



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:22 AM UTC

PDB ID : 1QDU / pdb_00001qdu
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF CASPASE-8 WITH THE
TRIPEPTIDE KETONE INHIBITOR ZEVD-DCBMK
Authors : Blanchard, H.; Grutter, M.G.
Deposited on : 1999-07-10
Resolution : 2.80 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

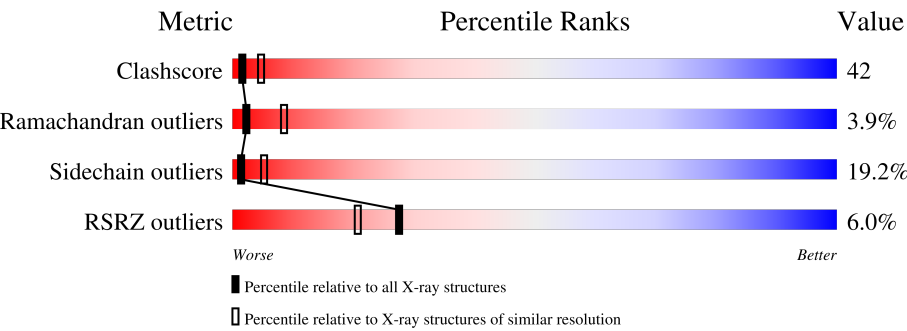
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	153	 6% 38% 41% 20% .
1	C	153	 5% 39% 46% 14% .
1	E	153	 7% 46% 37% 15% .
1	G	153	 8% 39% 44% 14% .
1	I	153	 7% 40% 41% 15% 5%
1	K	153	 5% 39% 48% 12% .
2	B	88	 5% 31% 47% 18% 5%

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Mol	Chain	Length	Quality of chain
2	D	88	
2	F	88	
2	H	88	
2	J	88	
2	L	88	
3	T	5	
3	U	5	
3	V	5	
3	W	5	
3	X	5	
3	Y	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11948 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 CASPASE-8 ALPHA-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	C	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	E	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	G	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	I	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	K	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	HIS	ASP	conflict	UNP Q14790
C	204	HIS	ASP	conflict	UNP Q14790
E	204	HIS	ASP	conflict	UNP Q14790
G	204	HIS	ASP	conflict	UNP Q14790
I	204	HIS	ASP	conflict	UNP Q14790
K	204	HIS	ASP	conflict	UNP Q14790

- Molecule 2 is a protein called CASPASE-8 BETA-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			712	447	123	136	6			
2	D	88	Total	C	N	O	S	0	0	0
			712	447	123	136	6			
2	F	88	Total	C	N	O	S	0	0	0
			712	447	123	136	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	88	Total	C	N	O	S	0	0	0
			712	447	123	136	6			
2	J	88	Total	C	N	O	S	0	0	0
			712	447	123	136	6			
2	L	88	Total	C	N	O	S	0	0	0
			712	447	123	136	6			

- Molecule 3 is a protein called PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	T	5	Total	C	N	O	8	0	1
			35	23	3	9			
3	U	5	Total	C	N	O	8	0	1
			35	23	3	9			
3	V	5	Total	C	N	O	8	0	1
			35	23	3	9			
3	W	5	Total	C	N	O	8	0	1
			35	23	3	9			
3	X	5	Total	C	N	O	8	0	1
			35	23	3	9			
3	Y	5	Total	C	N	O	8	0	1
			35	23	3	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	10	Total	O	0	0
			10	10		
4	C	16	Total	O	0	0
			16	16		
4	D	12	Total	O	0	0
			12	12		
4	E	15	Total	O	0	0
			15	15		
4	F	8	Total	O	0	0
			8	8		
4	V	3	Total	O	0	0
			3	3		
4	G	11	Total	O	0	0
			11	11		

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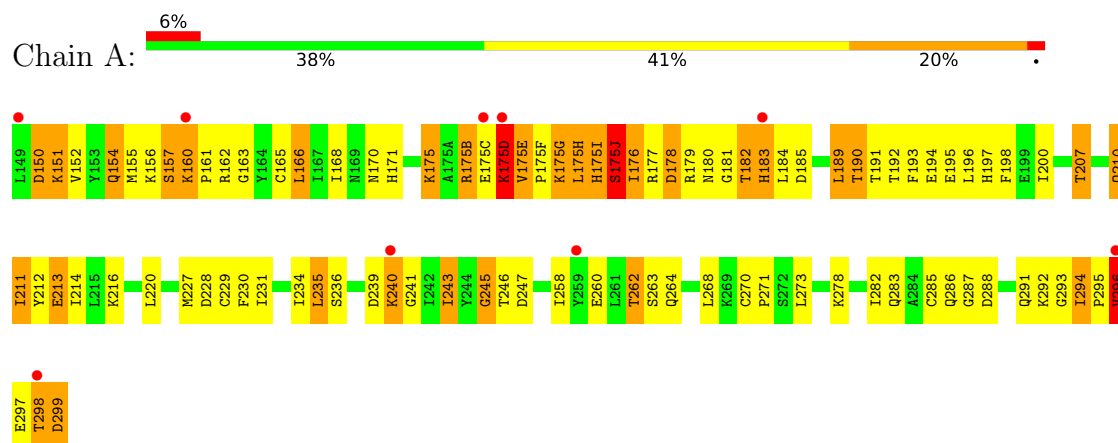
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	6	Total 6	O 6	0	0
4	I	6	Total 6	O 6	0	0
4	J	4	Total 4	O 4	0	0
4	K	20	Total 20	O 20	0	0
4	L	11	Total 11	O 11	0	0
4	Y	1	Total 1	O 1	0	0

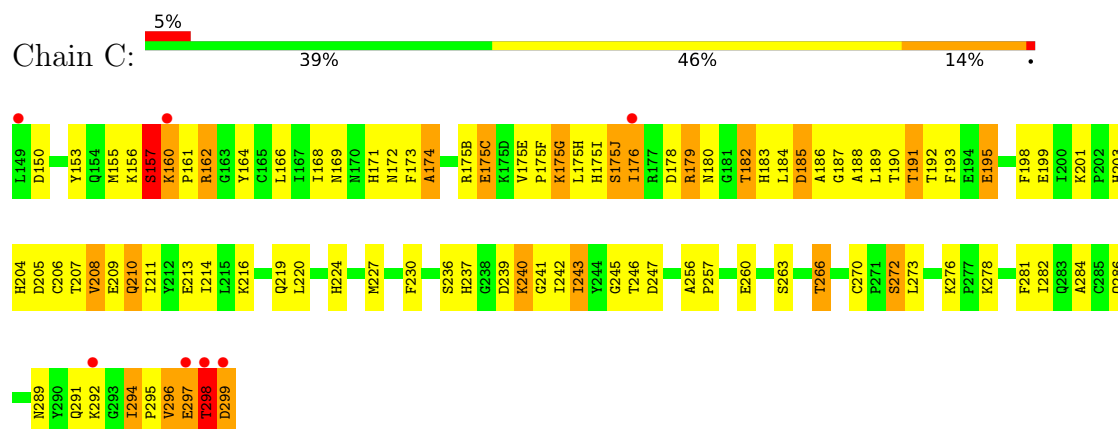
3 Residue-property plots [i](#)

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.

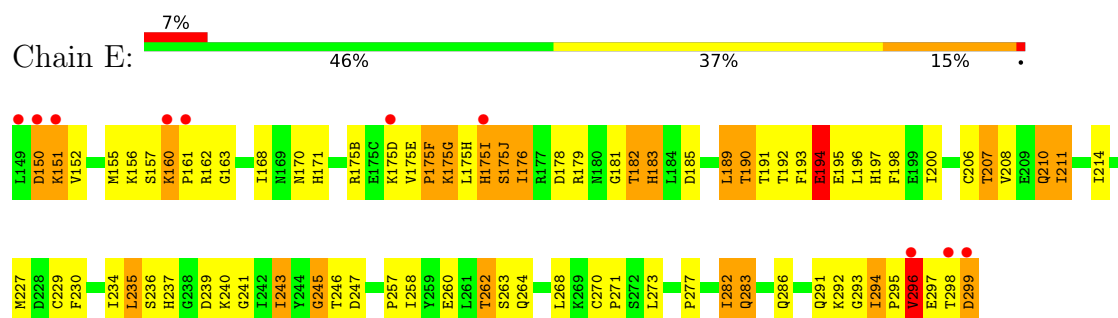
• Molecule 1: CASPASE-8 ALPHA-CHAIN



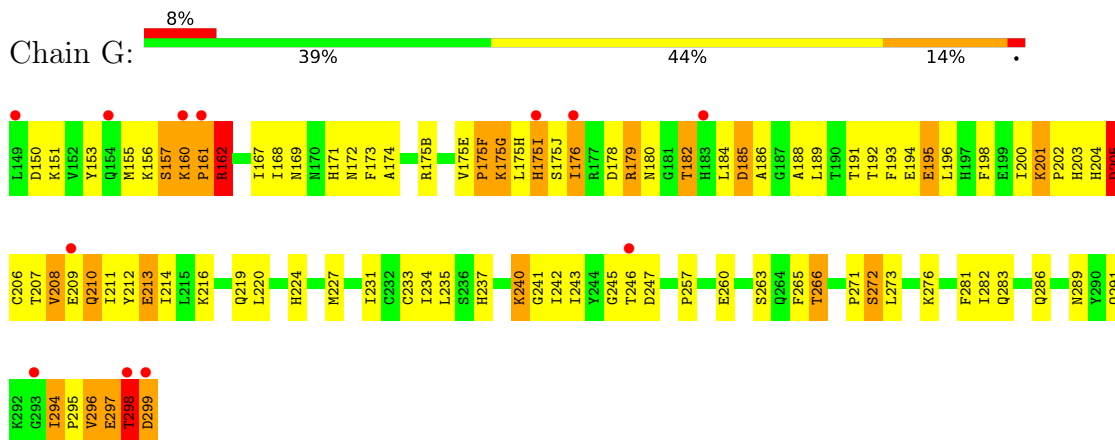
• Molecule 1: CASPASE-8 ALPHA-CHAIN



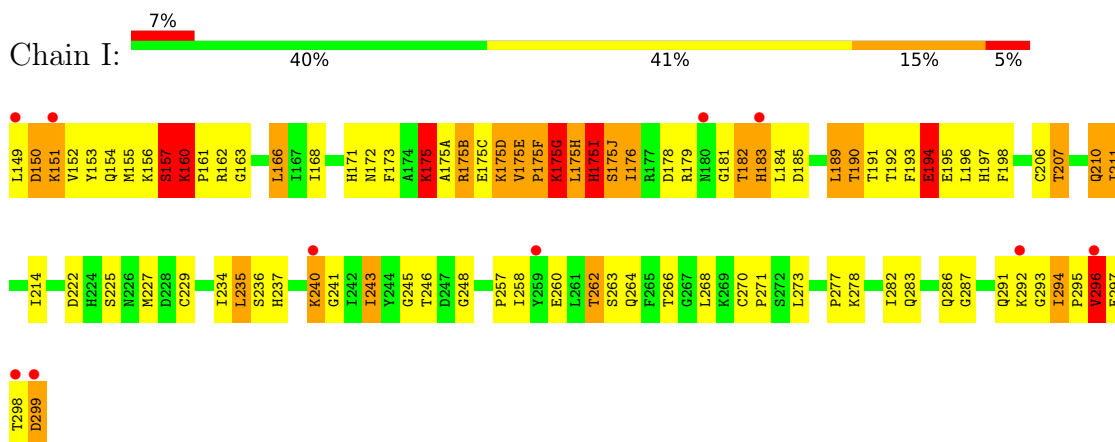
• Molecule 1: CASPASE-8 ALPHA-CHAIN



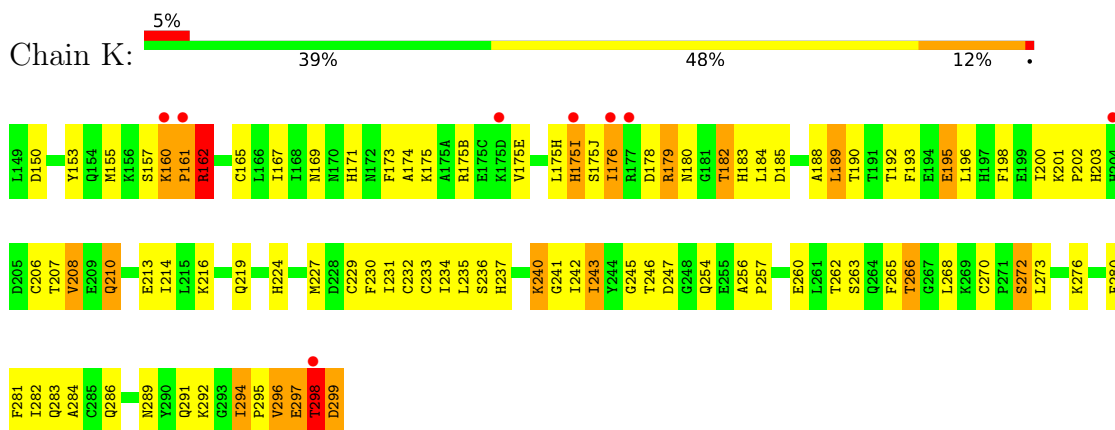
● Molecule 1: CASPASE-8 ALPHA-CHAIN



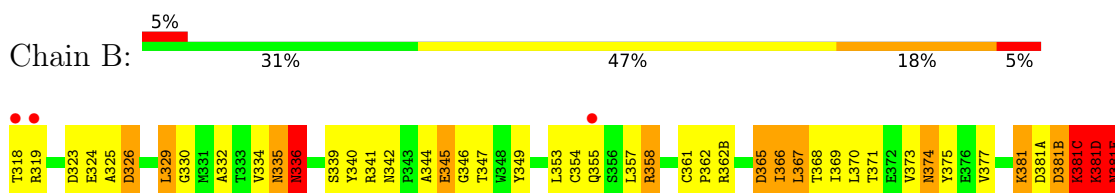
- Molecule 1: CASPASE-8 ALPHA-CHAIN



● Molecule 1: CASPASE-8 ALPHA-CHAIN

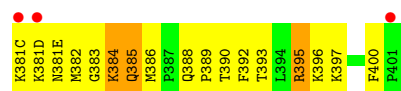


- Molecule 2: CASPASE-8 BETA-CHAIN

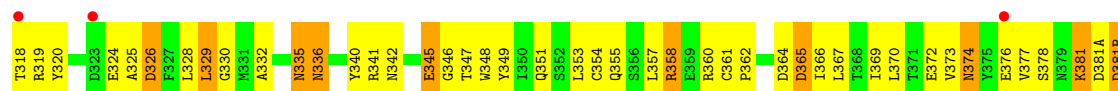




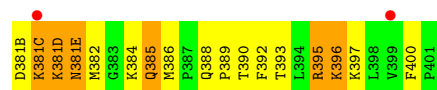
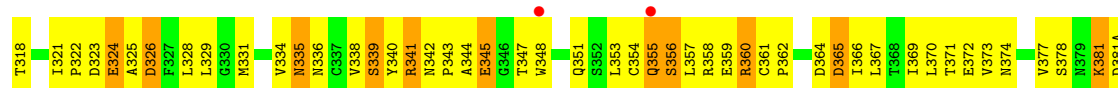
• Molecule 2: CASPASE-8 BETA-CHAIN



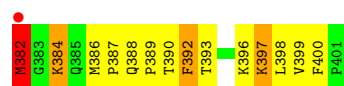
• Molecule 2: CASPASE-8 BETA-CHAIN



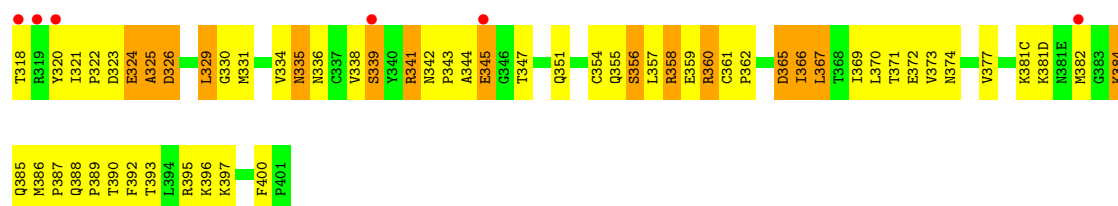
• Molecule 2: CASPASE-8 BETA-CHAIN



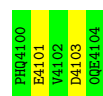
• Molecule 2: CASPASE-8 BETA-CHAIN



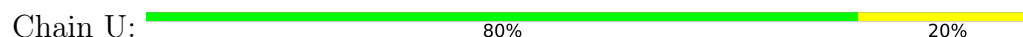
• Molecule 2: CASPASE-8 BETA-CHAIN



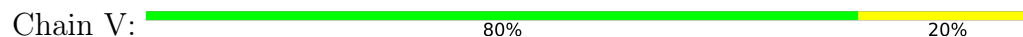
- Molecule 3: PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR



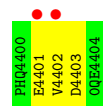
- Molecule 3: PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR



- Molecule 3: PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR



- Molecule 3: PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR



- Molecule 3: PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR



There are no outlier residues recorded for this chain.

- Molecule 3: PHQ-GLU-VAL-ASP-DICHLOROMETHYLKETONE INHIBITOR



PH4600
E4601
Y4602
D4603
Q4E4604

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 206.53Å 102.05Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80 100.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (100.00-2.80) 84.9 (100.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.302 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11948	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: 0QE, PHQ

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	0.67	0/1248	1.07	5/1682 (0.3%)
1	C	0.63	0/1248	1.00	8/1682 (0.5%)
1	E	0.66	0/1248	1.07	4/1682 (0.2%)
1	G	0.62	0/1248	0.99	8/1682 (0.5%)
1	I	0.63	0/1248	1.06	6/1682 (0.4%)
1	K	0.61	0/1248	1.00	3/1682 (0.2%)
2	B	0.65	0/726	1.05	6/981 (0.6%)
2	D	0.61	0/726	1.04	6/981 (0.6%)
2	F	0.58	0/726	1.04	5/981 (0.5%)
2	H	0.57	0/726	0.98	1/981 (0.1%)
2	J	0.57	0/726	1.04	5/981 (0.5%)
2	L	0.61	0/726	0.99	2/981 (0.2%)
3	T	1.86	0/23	1.75	0/30
3	U	1.97	0/23	1.68	0/30
3	V	2.05	0/23	1.77	0/30
3	W	2.02	0/23	1.75	0/30
3	X	2.06	0/23	1.76	0/30
3	Y	1.97	0/23	1.72	0/30
All	All	0.66	0/11982	1.04	59/16158 (0.4%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLU	N-CA-C	-7.47	102.74	111.03
2	L	392	PHE	N-CA-C	7.15	119.73	108.79
1	E	194	GLU	N-CA-C	-6.85	103.74	111.14
1	E	245	GLY	N-CA-C	-6.75	103.90	112.54
2	D	392	PHE	N-CA-C	6.64	118.29	108.60
1	K	245	GLY	N-CA-C	-6.63	102.18	112.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	326	ASP	N-CA-C	6.62	120.54	111.54
1	A	245	GLY	N-CA-C	-6.52	104.20	112.54
1	I	245	GLY	N-CA-C	-6.52	104.20	112.54
2	B	374	ASN	N-CA-C	-6.51	104.19	111.28
1	C	298	THR	N-CA-C	-6.46	97.85	108.12
1	G	245	GLY	N-CA-C	-6.46	102.45	112.85
1	C	245	GLY	N-CA-C	-6.43	101.50	112.30
1	G	298	THR	N-CA-C	-6.28	98.13	108.12
1	E	175(J)	SER	N-CA-C	6.28	120.98	112.88
2	F	326	ASP	N-CA-C	6.08	119.81	111.54
1	I	160	LYS	CA-C-N	-6.08	113.97	120.47
1	I	160	LYS	C-N-CA	-6.08	113.97	120.47
1	E	207	THR	N-CA-C	-6.06	102.68	110.19
1	K	298	THR	N-CA-C	-6.01	98.56	108.12
2	B	326	ASP	N-CA-C	6.01	119.85	111.74
2	J	392	PHE	N-CA-C	6.01	118.55	109.23
2	J	360	ARG	N-CA-C	5.93	120.57	112.68
2	F	335	ASN	N-CA-C	5.88	117.92	110.33
1	C	174	ALA	N-CA-C	-5.86	104.97	111.36
2	H	392	PHE	N-CA-C	5.83	117.71	108.79
1	A	178	ASP	N-CA-C	-5.82	102.29	110.50
1	G	201	LYS	CA-C-N	5.76	126.08	119.92
1	G	201	LYS	C-N-CA	5.76	126.08	119.92
1	C	185	ASP	N-CA-C	-5.74	104.72	110.97
1	I	175	LYS	N-CA-C	-5.71	104.75	110.97
2	J	335	ASN	N-CA-C	5.67	117.39	110.41
2	B	339	SER	N-CA-C	-5.64	100.59	109.50
1	A	207	THR	N-CA-C	-5.58	103.54	110.41
2	L	325	ALA	N-CA-C	5.55	117.49	110.33
2	B	388	GLN	N-CA-C	5.49	118.38	108.55
2	D	326	ASP	N-CA-C	5.48	119.00	111.54
2	F	374	ASN	N-CA-C	-5.47	105.31	111.28
1	G	194	GLU	N-CA-C	-5.47	105.22	111.07
1	G	185	ASP	N-CA-C	-5.45	105.03	110.97
2	F	340	TYR	N-CA-C	5.42	118.64	109.76
1	G	175(J)	SER	N-CA-C	5.42	119.87	112.88
2	J	324	GLU	N-CA-C	5.41	118.98	112.93
1	I	194	GLU	N-CA-C	-5.39	105.32	111.14
2	D	325	ALA	N-CA-C	5.36	117.24	110.33
1	C	175(C)	GLU	N-CA-C	5.32	117.99	111.82
2	B	335	ASN	N-CA-C	5.30	117.17	110.33
2	D	366	ILE	N-CA-C	5.30	116.02	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	392	PHE	N-CA-C	5.24	117.03	109.07
1	C	175(J)	SER	N-CA-C	5.24	119.63	112.88
1	A	175(J)	SER	N-CA-C	5.23	120.31	112.94
2	F	390	THR	N-CA-C	-5.19	100.23	109.06
1	K	185	ASP	N-CA-C	-5.19	105.31	110.97
1	I	207	THR	N-CA-C	-5.07	103.79	110.33
2	D	383	GLY	N-CA-C	5.04	121.12	112.51
1	G	265	PHE	N-CA-C	5.03	118.90	112.26
1	C	201	LYS	CA-C-N	5.03	125.01	120.03
1	C	201	LYS	C-N-CA	5.03	125.01	120.03
2	D	334	VAL	N-CA-C	-5.02	104.53	110.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1220	0	1198	114	0
1	C	1220	0	1198	112	0
1	E	1220	0	1198	105	0
1	G	1220	0	1198	124	0
1	I	1220	0	1198	106	0
1	K	1220	0	1198	115	0
2	B	712	0	707	88	0
2	D	712	0	707	82	0
2	F	712	0	707	81	0
2	H	712	0	707	80	0
2	J	712	0	707	78	0
2	L	712	0	707	81	0
3	T	35	0	25	3	0
3	U	35	0	25	1	0
3	V	35	0	25	2	0
3	W	35	0	25	3	0
3	X	35	0	25	0	0
3	Y	35	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	0	0	5	0
4	B	10	0	0	1	0
4	C	16	0	0	5	0
4	D	12	0	0	3	0
4	E	15	0	0	6	0
4	F	8	0	0	1	0
4	G	11	0	0	3	0
4	H	6	0	0	3	0
4	I	6	0	0	1	0
4	J	4	0	0	1	0
4	K	20	0	0	6	0
4	L	11	0	0	4	0
4	V	3	0	0	0	0
4	Y	1	0	0	0	0
All	All	11948	0	11580	977	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 42.

All (977) 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:E:207:THR:H	1:E:210:GLN:NE2	1.46	1.12
1:I:207:THR:H	1:I:210:GLN:NE2	1.45	1.11
2:F:318:THR:HA	1:G:297:GLU:HB2	1.30	1.10
2:J:318:THR:HA	1:K:297:GLU:HB2	1.32	1.07
2:B:318:THR:HA	1:C:297:GLU:HB2	1.31	1.07
1:C:160:LYS:HB2	1:C:161:PRO:HD3	1.30	1.06
1:G:160:LYS:HB2	1:G:161:PRO:HD3	1.33	1.06
1:K:160:LYS:HB2	1:K:161:PRO:HD3	1.36	1.05
1:A:207:THR:H	1:A:210:GLN:NE2	1.54	1.03
2:D:341:ARG:HB2	2:D:347:THR:HG22	1.39	1.03
4:E:93:HOH:O	2:F:349:TYR:HB3	1.60	1.02
2:H:341:ARG:HB2	2:H:347:THR:HG22	1.40	1.00
1:I:207:THR:H	1:I:210:GLN:HE21	1.12	0.97
2:L:341:ARG:HB2	2:L:347:THR:HG22	1.42	0.97
2:D:360:ARG:HH11	2:D:360:ARG:HB3	1.29	0.97
1:A:207:THR:H	1:A:210:GLN:HE21	1.12	0.93
2:F:386:MET:HE2	2:H:393:THR:HG23	1.51	0.92
2:F:393:THR:HG23	2:H:386:MET:HE2	1.51	0.92
2:H:360:ARG:HH11	2:H:360:ARG:HB3	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:LYS:HB2	2:H:323:ASP:HB2	1.50	0.91
1:E:207:THR:H	1:E:210:GLN:HE21	1.17	0.90
2:B:393:THR:HG23	2:D:386:MET:HE2	1.55	0.87
1:C:160:LYS:HB2	1:C:161:PRO:CD	2.04	0.87
1:E:179:ARG:HH12	1:E:182:THR:CG2	1.87	0.87
1:K:175(H):LEU:O	1:K:176:ILE:HG13	1.77	0.85
2:F:329:LEU:HD12	2:F:330:GLY:N	1.92	0.85
1:I:179:ARG:HH12	1:I:182:THR:HG21	1.41	0.85
1:I:292:LYS:HB2	2:L:323:ASP:HB2	1.57	0.85
1:I:179:ARG:HH12	1:I:182:THR:CG2	1.90	0.85
2:F:318:THR:HA	1:G:297:GLU:CB	2.08	0.84
1:A:292:LYS:HB2	2:D:323:ASP:HB2	1.59	0.83
2:F:396:LYS:NZ	1:G:299:ASP:HA	1.95	0.82
1:I:175(E):VAL:HG11	1:I:175(H):LEU:HG	1.61	0.82
2:B:318:THR:HA	1:C:297:GLU:CB	2.09	0.82
1:I:207:THR:N	1:I:210:GLN:HE21	1.77	0.82
1:E:151:LYS:HG3	2:F:396:LYS:HD3	1.61	0.81
1:E:207:THR:N	1:E:210:GLN:NE2	2.28	0.81
1:G:160:LYS:HB2	1:G:161:PRO:CD	2.10	0.81
2:D:370:LEU:HD22	4:D:42:HOH:O	1.81	0.81
2:L:360:ARG:HH11	2:L:360:ARG:HB3	1.42	0.80
1:E:207:THR:N	1:E:210:GLN:HE21	1.80	0.80
2:J:381:LYS:O	2:J:384:LYS:HE2	1.82	0.80
2:J:318:THR:HA	1:K:297:GLU:CB	2.10	0.79
1:E:179:ARG:HH12	1:E:182:THR:HG21	1.45	0.79
2:J:396:LYS:HZ3	1:K:299:ASP:HA	1.48	0.79
1:A:234:ILE:C	1:A:235:LEU:HD23	2.08	0.79
1:A:295:PRO:O	1:A:296:VAL:HG13	1.83	0.78
1:C:175(H):LEU:O	1:C:176:ILE:HG13	1.85	0.77
2:D:325:ALA:HA	2:D:393:THR:CG2	2.13	0.77
1:I:297:GLU:HB2	2:L:318:THR:HA	1.66	0.77
2:B:381(E):ASN:ND2	2:B:381(E):ASN:H	1.81	0.77
2:J:388:GLN:HE21	2:L:390:THR:HG21	1.50	0.77
2:J:386:MET:HE2	2:L:393:THR:HG23	1.66	0.76
1:I:207:THR:N	1:I:210:GLN:NE2	2.28	0.76
2:J:324:GLU:O	2:J:393:THR:HG21	1.86	0.76
1:A:297:GLU:HB2	2:D:318:THR:HA	1.66	0.76
1:C:207:THR:HG23	1:C:210:GLN:HE22	1.52	0.75
2:F:341:ARG:NH1	3:V:4303:ASP:OD1	2.19	0.75
1:E:295:PRO:O	1:E:296:VAL:HG13	1.87	0.75
1:I:295:PRO:O	1:I:296:VAL:HG13	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:385:GLN:HA	4:F:90:HOH:O	1.85	0.75
2:H:341:ARG:O	2:H:341:ARG:HG2	1.87	0.75
1:E:168:ILE:HD13	1:E:211:ILE:HG23	1.68	0.74
1:K:160:LYS:HB2	1:K:161:PRO:CD	2.14	0.74
2:D:325:ALA:HA	2:D:393:THR:HG21	1.68	0.73
1:A:179:ARG:HH12	1:A:182:THR:CG2	2.01	0.73
2:D:393:THR:HG22	2:D:393:THR:O	1.87	0.73
1:K:174:ALA:HA	1:K:175(B):ARG:NH1	2.04	0.73
2:D:371:THR:O	2:D:374:ASN:HB2	1.89	0.73
1:A:175:LYS:HB3	1:A:247:ASP:HA	1.70	0.73
1:E:297:GLU:HB2	2:H:318:THR:HA	1.69	0.73
1:A:207:THR:N	1:A:210:GLN:HE21	1.84	0.73
1:G:175(B):ARG:HG2	1:G:175(I):HIS:O	1.89	0.73
2:J:396:LYS:NZ	1:K:299:ASP:HA	2.04	0.73
1:G:227:MET:O	1:G:276:LYS:HE2	1.90	0.72
1:C:175(E):VAL:HG11	1:C:175(H):LEU:HD12	1.72	0.72
1:A:151:LYS:HG3	2:B:396:LYS:HD3	1.72	0.71
2:F:388:GLN:HE21	2:H:390:THR:HG21	1.56	0.71
2:J:324:GLU:HB2	1:K:291:GLN:HE22	1.55	0.71
1:I:175(E):VAL:CG1	1:I:175(H):LEU:HG	2.19	0.71
2:B:324:GLU:HB2	1:C:291:GLN:HE22	1.56	0.71
1:E:189:LEU:HD13	2:F:354:CYS:SG	2.30	0.71
1:I:151:LYS:HD2	1:I:152:VAL:H	1.55	0.71
1:C:203:HIS:HE1	4:C:40:HOH:O	1.73	0.71
2:J:373:VAL:O	2:J:377:VAL:HG23	1.90	0.71
1:C:188:ALA:O	1:C:192:THR:HG23	1.90	0.71
1:G:155:MET:HE2	2:H:400:PHE:HD2	1.56	0.71
2:B:342:ASN:ND2	2:B:345:GLU:HG2	2.06	0.70
1:C:175(B):ARG:NH2	1:C:178:ASP:OD1	2.24	0.70
2:F:396:LYS:HZ3	1:G:299:ASP:HA	1.55	0.70
2:J:393:THR:HG23	2:L:386:MET:HE2	1.71	0.70
2:B:329:LEU:HD12	2:B:330:GLY:N	2.07	0.70
1:G:175(H):LEU:O	1:G:176:ILE:HG13	1.91	0.70
2:L:393:THR:HG22	2:L:393:THR:O	1.92	0.70
1:A:151:LYS:HD2	1:A:152:VAL:H	1.57	0.69
4:E:132:HOH:O	1:G:151:LYS:HD2	1.91	0.69
1:G:176:ILE:HD12	1:G:176:ILE:O	1.92	0.69
2:F:386:MET:CE	2:H:393:THR:HG23	2.22	0.69
2:B:396:LYS:HZ3	1:C:299:ASP:HA	1.57	0.69
1:C:278:LYS:HE3	4:C:59:HOH:O	1.92	0.69
1:I:175(H):LEU:O	1:I:176:ILE:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:O	1:A:235:LEU:HD23	1.93	0.69
1:C:240:LYS:HD3	2:D:336:ASN:ND2	2.07	0.69
1:E:234:ILE:C	1:E:235:LEU:HD23	2.16	0.69
2:F:342:ASN:ND2	2:F:345:GLU:HG2	2.07	0.69
2:F:381:LYS:O	2:F:384:LYS:HE2	1.92	0.69
1:G:155:MET:HE2	2:H:400:PHE:CD2	2.28	0.69
2:L:324:GLU:HG2	4:L:63:HOH:O	1.93	0.68
1:G:282:ILE:HD13	2:H:329:LEU:HD11	1.74	0.68
1:E:175(B):ARG:HH22	1:E:178:ASP:CG	2.01	0.68
2:B:388:GLN:HE21	2:D:390:THR:HG21	1.58	0.68
1:I:207:THR:H	1:I:210:GLN:HE22	1.40	0.68
1:C:176:ILE:HD12	1:C:176:ILE:O	1.93	0.68
1:G:173:PHE:HB3	1:G:176:ILE:HD13	1.76	0.68
2:B:396:LYS:NZ	1:C:299:ASP:HA	2.09	0.68
2:J:342:ASN:ND2	2:J:345:GLU:HG2	2.08	0.68
1:C:155:MET:HE3	1:C:162:ARG:HD2	1.76	0.67
1:E:175(E):VAL:HG11	1:E:175(H):LEU:HG	1.74	0.67
1:E:160:LYS:HG3	1:E:161:PRO:HD3	1.76	0.67
2:H:356:SER:O	2:H:360:ARG:HG2	1.94	0.67
2:B:386:MET:SD	2:D:393:THR:HG23	2.34	0.67
1:G:175(E):VAL:CG2	1:G:175(H):LEU:HG	2.24	0.67
1:K:227:MET:O	1:K:276:LYS:HE2	1.93	0.67
2:D:365:ASP:O	2:D:369:ILE:HD12	1.95	0.67
1:I:160:LYS:HG3	1:I:161:PRO:HD3	1.75	0.67
2:J:329:LEU:HD12	2:J:330:GLY:N	2.09	0.67
1:K:273:LEU:HA	1:K:276:LYS:HD2	1.75	0.67
1:A:160:LYS:HG3	1:A:161:PRO:HD3	1.77	0.67
1:A:181:GLY:H	1:A:183:HIS:CE1	2.13	0.67
1:G:175(B):ARG:NH2	1:G:178:ASP:OD1	2.28	0.67
1:E:170:ASN:HB2	1:E:236:SER:HB2	1.77	0.66
1:E:175(B):ARG:HG3	1:E:176:ILE:HD12	1.76	0.66
1:I:207:THR:HG23	1:I:210:GLN:NE2	2.09	0.66
1:G:188:ALA:O	1:G:192:THR:HG23	1.95	0.66
1:K:175(B):ARG:NH2	1:K:178:ASP:OD1	2.28	0.66
2:H:393:THR:O	2:H:393:THR:HG22	1.95	0.66
2:B:381(E):ASN:H	2:B:381(E):ASN:HD22	1.43	0.66
1:E:175(B):ARG:HG3	1:E:176:ILE:CD1	2.25	0.66
2:L:341:ARG:NH1	3:Y:4603:ASP:OD1	2.29	0.66
1:C:203:HIS:CE1	4:C:40:HOH:O	2.46	0.66
2:H:365:ASP:HB2	2:H:397:LYS:HD2	1.78	0.66
2:L:325:ALA:HA	2:L:393:THR:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLU:HA	1:C:260:GLU:OE1	1.95	0.66
2:B:386:MET:HE2	2:D:393:THR:HG23	1.78	0.65
2:F:332:ALA:HB2	2:F:349:TYR:CD2	2.31	0.65
1:K:179:ARG:HD2	1:K:237:HIS:CE1	2.31	0.65
1:A:175(B):ARG:HG3	1:A:176:ILE:HD12	1.78	0.65
1:E:151:LYS:HD2	1:E:152:VAL:H	1.60	0.65
2:L:356:SER:O	2:L:360:ARG:HG2	1.97	0.65
1:G:169:ASN:HD22	1:G:186:ALA:HB2	1.61	0.65
2:F:393:THR:HG22	2:F:393:THR:O	1.97	0.65
2:D:341:ARG:O	2:D:341:ARG:HG2	1.96	0.65
1:E:271:PRO:HB3	4:E:89:HOH:O	1.96	0.65
1:K:175(E):VAL:HG11	1:K:175(H):LEU:HD12	1.79	0.65
1:I:168:ILE:HD13	1:I:211:ILE:HG23	1.78	0.65
1:K:184:LEU:N	1:K:184:LEU:HD12	2.12	0.65
2:F:354:CYS:HA	2:F:357:LEU:HD12	1.78	0.64
2:J:354:CYS:HA	2:J:357:LEU:HD12	1.79	0.64
1:E:163:GLY:HA3	1:E:229:CYS:O	1.97	0.64
1:G:175(E):VAL:HG11	1:G:175(H):LEU:HD12	1.79	0.64
1:A:297:GLU:HB2	2:D:318:THR:CA	2.27	0.64
1:E:207:THR:H	1:E:210:GLN:HE22	1.42	0.64
1:G:155:MET:HE3	1:G:162:ARG:HD2	1.80	0.64
2:J:386:MET:CE	2:L:393:THR:HG23	2.28	0.64
1:C:227:MET:O	1:C:276:LYS:HE2	1.97	0.64
1:E:268:LEU:O	1:E:271:PRO:HD3	1.98	0.64
1:K:232:CYS:HB2	4:K:126:HOH:O	1.96	0.64
1:A:175(H):LEU:O	1:A:176:ILE:HG13	1.98	0.64
2:F:325:ALA:HA	2:F:393:THR:CG2	2.28	0.64
2:F:324:GLU:H	1:G:291:GLN:HE21	1.46	0.64
1:C:207:THR:CG2	1:C:210:GLN:HE22	2.11	0.63
1:K:231:ILE:C	4:K:126:HOH:O	2.41	0.63
2:H:325:ALA:HA	2:H:393:THR:CG2	2.29	0.63
2:D:331:MET:HB2	2:D:388:GLN:O	1.99	0.63
2:F:324:GLU:O	2:F:393:THR:HG21	1.98	0.63
2:J:324:GLU:HB2	1:K:291:GLN:NE2	2.13	0.63
2:H:339:SER:O	3:W:4402:VAL:HA	1.99	0.63
1:K:263:SER:O	1:K:266:THR:HG23	1.99	0.63
1:A:293:GLY:HA3	2:B:384:LYS:HG3	1.80	0.62
1:I:151:LYS:HG3	2:J:396:LYS:HD3	1.80	0.62
2:D:356:SER:O	2:D:360:ARG:HG2	1.99	0.62
2:H:360:ARG:NH1	2:H:364:ASP:OD2	2.32	0.62
1:I:258:ILE:HD12	1:I:282:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:206:CYS:HB3	1:K:210:GLN:HB3	1.81	0.62
1:I:207:THR:HG23	1:I:210:GLN:HE22	1.63	0.62
1:G:179:ARG:HD2	1:G:237:HIS:CE1	2.34	0.62
2:L:341:ARG:O	2:L:341:ARG:HG2	2.00	0.62
1:E:175(H):LEU:O	1:E:176:ILE:HG13	1.99	0.62
1:E:155:MET:HE2	2:F:400:PHE:HD2	1.65	0.62
1:G:207:THR:HG23	1:G:210:GLN:HE22	1.64	0.62
1:K:169:ASN:HD21	1:K:182:THR:HB	1.65	0.61
1:C:263:SER:O	1:C:266:THR:HG23	1.99	0.61
2:J:341:ARG:HG3	2:J:347:THR:HG22	1.81	0.61
1:A:196:LEU:HD22	2:B:400:PHE:HB3	1.81	0.61
1:I:155:MET:HE2	2:J:400:PHE:HD2	1.63	0.61
2:J:386:MET:SD	2:L:393:THR:HG23	2.40	0.61
1:K:184:LEU:HD12	1:K:184:LEU:H	1.64	0.61
2:B:332:ALA:HB2	2:B:349:TYR:CD2	2.35	0.61
2:B:373:VAL:O	2:B:377:VAL:HG23	2.01	0.61
2:F:324:GLU:H	1:G:291:GLN:NE2	1.99	0.61
1:I:297:GLU:HB2	2:L:318:THR:CA	2.29	0.61
1:A:189:LEU:HD13	2:B:354:CYS:SG	2.40	0.61
1:C:155:MET:HE3	1:C:162:ARG:CD	2.31	0.61
2:F:388:GLN:HE21	2:H:390:THR:CG2	2.13	0.61
1:I:278:LYS:NZ	4:I:133:HOH:O	2.26	0.61
1:C:155:MET:HE2	2:D:400:PHE:HD1	1.64	0.60
2:D:360:ARG:HB3	2:D:360:ARG:NH1	2.10	0.60
1:G:200:ILE:HG22	1:G:202:PRO:HD3	1.82	0.60
2:B:386:MET:CE	2:D:393:THR:HG23	2.30	0.60
1:E:196:LEU:HD22	2:F:400:PHE:HB3	1.83	0.60
2:L:325:ALA:HA	2:L:393:THR:HG21	1.83	0.60
2:L:356:SER:HB3	2:L:369:ILE:HG23	1.82	0.60
2:D:393:THR:CG2	2:D:393:THR:O	2.48	0.60
2:F:318:THR:CA	1:G:297:GLU:HB2	2.20	0.60
2:F:324:GLU:HB2	1:G:291:GLN:HE22	1.66	0.60
1:C:179:ARG:HD2	1:C:237:HIS:CE1	2.36	0.60
1:K:155:MET:HE2	2:L:400:PHE:HD2	1.65	0.60
1:A:278:LYS:HE3	4:A:24:HOH:O	2.00	0.60
1:C:207:THR:HG23	1:C:210:GLN:NE2	2.15	0.60
1:I:155:MET:HE2	2:J:400:PHE:CD2	2.36	0.60
1:C:210:GLN:O	1:C:214:ILE:HG13	2.02	0.60
2:B:324:GLU:O	2:B:393:THR:HG21	2.01	0.60
1:E:297:GLU:HB2	2:H:318:THR:CA	2.31	0.60
2:H:371:THR:O	2:H:374:ASN:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:268:LEU:O	1:I:271:PRO:HD3	2.02	0.60
1:K:224:HIS:H	1:K:272:SER:HB2	1.67	0.60
2:B:381(E):ASN:O	2:B:382:MET:C	2.45	0.60
1:A:179:ARG:HH12	1:A:182:THR:HG21	1.64	0.60
1:C:175(B):ARG:HG2	1:C:175(I):HIS:O	2.01	0.60
1:I:191:THR:O	1:I:195:GLU:HG3	2.01	0.59
1:A:168:ILE:HD13	1:A:211:ILE:HG23	1.84	0.59
2:L:331:MET:HB2	2:L:388:GLN:O	2.02	0.59
2:F:373:VAL:O	2:F:377:VAL:HG23	2.02	0.59
1:A:155:MET:HE2	2:B:400:PHE:HD1	1.67	0.59
2:D:373:VAL:O	2:D:377:VAL:HG23	2.02	0.59
2:F:381(E):ASN:H	2:F:381(E):ASN:ND2	2.00	0.59
2:H:356:SER:HB3	2:H:369:ILE:HG23	1.84	0.59
2:H:357:LEU:O	2:H:361:CYS:HB2	2.01	0.59
2:J:388:GLN:HE21	2:L:390:THR:CG2	2.13	0.59
1:E:291:GLN:HB3	2:F:384:LYS:O	2.02	0.59
1:E:293:GLY:HA2	2:H:321:ILE:O	2.01	0.59
1:K:257:PRO:HB2	1:K:260:GLU:HG2	1.85	0.59
1:C:207:THR:HB	1:C:247:ASP:OD2	2.01	0.59
2:B:318:THR:CA	1:C:297:GLU:HB2	2.21	0.59
1:C:169:ASN:HD21	1:C:182:THR:HB	1.68	0.59
1:C:207:THR:OG1	1:C:210:GLN:NE2	2.36	0.59
2:F:360:ARG:HD2	2:F:364:ASP:OD2	2.03	0.59
1:G:172:ASN:HB3	1:G:205:ASP:OD2	2.02	0.59
2:H:341:ARG:HA	2:H:347:THR:HA	1.85	0.59
1:I:182:THR:O	1:I:183:HIS:C	2.46	0.59
1:I:283:GLN:HE21	2:J:347:THR:CB	2.16	0.59
1:G:241:GLY:H	1:G:286:GLN:NE2	2.00	0.59
2:B:341:ARG:CB	2:B:347:THR:HG22	2.32	0.58
2:D:360:ARG:NH1	2:D:364:ASP:OD2	2.36	0.58
1:E:182:THR:O	1:E:183:HIS:C	2.46	0.58
2:F:392:PHE:CZ	2:H:389:PRO:HG2	2.38	0.58
1:A:291:GLN:HB3	2:B:384:LYS:O	2.02	0.58
1:E:175(F):PRO:HG2	1:E:175(G):LYS:H	1.67	0.58
1:K:155:MET:HE3	1:K:162:ARG:CD	2.34	0.58
1:E:162:ARG:HG3	1:E:197:HIS:O	2.04	0.58
1:E:207:THR:HG23	1:E:210:GLN:NE2	2.18	0.58
1:E:295:PRO:C	1:E:296:VAL:HG22	2.28	0.58
2:J:381(E):ASN:O	2:J:382:MET:C	2.45	0.58
2:L:359:GLU:O	2:L:362:PRO:HD2	2.03	0.58
1:G:203:HIS:CD2	1:G:214:ILE:HD13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:GLY:HA3	1:I:229:CYS:O	2.02	0.58
1:E:175(E):VAL:CG1	1:E:175(H):LEU:HG	2.34	0.58
1:K:292:LYS:HE3	2:L:382:MET:HE2	1.85	0.58
1:C:171:HIS:C	1:C:171:HIS:CD2	2.82	0.58
1:C:242:ILE:C	1:C:242:ILE:HD12	2.28	0.58
2:D:360:ARG:HH11	2:D:360:ARG:CB	2.11	0.58
1:E:210:GLN:O	1:E:214:ILE:HG13	2.03	0.58
1:G:171:HIS:C	1:G:171:HIS:CD2	2.82	0.58
2:B:324:GLU:HB2	1:C:291:GLN:NE2	2.19	0.58
2:J:325:ALA:HA	2:J:393:THR:CG2	2.34	0.58
2:B:324:GLU:H	1:C:291:GLN:NE2	2.01	0.57
1:A:207:THR:N	1:A:210:GLN:NE2	2.38	0.57
1:E:155:MET:HE3	1:E:162:ARG:HD3	1.86	0.57
1:G:282:ILE:N	1:G:282:ILE:HD12	2.18	0.57
1:K:155:MET:HE2	2:L:400:PHE:CD2	2.38	0.57
2:B:354:CYS:HA	2:B:357:LEU:HD12	1.85	0.57
1:G:207:THR:HB	1:G:247:ASP:OD2	2.04	0.57
1:A:179:ARG:HH12	1:A:182:THR:HG23	1.69	0.57
2:B:325:ALA:HA	2:B:393:THR:CG2	2.34	0.57
1:C:155:MET:HE2	2:D:400:PHE:CD1	2.39	0.57
1:E:298:THR:O	1:E:299:ASP:OXT	2.22	0.57
1:G:175(E):VAL:HG21	1:G:175(H):LEU:HG	1.87	0.57
2:L:342:ASN:ND2	2:L:345:GLU:HG2	2.19	0.57
1:A:297:GLU:HB2	2:D:318:THR:N	2.19	0.57
2:F:390:THR:HG21	2:H:388:GLN:HE21	1.68	0.57
1:K:176:ILE:HD12	1:K:176:ILE:O	2.05	0.57
1:K:210:GLN:O	1:K:214:ILE:HG13	2.04	0.57
2:F:324:GLU:HB2	1:G:291:GLN:NE2	2.20	0.57
1:I:162:ARG:HG3	1:I:197:HIS:O	2.05	0.57
2:B:393:THR:HG22	2:B:393:THR:O	2.05	0.57
1:E:283:GLN:CD	4:E:93:HOH:O	2.48	0.57
2:F:341:ARG:CB	2:F:347:THR:HG22	2.35	0.57
1:G:207:THR:HG23	1:G:210:GLN:NE2	2.20	0.57
1:C:175(G):LYS:C	1:C:175(H):LEU:HD23	2.30	0.57
2:D:356:SER:HB3	2:D:369:ILE:HG23	1.87	0.57
2:F:353:LEU:HD12	2:F:353:LEU:O	2.05	0.57
1:K:260:GLU:OE1	1:K:260:GLU:HA	2.05	0.57
1:E:282:ILE:N	1:E:282:ILE:CD1	2.68	0.57
2:F:329:LEU:HD12	2:F:329:LEU:C	2.28	0.57
1:G:240:LYS:HA	2:H:335:ASN:HD21	1.70	0.57
1:I:293:GLY:HA2	2:L:321:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:173:PHE:HB3	1:K:176:ILE:HD13	1.86	0.56
2:L:360:ARG:NE	2:L:372:GLU:OE1	2.37	0.56
1:A:182:THR:O	1:A:183:HIS:C	2.47	0.56
1:G:216:LYS:HD2	1:G:220:LEU:HD11	1.87	0.56
2:L:322:PRO:HG2	2:L:325:ALA:HB2	1.87	0.56
1:E:262:THR:HG22	1:E:263:SER:N	2.20	0.56
1:I:175(H):LEU:O	1:I:175(J):SER:N	2.38	0.56
1:G:155:MET:HE3	1:G:162:ARG:CD	2.36	0.56
2:D:355:GLN:NE2	4:D:41:HOH:O	2.37	0.56
1:A:262:THR:HG22	1:A:263:SER:N	2.21	0.56
1:E:182:THR:O	1:E:185:ASP:N	2.38	0.56
2:F:381(D):LYS:C	2:F:382:MET:H	2.13	0.56
1:G:157:SER:OG	1:G:162:ARG:HA	2.06	0.56
1:E:229:CYS:HB2	1:E:277:PRO:HG2	1.87	0.56
1:G:263:SER:O	1:G:266:THR:HG23	2.05	0.56
2:H:360:ARG:HH11	2:H:360:ARG:CB	2.13	0.56
1:I:234:ILE:C	1:I:235:LEU:HD23	2.31	0.56
1:K:240:LYS:HD3	2:L:336:ASN:ND2	2.21	0.56
1:K:247:ASP:HB2	4:K:110:HOH:O	2.05	0.56
1:G:175(E):VAL:HG13	1:G:175(H):LEU:HB2	1.87	0.56
1:E:155:MET:HE2	2:F:400:PHE:CD2	2.39	0.56
1:C:289:ASN:O	2:D:338:VAL:HG13	2.05	0.55
1:E:234:ILE:O	1:E:235:LEU:HD23	2.05	0.55
1:G:185:ASP:OD2	2:H:347:THR:HG23	2.06	0.55
2:J:381(D):LYS:C	2:J:382:MET:H	2.13	0.55
2:D:359:GLU:O	2:D:362:PRO:HD2	2.05	0.55
1:E:179:ARG:HH12	1:E:182:THR:HG23	1.67	0.55
1:E:282:ILE:N	1:E:282:ILE:HD12	2.21	0.55
2:F:365:ASP:O	2:F:369:ILE:HD12	2.07	0.55
2:F:382:MET:HE3	2:F:382:MET:HA	1.87	0.55
1:I:295:PRO:C	1:I:296:VAL:HG22	2.31	0.55
1:K:175:LYS:HB3	1:K:247:ASP:HA	1.87	0.55
1:K:175(B):ARG:HG2	1:K:175(I):HIS:O	2.05	0.55
1:G:175(G):LYS:C	1:G:175(H):LEU:HD23	2.31	0.55
1:K:196:LEU:HG	4:K:106:HOH:O	2.07	0.55
2:B:381(B):ASP:O	2:B:381(D):LYS:N	2.39	0.55
2:H:342:ASN:ND2	2:H:345:GLU:HG2	2.22	0.55
2:J:318:THR:CA	1:K:297:GLU:HB2	2.22	0.55
1:K:155:MET:HE3	1:K:162:ARG:HD2	1.88	0.55
1:K:282:ILE:N	1:K:282:ILE:HD12	2.20	0.55
2:L:370:LEU:HD13	2:L:389:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:390:THR:CG2	2:H:388:GLN:HE21	2.20	0.55
2:H:325:ALA:HA	2:H:393:THR:HG21	1.87	0.55
1:E:191:THR:O	1:E:195:GLU:HG3	2.07	0.55
1:G:260:GLU:OE1	1:G:260:GLU:HA	2.07	0.55
1:A:175(D):LYS:HE2	4:A:33:HOH:O	2.05	0.55
2:J:361:CYS:N	2:J:362:PRO:HD2	2.22	0.55
1:I:262:THR:HG22	1:I:263:SER:N	2.21	0.55
1:A:268:LEU:O	1:A:271:PRO:HD3	2.07	0.54
1:G:240:LYS:HD3	2:H:336:ASN:ND2	2.21	0.54
1:A:191:THR:O	1:A:195:GLU:HG3	2.07	0.54
1:K:157:SER:OG	1:K:162:ARG:HA	2.08	0.54
1:K:281:PHE:C	1:K:282:ILE:HD12	2.32	0.54
1:I:175(B):ARG:HG2	1:I:175(I):HIS:O	2.07	0.54
1:G:206:CYS:HB3	1:G:210:GLN:HB3	1.90	0.54
1:G:296:VAL:HG13	1:G:297:GLU:N	2.22	0.54
1:A:175(B):ARG:HG3	1:A:176:ILE:CD1	2.37	0.54
2:F:365:ASP:HB2	2:F:397:LYS:HD3	1.88	0.54
1:G:299:ASP:HB3	4:H:122:HOH:O	2.07	0.54
2:H:365:ASP:O	2:H:369:ILE:HD12	2.08	0.54
1:A:151:LYS:HD2	1:A:152:VAL:N	2.22	0.54
1:A:175(E):VAL:HG11	1:A:175(H):LEU:HG	1.89	0.54
2:B:381:LYS:O	2:B:384:LYS:HE2	2.07	0.54
1:C:175(G):LYS:O	1:C:175(H):LEU:HD23	2.07	0.54
2:D:365:ASP:HB2	2:D:397:LYS:HD2	1.89	0.54
1:E:175(B):ARG:NH2	1:E:178:ASP:OD1	2.37	0.54
1:I:294:ILE:HD13	2:L:321:ILE:HG13	1.90	0.54
1:K:175(B):ARG:HG3	1:K:176:ILE:HD12	1.88	0.54
1:K:175(B):ARG:HG3	1:K:176:ILE:CD1	2.38	0.54
1:C:282:ILE:HD13	2:D:329:LEU:HD11	1.88	0.54
2:F:360:ARG:HH11	2:F:364:ASP:CG	2.16	0.54
2:J:393:THR:HG22	2:J:393:THR:O	2.07	0.54
1:A:283:GLN:HE21	2:B:347:THR:CB	2.20	0.54
1:A:285:CYS:SG	3:T:4103:ASP:N	2.80	0.54
1:A:192:THR:HG21	2:B:354:CYS:HB3	1.90	0.54
2:L:393:THR:O	2:L:393:THR:CG2	2.56	0.54
1:K:270:CYS:SG	1:K:273:LEU:HD12	2.47	0.54
2:F:393:THR:O	2:F:393:THR:CG2	2.56	0.53
1:I:175(E):VAL:HG21	1:I:248:GLY:HA3	1.89	0.53
2:J:332:ALA:HB2	2:J:349:TYR:CD2	2.43	0.53
2:J:381(E):ASN:ND2	2:J:381(E):ASN:H	2.06	0.53
2:J:389:PRO:HG3	4:J:94:HOH:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381(B):ASP:O	2:B:381(B):ASP:CG	2.51	0.53
2:B:381(D):LYS:C	2:B:382:MET:H	2.16	0.53
1:E:297:GLU:HB2	2:H:318:THR:N	2.22	0.53
1:G:184:LEU:N	1:G:184:LEU:HD12	2.24	0.53
1:K:171:HIS:CD2	1:K:171:HIS:C	2.86	0.53
1:C:166:LEU:HD13	1:C:230:PHE:CE1	2.44	0.53
1:C:270:CYS:SG	1:C:273:LEU:HD12	2.49	0.53
1:G:175(E):VAL:HG22	1:G:175(H):LEU:HG	1.90	0.53
2:J:371:THR:O	2:J:374:ASN:HB2	2.08	0.53
1:K:176:ILE:HA	4:K:88:HOH:O	2.08	0.53
1:C:296:VAL:HG13	1:C:297:GLU:N	2.23	0.53
2:H:325:ALA:HB1	2:H:395:ARG:HD3	1.90	0.53
1:G:157:SER:O	1:G:162:ARG:NH1	2.41	0.53
1:I:297:GLU:HB2	2:L:318:THR:N	2.24	0.53
2:B:361:CYS:N	2:B:362:PRO:HD2	2.24	0.53
2:L:342:ASN:C	2:L:344:ALA:H	2.15	0.53
1:E:291:GLN:HE21	2:H:322:PRO:HB2	1.72	0.53
1:G:210:GLN:O	1:G:214:ILE:HG13	2.08	0.53
1:A:177:ARG:HB2	4:B:15:HOH:O	2.07	0.53
1:C:180:ASN:O	2:D:343:PRO:HA	2.09	0.53
2:D:366:ILE:HD13	2:D:366:ILE:O	2.08	0.53
2:F:341:ARG:HD3	3:V:4303:ASP:OD1	2.08	0.53
1:I:151:LYS:HD2	1:I:152:VAL:N	2.23	0.53
1:I:196:LEU:HD22	2:J:400:PHE:HB3	1.90	0.53
1:K:192:THR:HA	1:K:195:GLU:HG3	1.91	0.53
1:E:206:CYS:HA	1:E:210:GLN:NE2	2.23	0.52
1:G:224:HIS:HB3	1:G:227:MET:HB2	1.91	0.52
1:C:175(G):LYS:HD2	1:C:175(H):LEU:HD21	1.92	0.52
1:G:153:TYR:OH	2:H:326:ASP:OD1	2.23	0.52
1:K:180:ASN:O	2:L:343:PRO:HA	2.10	0.52
1:A:175(E):VAL:CG1	1:A:175(H):LEU:HG	2.39	0.52
1:C:216:LYS:HD2	1:C:220:LEU:HD11	1.90	0.52
1:K:207:THR:HG23	1:K:210:GLN:HE22	1.74	0.52
2:B:371:THR:O	2:B:374:ASN:HB2	2.09	0.52
1:C:169:ASN:HD22	1:C:186:ALA:HB2	1.75	0.52
1:E:192:THR:HG21	2:F:354:CYS:HB3	1.91	0.52
2:F:393:THR:HG23	2:H:386:MET:CE	2.31	0.52
1:G:234:ILE:C	1:G:235:LEU:HD23	2.34	0.52
1:K:283:GLN:C	1:K:283:GLN:HE21	2.18	0.52
2:B:382:MET:HE3	2:B:382:MET:HA	1.91	0.52
2:B:388:GLN:HE21	2:D:390:THR:CG2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:PHE:HB3	1:C:176:ILE:HD13	1.91	0.52
1:C:192:THR:HA	1:C:195:GLU:HG3	1.90	0.52
2:D:342:ASN:C	2:D:344:ALA:H	2.17	0.52
2:H:396:LYS:HD3	4:H:81:HOH:O	2.09	0.52
1:K:296:VAL:HG13	1:K:297:GLU:N	2.25	0.52
1:I:185:ASP:O	1:I:189:LEU:HD22	2.09	0.52
2:J:324:GLU:H	1:K:291:GLN:HE21	1.58	0.52
1:G:192:THR:HA	1:G:195:GLU:HG3	1.91	0.52
1:G:224:HIS:H	1:G:272:SER:HB2	1.75	0.52
1:I:210:GLN:O	1:I:214:ILE:HG13	2.10	0.52
1:I:298:THR:O	1:I:299:ASP:OXT	2.28	0.52
1:E:190:THR:HG22	1:E:191:THR:N	2.24	0.52
2:F:381(E):ASN:O	2:F:382:MET:C	2.52	0.52
2:F:386:MET:SD	2:H:393:THR:HG23	2.49	0.52
1:G:184:LEU:HD12	1:G:184:LEU:H	1.73	0.52
1:I:161:PRO:O	1:I:197:HIS:O	2.28	0.52
1:A:283:GLN:NE2	2:B:347:THR:CB	2.73	0.52
2:B:341:ARG:HB2	2:B:347:THR:HG22	1.90	0.52
1:I:190:THR:HG22	1:I:191:THR:N	2.25	0.52
1:A:170:ASN:HB2	1:A:236:SER:HB2	1.92	0.51
1:A:210:GLN:O	1:A:214:ILE:HG13	2.10	0.51
1:C:224:HIS:HB3	1:C:227:MET:HB2	1.92	0.51
1:E:181:GLY:H	1:E:183:HIS:CE1	2.28	0.51
2:H:359:GLU:O	2:H:362:PRO:HD2	2.09	0.51
1:I:270:CYS:SG	1:I:273:LEU:HB2	2.50	0.51
1:C:185:ASP:OD2	2:D:347:THR:HG23	2.11	0.51
1:I:192:THR:HG21	2:J:354:CYS:HB3	1.92	0.51
2:L:357:LEU:O	2:L:361:CYS:HB2	2.09	0.51
2:J:341:ARG:HG3	2:J:347:THR:CG2	2.40	0.51
2:J:392:PHE:CZ	2:L:389:PRO:HG2	2.46	0.51
1:C:157:SER:O	1:C:160:LYS:C	2.53	0.51
2:D:381(E):ASN:C	2:D:382:MET:HG2	2.34	0.51
1:E:193:PHE:O	1:E:198:PHE:HB2	2.09	0.51
1:G:296:VAL:HG13	1:G:297:GLU:H	1.76	0.51
1:I:172:ASN:HA	1:I:178:ASP:OD1	2.11	0.51
2:B:353:LEU:HD12	2:B:353:LEU:O	2.11	0.51
1:E:257:PRO:HD2	1:E:260:GLU:HG3	1.93	0.51
1:E:283:GLN:HE21	2:F:347:THR:HG21	1.75	0.51
2:F:354:CYS:O	2:F:358:ARG:HG3	2.10	0.51
1:I:241:GLY:HA2	1:I:286:GLN:HE22	1.76	0.51
1:A:295:PRO:HB3	2:D:320:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:O	1:A:299:ASP:OXT	2.29	0.51
1:K:193:PHE:O	1:K:198:PHE:HB2	2.11	0.51
1:A:239:ASP:O	1:A:240:LYS:C	2.53	0.51
1:A:291:GLN:HE22	2:D:324:GLU:HB2	1.75	0.51
1:E:175(D):LYS:O	1:E:175(E):VAL:C	2.54	0.51
1:E:207:THR:HG23	1:E:210:GLN:HE22	1.76	0.51
2:F:319:ARG:O	1:G:295:PRO:HA	2.11	0.51
1:I:189:LEU:HD13	2:J:354:CYS:SG	2.50	0.51
2:J:319:ARG:O	1:K:295:PRO:HA	2.11	0.51
1:A:190:THR:HG22	1:A:191:THR:N	2.25	0.51
2:D:341:ARG:HD3	3:U:4203:ASP:OD1	2.10	0.51
1:G:175(F):PRO:O	1:G:175(H):LEU:N	2.43	0.51
1:C:153:TYR:OH	2:D:326:ASP:OD1	2.27	0.51
1:C:157:SER:OG	1:C:162:ARG:HA	2.11	0.51
2:J:325:ALA:HA	2:J:393:THR:HG22	1.91	0.51
1:K:240:LYS:HA	2:L:335:ASN:HD21	1.75	0.51
2:B:342:ASN:ND2	2:B:344:ALA:HB3	2.25	0.50
1:C:257:PRO:HB2	1:C:260:GLU:HG2	1.93	0.50
2:F:320:TYR:HE2	1:G:295:PRO:HG3	1.74	0.50
2:F:342:ASN:N	2:F:346:GLY:O	2.42	0.50
2:H:328:LEU:HD12	2:H:329:LEU:N	2.26	0.50
1:A:171:HIS:C	1:A:171:HIS:CD2	2.89	0.50
1:A:241:GLY:HA2	1:A:286:GLN:HE22	1.76	0.50
2:B:334:VAL:HG12	2:B:388:GLN:OE1	2.11	0.50
1:G:180:ASN:O	2:H:343:PRO:HA	2.11	0.50
2:J:341:ARG:CB	2:J:347:THR:HG22	2.41	0.50
2:B:381(B):ASP:O	2:B:381(C):LYS:C	2.54	0.50
2:B:393:THR:HG23	2:D:386:MET:CE	2.36	0.50
1:I:283:GLN:NE2	2:J:347:THR:HB	2.26	0.50
1:K:192:THR:HG22	2:L:358:ARG:CZ	2.42	0.50
1:A:182:THR:O	1:A:185:ASP:N	2.45	0.50
1:C:206:CYS:HB3	1:C:210:GLN:HB3	1.94	0.50
1:I:161:PRO:O	1:I:162:ARG:HB2	2.12	0.50
2:B:319:ARG:O	1:C:295:PRO:HA	2.11	0.50
2:B:342:ASN:HD21	2:B:344:ALA:HB3	1.76	0.50
1:C:175(E):VAL:CG2	1:C:175(H):LEU:HG	2.41	0.50
1:C:184:LEU:HD12	1:C:184:LEU:N	2.26	0.50
1:E:175(F):PRO:O	1:E:175(H):LEU:N	2.45	0.50
2:J:365:ASP:O	2:J:369:ILE:HD12	2.11	0.50
1:G:204:HIS:O	1:G:205:ASP:C	2.54	0.50
2:H:340:TYR:HA	3:W:4401:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:381(B):ASP:O	2:F:381(B):ASP:CG	2.52	0.50
1:G:273:LEU:HA	1:G:276:LYS:HD2	1.93	0.50
1:K:207:THR:HB	1:K:247:ASP:OD2	2.12	0.50
1:A:282:ILE:CD1	1:A:282:ILE:N	2.75	0.49
1:C:175(F):PRO:HB2	4:C:45:HOH:O	2.11	0.49
1:C:203:HIS:CD2	1:C:214:ILE:HD13	2.47	0.49
1:E:283:GLN:O	1:E:283:GLN:HG3	2.12	0.49
1:G:242:ILE:C	1:G:242:ILE:HD12	2.36	0.49
1:K:188:ALA:O	1:K:192:THR:HG23	2.11	0.49
1:K:200:ILE:HG22	1:K:202:PRO:HD3	1.93	0.49
1:K:242:ILE:HD12	1:K:242:ILE:C	2.37	0.49
2:L:334:VAL:HG12	2:L:388:GLN:OE1	2.12	0.49
1:A:193:PHE:O	1:A:198:PHE:HB2	2.11	0.49
1:K:179:ARG:HH12	1:K:182:THR:HG21	1.77	0.49
1:C:175(I):HIS:CD2	1:C:175(J):SER:HB3	2.47	0.49
1:G:207:THR:CG2	1:G:210:GLN:HE22	2.25	0.49
2:H:348:TRP:CZ3	2:H:381:LYS:HB2	2.47	0.49
1:A:175(B):ARG:HH22	1:A:178:ASP:CG	2.20	0.49
1:A:175(H):LEU:O	1:A:175(J):SER:N	2.45	0.49
2:B:324:GLU:H	1:C:291:GLN:HE21	1.59	0.49
2:H:342:ASN:ND2	2:H:345:GLU:CG	2.75	0.49
1:I:283:GLN:NE2	2:J:347:THR:CB	2.75	0.49
1:K:198:PHE:CE2	1:K:231:ILE:HG13	2.48	0.49
1:A:258:ILE:HD12	1:A:282:ILE:HG12	1.94	0.49
1:C:207:THR:CG2	1:C:210:GLN:NE2	2.74	0.49
2:D:325:ALA:HA	2:D:393:THR:HG22	1.93	0.49
2:F:361:CYS:N	2:F:362:PRO:HD2	2.28	0.49
1:G:289:ASN:O	2:H:338:VAL:HG13	2.12	0.49
1:A:220:LEU:HD22	4:A:16:HOH:O	2.13	0.49
1:A:161:PRO:HG2	1:A:227:MET:SD	2.52	0.49
1:A:282:ILE:N	1:A:282:ILE:HD12	2.28	0.49
1:A:260:GLU:OE1	1:A:260:GLU:HA	2.13	0.49
2:J:324:GLU:H	1:K:291:GLN:NE2	2.11	0.49
1:A:180:ASN:O	2:B:341:ARG:NE	2.45	0.49
2:B:365:ASP:O	2:B:369:ILE:HD12	2.12	0.49
1:C:169:ASN:OD1	1:C:169:ASN:C	2.55	0.49
1:I:179:ARG:HH12	1:I:182:THR:HG23	1.75	0.49
2:L:341:ARG:HA	2:L:347:THR:HA	1.95	0.49
1:A:155:MET:HE2	2:B:400:PHE:CD1	2.46	0.49
1:A:163:GLY:HA3	1:A:229:CYS:O	2.12	0.49
1:A:295:PRO:C	1:A:296:VAL:HG22	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:PRO:HG2	2:D:325:ALA:HB2	1.95	0.49
1:G:174:ALA:HA	1:G:175(B):ARG:NH1	2.28	0.49
2:H:328:LEU:HD12	2:H:328:LEU:C	2.37	0.49
1:I:291:GLN:HE22	2:L:324:GLU:HB2	1.77	0.49
2:L:365:ASP:O	2:L:369:ILE:HD12	2.13	0.49
1:A:291:GLN:HE21	2:D:322:PRO:HB2	1.78	0.48
1:G:286:GLN:HB3	2:H:335:ASN:HD22	1.78	0.48
2:J:365:ASP:HB2	2:J:397:LYS:HD3	1.95	0.48
2:J:397:LYS:NZ	4:L:131:HOH:O	2.45	0.48
1:A:168:ILE:HG21	1:A:211:ILE:HD13	1.95	0.48
1:A:175(H):LEU:HB3	1:A:176:ILE:HG12	1.95	0.48
1:G:257:PRO:HB2	1:G:260:GLU:HG2	1.93	0.48
1:I:155:MET:HE3	1:I:162:ARG:HD3	1.94	0.48
1:K:169:ASN:OD1	1:K:169:ASN:C	2.57	0.48
1:A:240:LYS:HG3	1:A:240:LYS:O	2.13	0.48
2:H:342:ASN:C	2:H:344:ALA:H	2.21	0.48
2:J:372:GLU:O	2:J:376:GLU:HG2	2.13	0.48
1:K:184:LEU:H	1:K:184:LEU:CD1	2.26	0.48
2:D:360:ARG:NE	2:D:372:GLU:OE1	2.45	0.48
1:C:175(E):VAL:HG22	1:C:175(H):LEU:HG	1.96	0.48
2:F:390:THR:HG21	2:H:388:GLN:NE2	2.29	0.48
2:H:360:ARG:NE	2:H:372:GLU:OE1	2.42	0.48
2:B:381(E):ASN:ND2	2:B:381(E):ASN:N	2.56	0.48
1:G:161:PRO:O	1:G:162:ARG:C	2.56	0.48
2:H:393:THR:O	2:H:393:THR:CG2	2.61	0.48
1:I:243:ILE:HD13	1:I:258:ILE:HD11	1.95	0.48
2:B:325:ALA:HA	2:B:393:THR:HG22	1.96	0.48
2:F:320:TYR:CE2	1:G:295:PRO:HG3	2.47	0.48
1:A:293:GLY:HA2	2:D:321:ILE:O	2.12	0.48
2:D:341:ARG:HA	2:D:347:THR:HA	1.95	0.48
1:G:179:ARG:HD2	1:G:237:HIS:ND1	2.28	0.48
2:B:365:ASP:HB2	2:B:397:LYS:HD3	1.95	0.48
1:E:171:HIS:C	1:E:171:HIS:CD2	2.91	0.48
1:I:282:ILE:N	1:I:282:ILE:HD12	2.28	0.48
1:I:291:GLN:HE21	2:L:322:PRO:HB2	1.79	0.48
2:H:325:ALA:HA	2:H:393:THR:HG22	1.96	0.48
2:H:331:MET:HB2	2:H:388:GLN:O	2.14	0.48
2:H:353:LEU:HD12	2:H:353:LEU:O	2.13	0.48
2:H:360:ARG:HB3	2:H:360:ARG:NH1	2.15	0.48
1:K:289:ASN:O	2:L:338:VAL:HG13	2.14	0.48
2:B:388:GLN:HG2	2:B:388:GLN:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:PHE:O	1:G:198:PHE:HB2	2.14	0.47
1:A:262:THR:CG2	1:A:263:SER:N	2.76	0.47
2:F:353:LEU:HD12	2:F:353:LEU:C	2.38	0.47
1:I:168:ILE:HG21	1:I:211:ILE:HD13	1.96	0.47
1:I:222:ASP:OD1	1:I:225:SER:HB2	2.15	0.47
1:A:241:GLY:H	1:A:286:GLN:NE2	2.12	0.47
1:A:294:ILE:HD13	2:D:321:ILE:HG13	1.96	0.47
2:B:392:PHE:CZ	2:D:389:PRO:HG2	2.49	0.47
1:C:257:PRO:HD2	1:C:260:GLU:HG3	1.97	0.47
2:F:341:ARG:HB2	2:F:347:THR:HG22	1.95	0.47
1:I:257:PRO:HD2	1:I:260:GLU:HG3	1.95	0.47
2:L:354:CYS:O	2:L:355:GLN:C	2.56	0.47
2:B:354:CYS:O	2:B:358:ARG:HG3	2.15	0.47
1:G:175(B):ARG:HG3	1:G:176:ILE:HD12	1.96	0.47
1:K:282:ILE:HD13	2:L:329:LEU:HD11	1.95	0.47
1:K:296:VAL:HG13	1:K:297:GLU:H	1.79	0.47
2:L:385:GLN:HA	4:L:143:HOH:O	2.14	0.47
2:B:386:MET:SD	2:D:393:THR:CG2	3.03	0.47
2:F:396:LYS:HZ1	1:G:299:ASP:HA	1.77	0.47
1:G:173:PHE:HE1	1:G:179:ARG:HG3	1.80	0.47
1:K:193:PHE:HA	1:K:196:LEU:HD12	1.96	0.47
2:L:325:ALA:HA	2:L:393:THR:HG22	1.95	0.47
1:E:295:PRO:O	1:E:296:VAL:HG22	2.14	0.47
1:K:206:CYS:HB3	1:K:210:GLN:CB	2.43	0.47
2:L:381(C):LYS:O	2:L:381(D):LYS:C	2.55	0.47
1:E:283:GLN:HE21	2:F:347:THR:CB	2.28	0.47
1:G:184:LEU:CD2	2:H:345:GLU:HA	2.45	0.47
1:G:191:THR:O	1:G:195:GLU:HG2	2.15	0.47
1:I:283:GLN:HG3	1:I:283:GLN:O	2.15	0.47
2:J:329:LEU:HD12	2:J:329:LEU:C	2.40	0.47
1:K:161:PRO:O	1:K:162:ARG:C	2.57	0.47
1:K:254:GLN:HG2	4:K:110:HOH:O	2.14	0.47
2:L:371:THR:O	2:L:374:ASN:HB2	2.15	0.47
2:L:381(C):LYS:HD3	2:L:381(C):LYS:HA	1.57	0.47
1:A:175(H):LEU:HB3	1:A:176:ILE:CG1	2.45	0.47
1:G:175(F):PRO:C	1:G:175(H):LEU:H	2.22	0.47
2:H:334:VAL:HG13	2:H:386:MET:O	2.15	0.47
1:A:229:CYS:SG	1:A:230:PHE:N	2.88	0.47
1:E:150:ASP:OD1	1:E:150:ASP:N	2.46	0.47
1:G:208:VAL:HG12	1:G:209:GLU:N	2.30	0.47
1:I:229:CYS:HB2	1:I:277:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:341:ARG:CG	2:J:347:THR:HG22	2.45	0.47
1:K:157:SER:O	1:K:160:LYS:C	2.58	0.47
1:C:179:ARG:HA	2:D:341:ARG:CZ	2.45	0.47
1:C:182:THR:O	1:C:185:ASP:HB2	2.15	0.47
2:F:329:LEU:HD12	2:F:330:GLY:H	1.76	0.47
2:J:362(B):ARG:HG2	2:J:362(B):ARG:HH11	1.80	0.47
1:C:224:HIS:H	1:C:272:SER:HB2	1.79	0.46
2:F:325:ALA:HA	2:F:393:THR:HG22	1.97	0.46
1:A:155:MET:HE3	1:A:162:ARG:HD3	1.97	0.46
1:A:207:THR:HG23	1:A:210:GLN:NE2	2.30	0.46
1:G:282:ILE:HD13	2:H:329:LEU:CD1	2.45	0.46
1:K:257:PRO:O	1:K:260:GLU:HB2	2.15	0.46
2:B:342:ASN:N	2:B:346:GLY:O	2.47	0.46
1:C:187:GLY:O	1:C:190:THR:HB	2.15	0.46
1:C:208:VAL:HG12	1:C:209:GLU:N	2.30	0.46
1:C:276:LYS:O	1:C:278:LYS:NZ	2.47	0.46
1:E:207:THR:O	1:E:211:ILE:HG13	2.15	0.46
2:H:354:CYS:O	2:H:355:GLN:C	2.58	0.46
2:H:373:VAL:O	2:H:377:VAL:HG23	2.16	0.46
1:E:168:ILE:HG21	1:E:211:ILE:HD13	1.98	0.46
1:G:257:PRO:O	1:G:260:GLU:HB2	2.15	0.46
1:I:171:HIS:CD2	1:I:171:HIS:C	2.93	0.46
2:L:339:SER:O	3:Y:4602:VAL:HA	2.16	0.46
1:A:154:GLN:HB3	4:A:30:HOH:O	2.16	0.46
1:E:151:LYS:HD2	1:E:152:VAL:N	2.29	0.46
1:E:155:MET:HG3	2:F:399:VAL:O	2.16	0.46
1:E:291:GLN:HE22	2:H:324:GLU:HB2	1.80	0.46
1:I:262:THR:CG2	1:I:263:SER:N	2.78	0.46
1:K:175(E):VAL:CG2	1:K:175(H):LEU:HG	2.45	0.46
2:B:375:TYR:HA	2:D:395:ARG:HG2	1.97	0.46
1:E:175(F):PRO:C	1:E:175(H):LEU:H	2.23	0.46
4:E:93:HOH:O	2:F:332:ALA:HB1	2.15	0.46
1:G:257:PRO:HD2	1:G:260:GLU:HG3	1.97	0.46
1:I:210:GLN:HE21	1:I:210:GLN:HB2	1.53	0.46
1:I:236:SER:OG	1:I:237:HIS:N	2.49	0.46
2:J:390:THR:CG2	2:L:388:GLN:HE21	2.29	0.46
1:C:291:GLN:O	2:D:384:LYS:HB2	2.16	0.46
1:G:175(G):LYS:HD2	1:G:175(H):LEU:CD2	2.45	0.46
1:K:167:ILE:O	1:K:167:ILE:HG22	2.15	0.46
1:A:155:MET:HG3	2:B:399:VAL:O	2.16	0.46
2:D:354:CYS:O	2:D:357:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:LYS:O	1:E:240:LYS:HG3	2.15	0.46
1:G:167:ILE:HG22	1:G:167:ILE:O	2.15	0.46
1:K:153:TYR:OH	2:L:326:ASP:OD1	2.33	0.46
1:K:200:ILE:HG22	1:K:201:LYS:N	2.31	0.46
1:K:241:GLY:H	1:K:286:GLN:NE2	2.13	0.46
2:L:342:ASN:C	2:L:344:ALA:N	2.73	0.46
2:D:342:ASN:C	2:D:344:ALA:N	2.74	0.46
2:D:342:ASN:ND2	2:D:345:GLU:HG2	2.31	0.46
1:E:271:PRO:C	1:E:273:LEU:H	2.24	0.46
1:A:287:GLY:HA3	2:B:336:ASN:C	2.41	0.46
1:C:193:PHE:O	1:C:198:PHE:HB2	2.16	0.46
1:G:200:ILE:HG22	1:G:201:LYS:N	2.31	0.46
1:I:150:ASP:OD1	1:I:150:ASP:N	2.47	0.46
1:I:297:GLU:OE2	1:I:298:THR:O	2.34	0.46
1:K:175(H):LEU:O	1:K:175(J):SER:N	2.49	0.46
1:C:204:HIS:O	1:C:205:ASP:C	2.59	0.45
2:L:342:ASN:ND2	2:L:345:GLU:CG	2.79	0.45
1:A:297:GLU:OE1	2:D:319:ARG:HD2	2.16	0.45
1:I:270:CYS:SG	1:I:270:CYS:O	2.74	0.45
2:J:381(B):ASP:CG	2:J:381(B):ASP:O	2.58	0.45
2:J:392:PHE:O	2:L:389:PRO:HD2	2.16	0.45
1:C:161:PRO:O	1:C:162:ARG:C	2.59	0.45
1:C:296:VAL:HG13	1:C:297:GLU:H	1.81	0.45
2:D:381:LYS:O	2:D:384:LYS:HE2	2.17	0.45
2:H:377:VAL:CG1	2:H:385:GLN:HG2	2.46	0.45
2:D:339:SER:HA	2:D:385:GLN:OE1	2.16	0.45
1:G:193:PHE:HA	1:G:196:LEU:HD12	1.98	0.45
1:I:175(B):ARG:HG3	1:I:176:ILE:HD12	1.98	0.45
1:I:192:THR:HG22	2:J:358:ARG:HG2	1.98	0.45
2:J:342:ASN:N	2:J:346:GLY:O	2.46	0.45
1:G:169:ASN:C	1:G:169:ASN:OD1	2.60	0.45
1:K:294:ILE:O	1:K:294:ILE:HG12	2.17	0.45
1:A:179:ARG:HA	2:B:341:ARG:CZ	2.46	0.45
1:E:175(F):PRO:C	1:E:175(H):LEU:N	2.74	0.45
1:E:239:ASP:O	1:E:240:LYS:C	2.59	0.45
1:E:291:GLN:NE2	2:H:324:GLU:H	2.14	0.45
2:F:374:ASN:OD1	2:F:387:PRO:HB2	2.16	0.45
1:A:162:ARG:HG3	1:A:197:HIS:O	2.16	0.45
1:C:179:ARG:HH12	1:C:182:THR:HG21	1.82	0.45
2:D:342:ASN:ND2	2:D:345:GLU:CG	2.79	0.45
1:G:182:THR:O	1:G:185:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:ARG:HA	2:L:341:ARG:CZ	2.45	0.45
1:K:202:PRO:O	1:K:203:HIS:ND1	2.49	0.45
1:C:292:LYS:HE3	2:D:382:MET:HE2	1.98	0.45
1:E:168:ILE:CD1	1:E:211:ILE:HG23	2.41	0.45
1:G:271:PRO:HG3	4:G:82:HOH:O	2.17	0.45
1:K:155:MET:HE3	1:K:162:ARG:HD3	1.98	0.45
1:A:150:ASP:N	1:A:150:ASP:OD1	2.48	0.45
1:A:216:LYS:O	1:A:220:LEU:HG	2.16	0.45
2:B:393:THR:CG2	2:B:393:THR:O	2.65	0.45
1:C:236:SER:O	1:C:284:ALA:HA	2.17	0.45
1:E:200:ILE:HD13	1:E:200:ILE:N	2.31	0.45
2:F:347:THR:O	2:F:351:GLN:HB2	2.17	0.45
1:I:181:GLY:H	1:I:183:HIS:CE1	2.35	0.45
2:J:323:ASP:HB2	1:K:292:LYS:O	2.16	0.45
2:J:386:MET:SD	2:L:393:THR:CG2	3.05	0.45
2:L:365:ASP:HB2	2:L:397:LYS:HD2	1.98	0.45
1:C:203:HIS:CG	1:C:214:ILE:HD13	2.52	0.45
2:D:377:VAL:CG1	2:D:385:GLN:HG2	2.47	0.45
2:F:325:ALA:HA	2:F:393:THR:HG21	1.97	0.45
1:I:160:LYS:CG	1:I:161:PRO:HD3	2.45	0.45
1:A:243:ILE:HA	1:A:243:ILE:HD12	1.56	0.44
2:D:370:LEU:HD13	2:D:389:PRO:HB3	1.99	0.44
1:G:179:ARG:NH2	1:G:182:THR:HG23	2.33	0.44
1:G:184:LEU:HD22	2:H:345:GLU:HA	1.98	0.44
1:G:297:GLU:OE1	1:G:297:GLU:HA	2.17	0.44
1:A:200:ILE:N	1:A:200:ILE:HD13	2.31	0.44
1:E:208:VAL:HG23	1:E:245:GLY:HA3	1.99	0.44
1:G:191:THR:O	1:G:195:GLU:CG	2.65	0.44
1:G:207:THR:HB	1:G:247:ASP:CG	2.43	0.44
2:H:381(C):LYS:O	2:H:381(D):LYS:C	2.60	0.44
2:B:340:TYR:HA	3:T:4101:GLU:O	2.17	0.44
2:B:390:THR:CG2	2:D:388:GLN:HE21	2.31	0.44
1:G:169:ASN:ND2	1:G:186:ALA:HB2	2.29	0.44
1:G:175(B):ARG:HG3	1:G:176:ILE:CD1	2.47	0.44
1:I:175(F):PRO:C	1:I:175(H):LEU:N	2.74	0.44
1:K:236:SER:O	1:K:284:ALA:HA	2.18	0.44
1:C:164:TYR:N	4:C:51:HOH:O	2.39	0.44
1:C:207:THR:HB	1:C:247:ASP:CG	2.42	0.44
2:J:388:GLN:NE2	2:L:390:THR:HG21	2.27	0.44
1:K:242:ILE:HG22	1:K:257:PRO:HA	1.99	0.44
1:K:291:GLN:O	2:L:384:LYS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:CYS:O	1:A:270:CYS:SG	2.75	0.44
1:E:243:ILE:HD13	1:E:258:ILE:HD11	2.00	0.44
1:E:270:CYS:SG	1:E:273:LEU:HB2	2.57	0.44
2:L:360:ARG:HH11	2:L:360:ARG:CB	2.20	0.44
1:E:294:ILE:HD13	2:H:321:ILE:HG13	2.00	0.44
2:B:399:VAL:HG22	2:B:400:PHE:N	2.33	0.44
1:C:179:ARG:NH2	1:C:182:THR:HG23	2.33	0.44
1:G:291:GLN:OE1	1:G:291:GLN:HA	2.18	0.44
1:I:162:ARG:HG2	1:I:162:ARG:HH11	1.82	0.44
1:I:173:PHE:HB3	1:I:176:ILE:HD13	1.99	0.44
1:I:240:LYS:O	1:I:240:LYS:HG3	2.18	0.44
2:J:386:MET:HE3	2:J:387:PRO:HD2	2.00	0.44
1:A:207:THR:O	1:A:211:ILE:HG13	2.18	0.44
1:A:283:GLN:NE2	2:B:347:THR:HB	2.33	0.44
1:E:270:CYS:SG	1:E:270:CYS:O	2.76	0.44
1:G:281:PHE:C	1:G:282:ILE:HD12	2.42	0.44
2:H:342:ASN:C	2:H:344:ALA:N	2.76	0.44
1:I:175:LYS:O	1:I:175(A):ALA:C	2.60	0.44
1:A:212:TYR:O	1:A:213:GLU:C	2.61	0.44
2:B:329:LEU:HD12	2:B:329:LEU:C	2.42	0.44
2:H:341:ARG:NH1	3:W:4403:ASP:OD1	2.51	0.44
1:I:166:LEU:N	1:I:166:LEU:HD23	2.33	0.44
1:K:207:THR:OG1	1:K:210:GLN:NE2	2.51	0.44
1:A:166:LEU:N	1:A:166:LEU:HD23	2.33	0.43
1:C:168:ILE:CD1	1:C:211:ILE:HG23	2.48	0.43
1:C:242:ILE:HG22	1:C:257:PRO:HA	2.00	0.43
2:D:348:TRP:CZ3	2:D:381:LYS:HB2	2.53	0.43
1:G:182:THR:HG23	4:G:99:HOH:O	2.18	0.43
1:K:207:THR:HG23	1:K:210:GLN:NE2	2.33	0.43
1:A:161:PRO:O	1:A:162:ARG:HB2	2.16	0.43
1:A:210:GLN:HE21	1:A:210:GLN:HB2	1.59	0.43
1:A:291:GLN:NE2	2:D:324:GLU:H	2.16	0.43
1:C:294:ILE:O	1:C:294:ILE:HG12	2.14	0.43
2:D:367:LEU:HD12	2:D:367:LEU:HA	1.70	0.43
1:I:175(F):PRO:O	1:I:175(H):LEU:N	2.51	0.43
1:K:184:LEU:N	1:K:184:LEU:CD1	2.81	0.43
1:K:207:THR:HB	1:K:247:ASP:CG	2.43	0.43
1:K:298:THR:O	1:K:299:ASP:C	2.61	0.43
1:C:184:LEU:HD12	1:C:184:LEU:H	1.82	0.43
1:C:207:THR:O	1:C:208:VAL:C	2.60	0.43
1:E:229:CYS:SG	1:E:230:PHE:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:347:THR:O	2:H:351:GLN:HG2	2.18	0.43
1:K:243:ILE:CD1	1:K:256:ALA:HB3	2.48	0.43
1:K:286:GLN:HB3	2:L:335:ASN:HD22	1.83	0.43
1:C:155:MET:HE3	1:C:155:MET:HB3	1.79	0.43
2:F:328:LEU:HD12	2:F:329:LEU:N	2.33	0.43
2:J:354:CYS:O	2:J:355:GLN:C	2.62	0.43
1:K:175(E):VAL:HG22	1:K:175(H):LEU:HG	1.99	0.43
2:F:328:LEU:HD12	2:F:328:LEU:C	2.44	0.43
1:K:207:THR:CG2	1:K:210:GLN:HE22	2.31	0.43
2:B:354:CYS:O	2:B:355:GLN:C	2.61	0.43
1:C:282:ILE:HD12	1:C:282:ILE:N	2.33	0.43
1:E:175(H):LEU:O	1:E:175(I):HIS:C	2.60	0.43
1:E:262:THR:CG2	1:E:263:SER:N	2.78	0.43
2:J:342:ASN:HD21	2:J:344:ALA:HB3	1.83	0.43
1:K:179:ARG:NH2	1:K:182:THR:HG23	2.32	0.43
1:K:282:ILE:N	1:K:282:ILE:CD1	2.82	0.43
1:K:292:LYS:HE3	2:L:382:MET:CE	2.48	0.43
1:A:207:THR:HG23	1:A:210:GLN:HE22	1.84	0.43
1:C:191:THR:HG22	1:C:195:GLU:OE2	2.19	0.43
2:F:332:ALA:CB	2:F:349:TYR:CD2	2.99	0.43
1:G:179:ARG:HA	2:H:341:ARG:CZ	2.49	0.43
1:I:243:ILE:HA	1:I:243:ILE:HD12	1.64	0.43
2:J:321:ILE:O	1:K:294:ILE:HD13	2.18	0.43
2:J:342:ASN:ND2	2:J:344:ALA:HB3	2.33	0.43
2:L:342:ASN:O	2:L:344:ALA:N	2.52	0.43
1:A:287:GLY:HA3	2:B:336:ASN:HA	1.99	0.43
1:A:297:GLU:OE2	1:A:298:THR:O	2.37	0.43
1:C:240:LYS:HD3	2:D:336:ASN:HD21	1.79	0.43
1:E:155:MET:HE3	1:E:162:ARG:CD	2.48	0.43
1:A:160:LYS:CG	1:A:161:PRO:HD3	2.46	0.43
2:B:341:ARG:HG3	2:B:347:THR:HG22	2.01	0.43
1:C:239:ASP:O	1:C:240:LYS:C	2.61	0.43
1:C:273:LEU:HA	1:C:276:LYS:HD2	2.00	0.43
2:D:328:LEU:HD12	2:D:329:LEU:N	2.34	0.43
1:E:175(H):LEU:O	1:E:175(J):SER:N	2.52	0.43
2:F:353:LEU:HD11	2:F:357:LEU:HD11	2.00	0.43
1:G:157:SER:O	1:G:160:LYS:C	2.61	0.43
1:I:206:CYS:HA	1:I:210:GLN:NE2	2.33	0.43
1:K:234:ILE:C	1:K:235:LEU:HD23	2.44	0.43
2:B:367:LEU:HD12	2:B:367:LEU:HA	1.80	0.42
1:E:243:ILE:HA	1:E:243:ILE:HD12	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:342:ASN:HD22	2:L:345:GLU:CG	2.32	0.42
1:A:176:ILE:HG13	1:A:176:ILE:H	1.53	0.42
1:A:270:CYS:SG	1:A:273:LEU:HB2	2.59	0.42
2:B:366:ILE:HG21	2:B:398:LEU:HD23	2.01	0.42
1:C:172:ASN:HB3	1:C:205:ASP:OD2	2.19	0.42
1:E:283:GLN:NE2	4:E:93:HOH:O	2.53	0.42
2:F:348:TRP:CG	2:F:381:LYS:HD2	2.54	0.42
2:F:354:CYS:O	2:F:355:GLN:C	2.62	0.42
2:L:366:ILE:CG2	2:L:367:LEU:N	2.81	0.42
1:G:179:ARG:NH2	4:G:99:HOH:O	2.52	0.42
1:E:160:LYS:CG	1:E:161:PRO:HD3	2.47	0.42
1:E:241:GLY:HA2	1:E:286:GLN:HE22	1.85	0.42
1:E:297:GLU:OE2	1:E:298:THR:O	2.38	0.42
2:F:372:GLU:O	2:F:376:GLU:HG2	2.19	0.42
1:G:207:THR:CG2	1:G:210:GLN:NE2	2.82	0.42
2:H:342:ASN:HD22	2:H:345:GLU:CG	2.32	0.42
1:A:155:MET:HE3	1:A:162:ARG:CD	2.50	0.42
1:E:163:GLY:HA2	1:E:227:MET:SD	2.60	0.42
1:G:189:LEU:HD22	1:G:233:CYS:SG	2.59	0.42
1:G:282:ILE:N	1:G:282:ILE:CD1	2.82	0.42
1:I:175(F):PRO:C	1:I:175(H):LEU:H	2.27	0.42
1:I:179:ARG:HG2	1:I:237:HIS:CE1	2.54	0.42
1:I:206:CYS:HB3	1:I:210:GLN:HB3	2.01	0.42
1:K:207:THR:O	1:K:208:VAL:C	2.62	0.42
1:C:282:ILE:HD13	2:D:329:LEU:CD1	2.49	0.42
1:G:175(G):LYS:O	1:G:175(H):LEU:HD23	2.20	0.42
2:J:390:THR:HG21	2:L:388:GLN:HE21	1.84	0.42
1:K:189:LEU:HD22	1:K:233:CYS:SG	2.60	0.42
2:B:381(B):ASP:O	2:B:381(B):ASP:OD1	2.37	0.42
2:D:381(C):LYS:O	2:D:381(D):LYS:C	2.62	0.42
1:I:155:MET:HG3	2:J:399:VAL:O	2.19	0.42
1:I:295:PRO:HB3	2:L:320:TYR:CE1	2.55	0.42
1:K:182:THR:O	1:K:183:HIS:C	2.62	0.42
2:L:366:ILE:HA	2:L:369:ILE:HD12	2.01	0.42
1:A:160:LYS:CB	1:A:161:PRO:HD3	2.50	0.42
2:B:362(B):ARG:HG2	2:B:362(B):ARG:HH11	1.85	0.42
1:C:241:GLY:H	1:C:286:GLN:NE2	2.18	0.42
2:J:342:ASN:HD22	2:J:345:GLU:HG2	1.84	0.42
2:J:382:MET:HE3	2:J:382:MET:HA	2.02	0.42
1:K:224:HIS:H	1:K:272:SER:CB	2.32	0.42
1:K:229:CYS:SG	1:K:230:PHE:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:ILE:O	1:G:235:LEU:HD23	2.20	0.42
1:G:297:GLU:C	1:G:297:GLU:CD	2.88	0.42
1:I:193:PHE:O	1:I:198:PHE:HB2	2.20	0.42
2:J:360:ARG:HD2	2:J:364:ASP:OD2	2.20	0.42
2:L:347:THR:O	2:L:351:GLN:HG2	2.19	0.42
1:A:184:LEU:HD23	2:B:345:GLU:C	2.44	0.41
1:C:243:ILE:CD1	1:C:256:ALA:HB3	2.49	0.41
2:D:334:VAL:HG13	2:D:386:MET:O	2.20	0.41
1:E:161:PRO:HG2	1:E:227:MET:SD	2.59	0.41
2:H:348:TRP:CE3	2:H:381:LYS:HB2	2.54	0.41
1:I:175(H):LEU:O	1:I:175(I):HIS:C	2.61	0.41
1:I:287:GLY:HA3	2:J:336:ASN:C	2.45	0.41
1:I:287:GLY:HA3	2:J:336:ASN:HA	2.02	0.41
1:A:271:PRO:C	1:A:273:LEU:H	2.28	0.41
2:B:365:ASP:O	2:B:368:THR:HB	2.21	0.41
2:H:370:LEU:HD23	2:H:370:LEU:HA	1.90	0.41
1:I:157:SER:OG	1:I:162:ARG:N	2.52	0.41
1:C:157:SER:O	1:C:162:ARG:NH1	2.53	0.41
2:D:347:THR:O	2:D:351:GLN:HG2	2.20	0.41
1:G:203:HIS:CG	1:G:214:ILE:HD13	2.55	0.41
1:I:161:PRO:HG2	1:I:227:MET:SD	2.60	0.41
1:A:165:CYS:HA	1:A:231:ILE:O	2.20	0.41
2:B:370:LEU:HD13	2:B:389:PRO:HB3	2.03	0.41
1:C:174:ALA:HA	1:C:175(B):ARG:NH1	2.36	0.41
1:C:175(B):ARG:HG3	1:C:176:ILE:CD1	2.50	0.41
1:I:175(E):VAL:CG2	1:I:248:GLY:HA3	2.50	0.41
1:I:260:GLU:OE1	1:I:260:GLU:HA	2.20	0.41
2:L:354:CYS:O	2:L:358:ARG:HG3	2.20	0.41
1:A:157:SER:HB3	1:A:228:ASP:HB2	2.01	0.41
2:B:386:MET:HE3	2:B:387:PRO:HD2	2.02	0.41
1:C:156:LYS:C	1:C:162:ARG:HH12	2.28	0.41
1:E:161:PRO:O	1:E:162:ARG:HB2	2.20	0.41
1:G:193:PHE:CE2	1:G:231:ILE:HD13	2.55	0.41
1:G:203:HIS:CD2	1:G:214:ILE:CD1	3.03	0.41
1:I:190:THR:O	1:I:194:GLU:HB2	2.21	0.41
1:K:203:HIS:CD2	1:K:214:ILE:HD13	2.55	0.41
1:A:263:SER:HB2	4:A:26:HOH:O	2.21	0.41
2:D:365:ASP:CB	2:D:397:LYS:HD2	2.51	0.41
1:G:283:GLN:HE21	1:G:283:GLN:C	2.28	0.41
1:I:149:LEU:C	1:I:149:LEU:HD23	2.46	0.41
1:C:175(C):GLU:O	1:C:175(C):GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:THR:O	1:C:183:HIS:C	2.63	0.41
1:C:240:LYS:HA	2:D:335:ASN:HD21	1.85	0.41
2:F:370:LEU:HD13	2:F:389:PRO:HB3	2.02	0.41
1:G:202:PRO:O	1:G:203:HIS:ND1	2.53	0.41
1:G:212:TYR:O	1:G:213:GLU:C	2.64	0.41
1:I:153:TYR:OH	2:J:326:ASP:OD1	2.33	0.41
2:L:386:MET:HE3	2:L:387:PRO:HD2	2.02	0.41
1:A:291:GLN:HB3	2:B:384:LYS:C	2.46	0.41
2:B:323:ASP:HB2	1:C:292:LYS:O	2.21	0.41
2:B:393:THR:O	2:B:394:LEU:C	2.64	0.41
1:C:298:THR:O	1:C:299:ASP:C	2.63	0.41
2:D:354:CYS:O	2:D:355:GLN:C	2.63	0.41
1:G:156:LYS:O	1:G:157:SER:C	2.64	0.41
1:G:299:ASP:CB	4:H:122:HOH:O	2.68	0.41
1:K:262:THR:HA	1:K:280:PHE:CZ	2.56	0.41
1:A:175(H):LEU:C	1:A:175(J):SER:N	2.78	0.41
1:A:185:ASP:O	1:A:189:LEU:HD22	2.21	0.41
1:A:288:ASP:OD1	1:A:288:ASP:N	2.54	0.41
1:C:281:PHE:C	1:C:282:ILE:HD12	2.46	0.41
2:D:349:TYR:N	4:D:50:HOH:O	2.23	0.41
1:E:245:GLY:C	1:E:247:ASP:H	2.29	0.41
1:E:271:PRO:C	1:E:273:LEU:N	2.78	0.41
1:G:168:ILE:CD1	1:G:211:ILE:HG23	2.51	0.41
2:L:373:VAL:O	2:L:377:VAL:HG23	2.21	0.41
1:C:243:ILE:H	1:C:243:ILE:HG13	1.62	0.41
2:D:377:VAL:HG11	2:D:385:GLN:HG2	2.03	0.41
1:E:190:THR:O	1:E:194:GLU:HB2	2.21	0.41
2:J:369:ILE:O	2:J:373:VAL:HG23	2.21	0.41
1:K:175(I):HIS:CD2	1:K:175(J):SER:HB3	2.56	0.41
1:A:241:GLY:CA	1:A:286:GLN:HE22	2.35	0.40
1:G:298:THR:O	1:G:299:ASP:C	2.64	0.40
1:I:282:ILE:N	1:I:282:ILE:CD1	2.84	0.40
1:I:291:GLN:NE2	2:L:324:GLU:H	2.19	0.40
2:J:366:ILE:HG21	2:J:398:LEU:HD23	2.03	0.40
2:J:381(D):LYS:C	2:J:382:MET:N	2.78	0.40
1:K:289:ASN:HB2	2:L:336:ASN:O	2.21	0.40
1:E:258:ILE:HD12	1:E:282:ILE:HG12	2.03	0.40
1:I:294:ILE:HG22	1:K:268:LEU:HD21	2.04	0.40
2:J:392:PHE:CE2	2:L:389:PRO:HG2	2.56	0.40
1:K:165:CYS:HA	1:K:231:ILE:O	2.21	0.40
1:E:179:ARG:HG2	1:E:237:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:378:SER:O	2:F:384:LYS:NZ	2.53	0.40
2:H:378:SER:O	2:H:384:LYS:HE2	2.22	0.40
2:H:381(E):ASN:C	2:H:382:MET:HG2	2.47	0.40
1:I:179:ARG:HA	2:J:341:ARG:CZ	2.51	0.40
1:K:265:PHE:CD1	1:K:265:PHE:N	2.89	0.40
1:G:294:ILE:O	1:G:294:ILE:HG12	2.20	0.40
2:H:381(C):LYS:HD3	2:H:381(C):LYS:HA	1.69	0.40
1:I:175(G):LYS:HG3	1:I:175(H):LEU:HD23	2.03	0.40
2:L:397:LYS:HA	4:L:124:HOH:O	2.20	0.40
1:A:245:GLY:C	1:A:247:ASP:H	2.29	0.40
2:B:341:ARG:NH1	3:T:4103:ASP:OD1	2.52	0.40
2:B:370:LEU:HA	2:B:370:LEU:HD23	1.84	0.40
1:E:179:ARG:HA	2:F:341:ARG:CZ	2.51	0.40
1:E:179:ARG:CD	1:E:236:SER:HA	2.51	0.40
2:L:329:LEU:HD12	2:L:330:GLY:N	2.36	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	151/153 (99%)	125 (83%)	20 (13%)	6 (4%)	2	8
1	C	151/153 (99%)	121 (80%)	23 (15%)	7 (5%)	2	6
1	E	151/153 (99%)	125 (83%)	21 (14%)	5 (3%)	3	11
1	G	151/153 (99%)	125 (83%)	15 (10%)	11 (7%)	1	2
1	I	151/153 (99%)	126 (83%)	18 (12%)	7 (5%)	2	6
1	K	151/153 (99%)	125 (83%)	19 (13%)	7 (5%)	2	6
2	B	86/88 (98%)	74 (86%)	8 (9%)	4 (5%)	2	6
2	D	86/88 (98%)	70 (81%)	15 (17%)	1 (1%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	86/88 (98%)	76 (88%)	8 (9%)	2 (2%)	5	18
2	H	86/88 (98%)	70 (81%)	15 (17%)	1 (1%)	10	34
2	J	86/88 (98%)	76 (88%)	6 (7%)	4 (5%)	2	6
2	L	86/88 (98%)	71 (83%)	14 (16%)	1 (1%)	10	34
3	T	1/5 (20%)	1 (100%)	0	0	100	100
3	U	1/5 (20%)	1 (100%)	0	0	100	100
3	V	1/5 (20%)	1 (100%)	0	0	100	100
3	W	1/5 (20%)	1 (100%)	0	0	100	100
3	X	1/5 (20%)	1 (100%)	0	0	100	100
3	Y	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1428/1476 (97%)	1190 (83%)	182 (13%)	56 (4%)	2	8

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	175(D)	LYS
1	A	296	VAL
2	B	381(C)	LYS
2	B	381(D)	LYS
1	C	296	VAL
1	E	157	SER
1	E	296	VAL
2	F	381(D)	LYS
1	G	296	VAL
1	I	157	SER
1	I	175(D)	LYS
1	I	175(I)	HIS
1	I	296	VAL
2	J	381(D)	LYS
1	K	175(I)	HIS
1	K	296	VAL
1	A	175(I)	HIS
1	C	266	THR
1	E	175(G)	LYS
2	F	336	ASN
1	G	175(G)	LYS
1	G	240	LYS

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Mol	Chain	Res	Type
1	G	266	THR
1	I	266	THR
1	K	266	THR
2	B	336	ASN
1	C	175(G)	LYS
1	C	240	LYS
2	D	345	GLU
1	E	175(F)	PRO
1	E	175(I)	HIS
1	G	175(I)	HIS
2	H	345	GLU
2	J	336	ASN
2	J	381(C)	LYS
1	K	162	ARG
1	K	240	LYS
2	L	345	GLU
2	B	381(E)	ASN
1	C	157	SER
1	G	162	ARG
1	G	175(F)	PRO
1	G	205	ASP
1	I	175(G)	LYS
1	I	240	LYS
2	J	382	MET
1	A	175(G)	LYS
1	A	240	LYS
1	C	160	LYS
1	C	191	THR
1	G	157	SER
1	G	160	LYS
1	K	160	LYS
1	K	161	PRO
1	G	161	PRO

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	135/135 (100%)	102 (76%)	33 (24%)	1	2
1	C	135/135 (100%)	115 (85%)	20 (15%)	3	10
1	E	135/135 (100%)	113 (84%)	22 (16%)	2	8
1	G	135/135 (100%)	117 (87%)	18 (13%)	4	14
1	I	135/135 (100%)	101 (75%)	34 (25%)	0	2
1	K	135/135 (100%)	115 (85%)	20 (15%)	3	10
2	B	81/81 (100%)	63 (78%)	18 (22%)	1	3
2	D	81/81 (100%)	66 (82%)	15 (18%)	1	6
2	F	81/81 (100%)	63 (78%)	18 (22%)	1	3
2	H	81/81 (100%)	60 (74%)	21 (26%)	0	2
2	J	81/81 (100%)	63 (78%)	18 (22%)	1	3
2	L	81/81 (100%)	66 (82%)	15 (18%)	1	6
3	T	3/3 (100%)	3 (100%)	0	100	100
3	U	3/3 (100%)	3 (100%)	0	100	100
3	V	3/3 (100%)	3 (100%)	0	100	100
3	W	3/3 (100%)	3 (100%)	0	100	100
3	X	3/3 (100%)	3 (100%)	0	100	100
3	Y	3/3 (100%)	3 (100%)	0	100	100
All	All	1314/1314 (100%)	1062 (81%)	252 (19%)	1	5

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ASP
1	A	151	LYS
1	A	154	GLN
1	A	156	LYS
1	A	160	LYS
1	A	166	LEU
1	A	175	LYS
1	A	175(B)	ARG
1	A	175(C)	GLU
1	A	175(D)	LYS
1	A	175(E)	VAL
1	A	175(F)	PRO
1	A	175(G)	LYS
1	A	175(H)	LEU

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Mol	Chain	Res	Type
1	A	175(I)	HIS
1	A	175(J)	SER
1	A	176	ILE
1	A	182	THR
1	A	183	HIS
1	A	189	LEU
1	A	190	THR
1	A	210	GLN
1	A	211	ILE
1	A	213	GLU
1	A	235	LEU
1	A	243	ILE
1	A	246	THR
1	A	262	THR
1	A	264	GLN
1	A	294	ILE
1	A	296	VAL
1	A	298	THR
1	A	299	ASP
2	B	326	ASP
2	B	329	LEU
2	B	335	ASN
2	B	336	ASN
2	B	345	GLU
2	B	358	ARG
2	B	365	ASP
2	B	366	ILE
2	B	367	LEU
2	B	381	LYS
2	B	381(A)	ASP
2	B	381(B)	ASP
2	B	381(C)	LYS
2	B	381(D)	LYS
2	B	381(E)	ASN
2	B	382	MET
2	B	384	LYS
2	B	397	LYS
1	C	150	ASP
1	C	157	SER
1	C	162	ARG
1	C	176	ILE
1	C	179	ARG

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Mol	Chain	Res	Type
1	C	182	THR
1	C	189	LEU
1	C	195	GLU
1	C	199	GLU
1	C	208	VAL
1	C	210	GLN
1	C	213	GLU
1	C	219	GLN
1	C	243	ILE
1	C	246	THR
1	C	272	SER
1	C	294	ILE
1	C	297	GLU
1	C	298	THR
1	C	299	ASP
2	D	324	GLU
2	D	326	ASP
2	D	335	ASN
2	D	339	SER
2	D	341	ARG
2	D	356	SER
2	D	358	ARG
2	D	360	ARG
2	D	365	ASP
2	D	366	ILE
2	D	367	LEU
2	D	384	LYS
2	D	385	GLN
2	D	395	ARG
2	D	396	LYS
1	E	150	ASP
1	E	151	LYS
1	E	156	LYS
1	E	160	LYS
1	E	176	ILE
1	E	182	THR
1	E	183	HIS
1	E	189	LEU
1	E	190	THR
1	E	194	GLU
1	E	210	GLN
1	E	211	ILE

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Mol	Chain	Res	Type
1	E	235	LEU
1	E	243	ILE
1	E	246	THR
1	E	262	THR
1	E	264	GLN
1	E	282	ILE
1	E	283	GLN
1	E	294	ILE
1	E	296	VAL
1	E	299	ASP
2	F	326	ASP
2	F	329	LEU
2	F	335	ASN
2	F	336	ASN
2	F	345	GLU
2	F	358	ARG
2	F	365	ASP
2	F	366	ILE
2	F	367	LEU
2	F	381	LYS
2	F	381(A)	ASP
2	F	381(B)	ASP
2	F	381(C)	LYS
2	F	381(D)	LYS
2	F	381(E)	ASN
2	F	382	MET
2	F	384	LYS
2	F	397	LYS
1	G	150	ASP
1	G	162	ARG
1	G	176	ILE
1	G	179	ARG
1	G	182	THR
1	G	195	GLU
1	G	205	ASP
1	G	208	VAL
1	G	210	GLN
1	G	213	GLU
1	G	219	GLN
1	G	243	ILE
1	G	246	THR
1	G	272	SER

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Mol	Chain	Res	Type
1	G	294	ILE
1	G	297	GLU
1	G	298	THR
1	G	299	ASP
2	H	324	GLU
2	H	326	ASP
2	H	335	ASN
2	H	339	SER
2	H	341	ARG
2	H	355	GLN
2	H	356	SER
2	H	358	ARG
2	H	360	ARG
2	H	365	ASP
2	H	366	ILE
2	H	367	LEU
2	H	381	LYS
2	H	381(A)	ASP
2	H	381(B)	ASP
2	H	381(C)	LYS
2	H	381(D)	LYS
2	H	381(E)	ASN
2	H	385	GLN
2	H	395	ARG
2	H	396	LYS
1	I	150	ASP
1	I	151	LYS
1	I	154	GLN
1	I	156	LYS
1	I	157	SER
1	I	160	LYS
1	I	166	LEU
1	I	175	LYS
1	I	175(B)	ARG
1	I	175(C)	GLU
1	I	175(D)	LYS
1	I	175(E)	VAL
1	I	175(F)	PRO
1	I	175(G)	LYS
1	I	175(H)	LEU
1	I	175(I)	HIS
1	I	175(J)	SER

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Mol	Chain	Res	Type
1	I	176	ILE
1	I	182	THR
1	I	183	HIS
1	I	184	LEU
1	I	189	LEU
1	I	190	THR
1	I	194	GLU
1	I	210	GLN
1	I	211	ILE
1	I	235	LEU
1	I	243	ILE
1	I	246	THR
1	I	262	THR
1	I	264	GLN
1	I	294	ILE
1	I	296	VAL
1	I	299	ASP
2	J	326	ASP
2	J	329	LEU
2	J	335	ASN
2	J	336	ASN
2	J	345	GLU
2	J	358	ARG
2	J	365	ASP
2	J	366	ILE
2	J	367	LEU
2	J	381	LYS
2	J	381(A)	ASP
2	J	381(B)	ASP
2	J	381(C)	LYS
2	J	381(D)	LYS
2	J	381(E)	ASN
2	J	382	MET
2	J	384	LYS
2	J	397	LYS
1	K	150	ASP
1	K	162	ARG
1	K	176	ILE
1	K	179	ARG
1	K	182	THR
1	K	189	LEU
1	K	190	THR

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Mol	Chain	Res	Type
1	K	195	GLU
1	K	208	VAL
1	K	210	GLN
1	K	213	GLU
1	K	216	LYS
1	K	219	GLN
1	K	243	ILE
1	K	246	THR
1	K	272	SER
1	K	294	ILE
1	K	297	GLU
1	K	298	THR
1	K	299	ASP
2	L	324	GLU
2	L	326	ASP
2	L	329	LEU
2	L	335	ASN
2	L	339	SER
2	L	341	ARG
2	L	356	SER
2	L	358	ARG
2	L	360	ARG
2	L	365	ASP
2	L	366	ILE
2	L	367	LEU
2	L	384	LYS
2	L	395	ARG
2	L	396	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	175(I)	HIS
1	A	183	HIS
1	A	210	GLN
1	A	286	GLN
1	A	291	GLN
2	B	335	ASN
2	B	381(E)	ASN
1	C	169	ASN
1	C	175(I)	HIS

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Mol	Chain	Res	Type
1	C	203	HIS
1	C	210	GLN
1	C	286	GLN
1	C	291	GLN
2	D	335	ASN
2	D	336	ASN
1	E	210	GLN
1	E	286	GLN
1	E	291	GLN
2	F	381(E)	ASN
1	G	169	ASN
1	G	175(I)	HIS
1	G	210	GLN
1	G	264	GLN
1	G	286	GLN
1	G	291	GLN
2	H	335	ASN
2	H	336	ASN
2	H	355	GLN
1	I	154	GLN
1	I	171	HIS
1	I	210	GLN
1	I	286	GLN
1	I	291	GLN
2	J	335	ASN
2	J	381(E)	ASN
2	J	388	GLN
1	K	169	ASN
1	K	210	GLN
1	K	264	GLN
1	K	283	GLN
1	K	286	GLN
1	K	291	GLN
2	L	335	ASN
2	L	336	ASN
2	L	355	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	153/153 (100%)	0.41	9 (5%) 28 21	19, 38, 80, 100	0
1	C	153/153 (100%)	0.50	7 (4%) 37 29	21, 45, 77, 100	0
1	E	153/153 (100%)	0.55	10 (6%) 25 18	23, 42, 86, 100	0
1	G	153/153 (100%)	0.66	12 (7%) 19 14	21, 49, 89, 100	0
1	I	153/153 (100%)	0.54	10 (6%) 25 18	18, 45, 81, 100	0
1	K	153/153 (100%)	0.48	8 (5%) 33 25	22, 44, 85, 100	0
2	B	88/88 (100%)	0.28	4 (4%) 38 30	21, 39, 72, 100	0
2	D	88/88 (100%)	0.49	5 (5%) 29 22	26, 41, 79, 100	0
2	F	88/88 (100%)	0.55	5 (5%) 29 22	20, 48, 82, 100	0
2	H	88/88 (100%)	0.61	4 (4%) 38 30	20, 51, 94, 100	0
2	J	88/88 (100%)	0.57	6 (6%) 23 17	25, 46, 82, 98	0
2	L	88/88 (100%)	0.56	6 (6%) 23 17	22, 47, 94, 100	0
3	T	3/5 (60%)	1.18	0 100 100	51, 51, 54, 64	0
3	U	3/5 (60%)	1.16	0 100 100	51, 51, 60, 70	0
3	V	3/5 (60%)	1.00	0 100 100	58, 58, 60, 67	0
3	W	3/5 (60%)	1.55	2 (66%) 0 0	57, 57, 67, 74	0
3	X	3/5 (60%)	1.62	0 100 100	61, 61, 64, 70	0
3	Y	3/5 (60%)	1.22	0 100 100	53, 53, 58, 60	0
All	All	1464/1476 (99%)	0.53	88 (6%) 27 21	18, 45, 86, 100	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	298	THR	6.2
1	I	298	THR	6.1
1	C	298	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	298	THR	5.7
1	K	298	THR	4.4
1	I	296	VAL	4.1
1	E	175(I)	HIS	4.0
1	A	183	HIS	3.9
1	K	175(I)	HIS	3.8
1	I	149	LEU	3.8
1	C	149	LEU	3.8
1	C	160	LYS	3.8
1	G	299	ASP	3.7
1	A	149	LEU	3.7
1	I	183	HIS	3.6
1	G	183	HIS	3.5
1	E	160	LYS	3.5
1	G	209	GLU	3.4
1	K	160	LYS	3.4
1	E	149	LEU	3.4
1	C	299	ASP	3.4
1	G	160	LYS	3.2
1	E	299	ASP	3.0
1	A	175(D)	LYS	3.0
1	K	161	PRO	3.0
2	L	319	ARG	2.9
2	B	318	THR	2.9
1	G	293	GLY	2.9
2	J	382	MET	2.8
1	K	204	HIS	2.7
1	E	150	ASP	2.7
2	B	355	GLN	2.7
1	A	160	LYS	2.6
2	F	382	MET	2.6
1	I	151	LYS	2.6
2	D	381(D)	LYS	2.6
2	L	345	GLU	2.6
2	L	382	MET	2.5
2	F	318	THR	2.5
1	K	176	ILE	2.5
1	C	297	GLU	2.5
1	E	175(D)	LYS	2.5
2	L	318	THR	2.4
2	D	336	ASN	2.4
1	E	161	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	381(D)	LYS	2.4
1	I	259	TYR	2.4
2	H	381(C)	LYS	2.4
2	J	381(A)	ASP	2.3
1	A	298	THR	2.3
1	I	180	ASN	2.3
1	G	149	LEU	2.3
1	K	175(D)	LYS	2.3
3	W	4402	VAL	2.3
3	W	4401	GLU	2.3
1	G	246	THR	2.3
2	J	362	PRO	2.3
1	C	292	LYS	2.2
1	K	177	ARG	2.2
2	F	376	GLU	2.2
1	I	240	LYS	2.2
2	H	399	VAL	2.2
2	L	339	SER	2.2
2	B	382	MET	2.2
2	D	401	PRO	2.2
2	H	348	TRP	2.2
1	G	161	PRO	2.2
2	F	323	ASP	2.2
2	J	318	THR	2.2
2	D	381(C)	LYS	2.2
2	L	320	TYR	2.2
1	G	176	ILE	2.1
2	D	355	GLN	2.1
1	I	299	ASP	2.1
1	A	259	TYR	2.1
2	H	355	GLN	2.1
1	G	175(I)	HIS	2.1
1	A	240	LYS	2.1
1	I	292	LYS	2.1
1	A	296	VAL	2.1
1	C	176	ILE	2.1
1	E	151	LYS	2.0
1	G	154	GLN	2.0
2	J	376	GLU	2.0
2	B	319	ARG	2.0
2	J	321	ILE	2.0
1	A	175(C)	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	296	VAL	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.