL:HG12	2.21	0.40
1:B:97:THR:C	1:B:99:LEU:H	2.29	0.40
1:B:117:ALA:O	1:B:121:PRO:CD	2.58	0.40
1:B:281:CYS:SG	1:B:282:LEU:N	2.94	0.40
1:A:69:ARG:O	1:A:70:VAL:HB	2.21	0.40
1:A:286:LEU:HB3	1:A:287:LEU:H	1.71	0.40
1:B:262:PHE:CZ	1:B:270:PHE:HD2	2.33	0.40
1:A:233:LEU:HA	1:A:238:LEU:HG	2.02	0.40
1:A:267:ASN:O	1:A:268:LYS:C	2.64	0.40
1:B:294:PHE:CE2	1:B:297:MET:SD	3.14	0.40
1:B:342:LEU:HA	1:B:345:ILE:CG2	2.52	0.40
1:A:15:LEU:O	1:A:19:VAL:HG12	2.21	0.40
1:A:95:SER:O	1:A:96:LEU:C	2.63	0.40
1:A:238:LEU:HD13	1:A:238:LEU:HA	1.95	0.40
1:A:265:ARG:O	1:A:267:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLY:O	1:A:324:ALA:C	2.64	0.40
1:B:84:MET:CG	1:B:162:ARG:HH12	2.23	0.40
1:B:195:ARG:C	1:B:197:LEU:H	2.30	0.40
1:B:323:GLY:O	1:B:324:ALA:C	2.64	0.40
1:B:376:ILE:O	1:B:376:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

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	373/375 (100%)	268 (72%)	67 (18%)	38 (10%)	0	6
1	B	373/375 (100%)	268 (72%)	67 (18%)	38 (10%)	0	6
All	All	746/750 (100%)	536 (72%)	134 (18%)	76 (10%)	0	6

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	69	ARG
1	A	87	THR
1	A	97	THR
1	A	180	ALA
1	A	212	TYR
1	A	233	LEU
1	A	235	GLY
1	A	266	PRO
1	A	267	ASN
1	A	268	LYS
1	A	288	MET
1	A	289	TRP

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Mol	Chain	Res	Type
1	A	291	PRO
1	A	352	SER
1	A	355	ALA
1	B	42	GLU
1	B	69	ARG
1	B	87	THR
1	B	97	THR
1	B	180	ALA
1	B	212	TYR
1	B	233	LEU
1	B	235	GLY
1	B	266	PRO
1	B	267	ASN
1	B	268	LYS
1	B	288	MET
1	B	289	TRP
1	B	291	PRO
1	B	352	SER
1	B	355	ALA
1	A	61	LEU
1	A	70	VAL
1	A	74	PRO
1	A	76	ILE
1	A	98	VAL
1	A	156	ASP
1	A	184	PRO
1	A	200	TYR
1	A	350	LEU
1	A	353	LEU
1	A	382	PRO
1	B	61	LEU
1	B	70	VAL
1	B	74	PRO
1	B	76	ILE
1	B	98	VAL
1	B	156	ASP
1	B	184	PRO
1	B	200	TYR
1	B	350	LEU
1	B	353	LEU
1	B	382	PRO
1	A	24	GLN

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Mol	Chain	Res	Type
1	A	132	HIS
1	A	158	MET
1	A	234	MET
1	B	24	GLN
1	B	132	HIS
1	B	158	MET
1	B	234	MET
1	A	33	ASP
1	A	273	LEU
1	B	33	ASP
1	B	273	LEU
1	A	59	SER
1	A	72	ARG
1	B	72	ARG
1	B	59	SER
1	A	326	GLU
1	B	326	GLU
1	A	143	VAL
1	A	328	PHE
1	B	143	VAL
1	B	328	PHE

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	295/295 (100%)	222 (75%)	73 (25%)	1	4
1	B	295/295 (100%)	223 (76%)	72 (24%)	1	4
All	All	590/590 (100%)	445 (75%)	145 (25%)	1	4

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	15	LEU

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Mol	Chain	Res	Type
1	A	19	VAL
1	A	21	GLN
1	A	22	MET
1	A	25	THR
1	A	26	ILE
1	A	27	TYR
1	A	38	LEU
1	A	42	GLU
1	A	54	LEU
1	A	60	GLN
1	A	65	PRO
1	A	73	ARG
1	A	77	LEU
1	A	84	MET
1	A	87	THR
1	A	89	VAL
1	A	91	VAL
1	A	99	LEU
1	A	100	ILE
1	A	105	MET
1	A	110	THR
1	A	118	ARG
1	A	121	PRO
1	A	122	ARG
1	A	125	TYR
1	A	132	HIS
1	A	138	ASN
1	A	141	ILE
1	A	143	VAL
1	A	144	SER
1	A	154	LEU
1	A	159	TRP
1	A	161	TRP
1	A	164	CYS
1	A	166	LEU
1	A	167	PHE
1	A	168	LEU
1	A	175	VAL
1	A	179	MET
1	A	182	TRP
1	A	186	THR
1	A	187	ARG

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Mol	Chain	Res	Type
1	A	194	THR
1	A	195	ARG
1	A	201	LYS
1	A	202	THR
1	A	203	LEU
1	A	206	ASN
1	A	243	MET
1	A	250	ILE
1	A	252	PRO
1	A	265	ARG
1	A	266	PRO
1	A	267	ASN
1	A	268	LYS
1	A	275	TRP
1	A	282	LEU
1	A	283	LEU
1	A	287	LEU
1	A	290	ILE
1	A	291	PRO
1	A	296	VAL
1	A	297	MET
1	A	310	PHE
1	A	334	THR
1	A	338	LEU
1	A	344	ASN
1	A	353	LEU
1	A	360	THR
1	A	365	LEU
1	A	376	ILE
1	B	10	LEU
1	B	15	LEU
1	B	19	VAL
1	B	21	GLN
1	B	22	MET
1	B	26	ILE
1	B	27	TYR
1	B	38	LEU
1	B	42	GLU
1	B	54	LEU
1	B	60	GLN
1	B	65	PRO
1	B	73	ARG

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Mol	Chain	Res	Type
1	B	77	LEU
1	B	84	MET
1	B	87	THR
1	B	89	VAL
1	B	91	VAL
1	B	99	LEU
1	B	100	ILE
1	B	105	MET
1	B	110	THR
1	B	118	ARG
1	B	121	PRO
1	B	122	ARG
1	B	125	TYR
1	B	132	HIS
1	B	138	ASN
1	B	141	ILE
1	B	143	VAL
1	B	144	SER
1	B	154	LEU
1	B	159	TRP
1	B	161	TRP
1	B	164	CYS
1	B	166	LEU
1	B	167	PHE
1	B	168	LEU
1	B	175	VAL
1	B	179	MET
1	B	182	TRP
1	B	186	THR
1	B	187	ARG
1	B	194	THR
1	B	195	ARG
1	B	201	LYS
1	B	202	THR
1	B	203	LEU
1	B	206	ASN
1	B	243	MET
1	B	250	ILE
1	B	252	PRO
1	B	265	ARG
1	B	266	PRO
1	B	267	ASN

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Mol	Chain	Res	Type
1	B	268	LYS
1	B	275	TRP
1	B	282	LEU
1	B	283	LEU
1	B	287	LEU
1	B	290	ILE
1	B	291	PRO
1	B	296	VAL
1	B	297	MET
1	B	310	PHE
1	B	334	THR
1	B	338	LEU
1	B	344	ASN
1	B	353	LEU
1	B	360	THR
1	B	365	LEU
1	B	376	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	106	GLN
1	A	206	ASN
1	A	298	ASN
1	B	60	GLN
1	B	106	GLN
1	B	206	ASN
1	B	298	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	375/375 (100%)	0.80	41 (10%)	10 7	80, 80, 80, 80	0
1	B	375/375 (100%)	0.84	51 (13%)	7 5	80, 80, 80, 80	0
All	All	750/750 (100%)	0.82	92 (12%)	8 6	80, 80, 80, 80	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	THR	6.3
1	A	300	TRP	5.3
1	A	27	TYR	4.9
1	A	52	TYR	4.6
1	A	115	VAL	4.3
1	A	311	PHE	4.2
1	A	315	MET	4.0
1	B	27	TYR	3.9
1	B	304	VAL	3.9
1	A	312	GLY	3.9
1	B	48	VAL	3.8
1	B	134	ASN	3.8
1	B	86	ALA	3.8
1	B	31	ILE	3.7
1	A	239	GLY	3.7
1	A	60	GLN	3.5
1	B	80	MET	3.5
1	A	352	SER	3.5
1	B	161	TRP	3.5
1	B	60	GLN	3.4
1	A	366	GLY	3.4
1	A	369	MET	3.2
1	B	303	LEU	3.2
1	A	136	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	56	TYR	3.1
1	B	79	GLY	3.1
1	A	118	ARG	3.1
1	A	111	GLY	3.1
1	A	209	PHE	3.0
1	A	24	GLN	2.9
1	B	118	ARG	2.9
1	A	303	LEU	2.9
1	B	19	VAL	2.9
1	B	144	SER	2.9
1	B	104	ALA	2.9
1	B	113	GLY	2.9
1	B	133	ALA	2.8
1	B	165	TYR	2.8
1	A	276	GLN	2.8
1	A	353	LEU	2.8
1	B	147	LEU	2.7
1	A	108	MET	2.7
1	B	119	THR	2.7
1	B	169	LEU	2.7
1	B	106	GLN	2.7
1	B	150	LEU	2.7
1	B	70	VAL	2.6
1	B	352	SER	2.6
1	B	107	GLY	2.6
1	B	300	TRP	2.5
1	A	297	MET	2.5
1	A	310	PHE	2.5
1	B	66	ILE	2.5
1	B	316	LEU	2.5
1	A	313	ALA	2.5
1	B	30	ALA	2.5
1	B	75	VAL	2.5
1	A	314	GLY	2.5
1	B	311	PHE	2.4
1	A	268	LYS	2.4
1	B	239	GLY	2.4
1	B	173	ALA	2.4
1	A	365	LEU	2.4
1	B	101	ALA	2.4
1	B	109	GLY	2.4
1	A	306	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	251	LEU	2.3
1	B	52	TYR	2.3
1	A	13	LEU	2.3
1	B	71	GLY	2.3
1	A	80	MET	2.3
1	A	105	MET	2.3
1	B	180	ALA	2.3
1	B	102	ALA	2.2
1	A	56	TYR	2.2
1	B	21	GLN	2.2
1	B	108	MET	2.2
1	B	28	ILE	2.2
1	B	328	PHE	2.2
1	B	307	ALA	2.2
1	B	315	MET	2.2
1	B	17	VAL	2.2
1	A	250	ILE	2.2
1	A	272	THR	2.2
1	A	106	GLN	2.1
1	A	104	ALA	2.1
1	A	21	GLN	2.1
1	B	112	VAL	2.1
1	B	170	VAL	2.1
1	A	70	VAL	2.1
1	A	48	VAL	2.0
1	B	367	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.