Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 10:17 AM EDT

PDB ID	:	1QDU
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 (i) 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 (i)) were used in the production of this report:

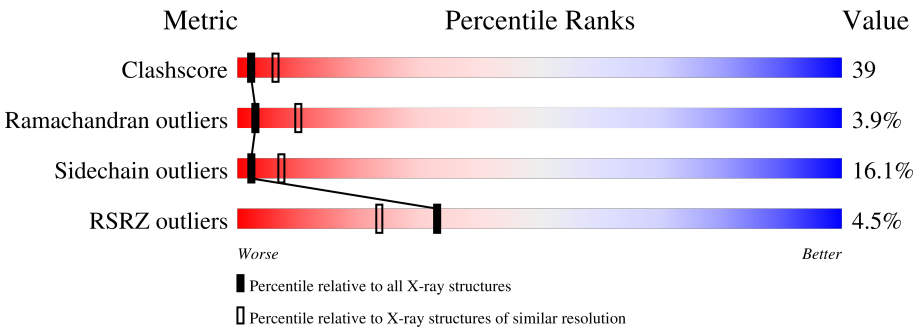
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	.%, 42%, 44%, 13%, •
1	C	153	3%, 44%, 45%, 10%, •
1	E	153	3%, 47%, 41%, 10%, •
1	G	153	7%, 45%, 41%, 12%, •
1	I	153	4%, 43%, 43%, 12%, •
1	K	153	3%, 44%, 44%, 11%, •
2	B	88	3%, 35%, 51%, 10%, •

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Mol	Chain	Length	Quality of chain
2	D	88	7% 32% 52% 16%
2	F	88	9% 36% 53% 10%
2	H	88	8% 33% 53% 14%
2	J	88	6% 36% 50% 10%
2	L	88	7% 35% 51% 14%
3	T	5	60% 40%
3	U	5	60% 20% 20%
3	V	5	60% 20% 20%
3	W	5	40% 20% 40%
3	X	5	60% 40%
3	Y	5	40% 40% 20%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	153	1220	774	208	228	10	0	0	0
1	C	153	1220	774	208	228	10	0	0	0
1	E	153	1220	774	208	228	10	0	0	0
1	G	153	1220	774	208	228	10	0	0	0
1	I	153	1220	774	208	228	10	0	0	0
1	K	153	1220	774	208	228	10	0	0	0

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
			Total	C	N	O	S			
2	B	88	712	447	123	136	6	0	0	0
2	D	88	712	447	123	136	6	0	0	0
2	F	88	712	447	123	136	6	0	0	0

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

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

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

- Molecule 4 is water.

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

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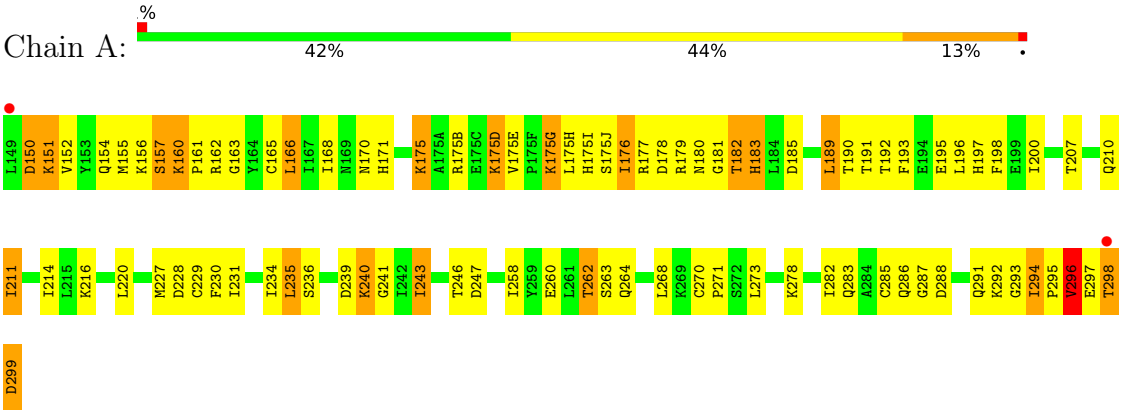
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	6	6	6	0	0
			Total	O		
4	I	6	6	6	0	0
			Total	O		
4	J	4	4	4	0	0
			Total	O		
4	K	20	20	20	0	0
			Total	O		
4	L	11	11	11	0	0
			Total	O		
4	Y	1	1	1	0	0

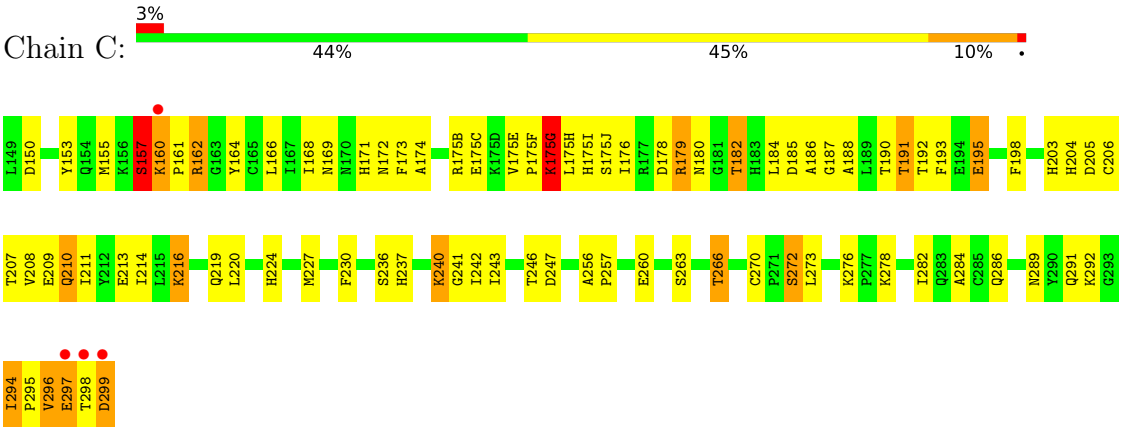
3 Residue-property plots (i)

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.

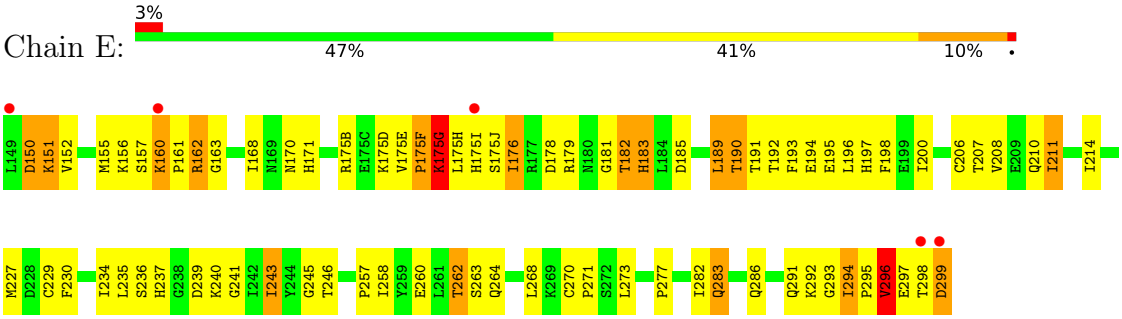
• Molecule 1: CASPASE-8 ALPHA-CHAIN



• Molecule 1: CASPASE-8 ALPHA-CHAIN

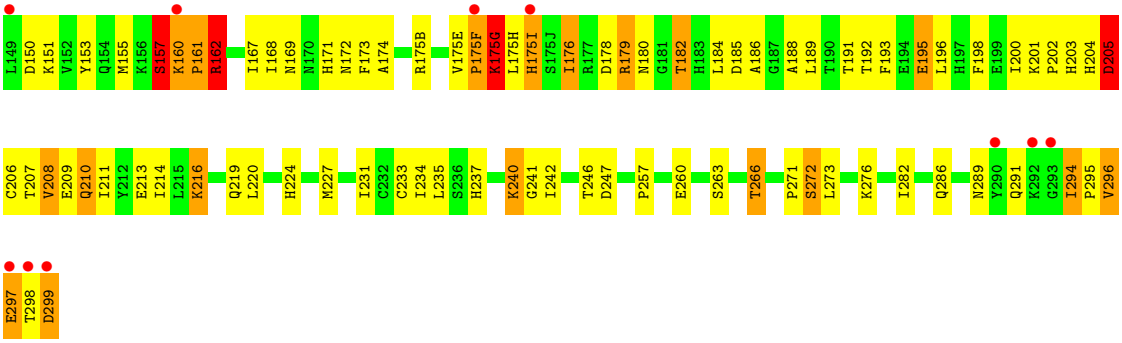


• Molecule 1: CASPASE-8 ALPHA-CHAIN



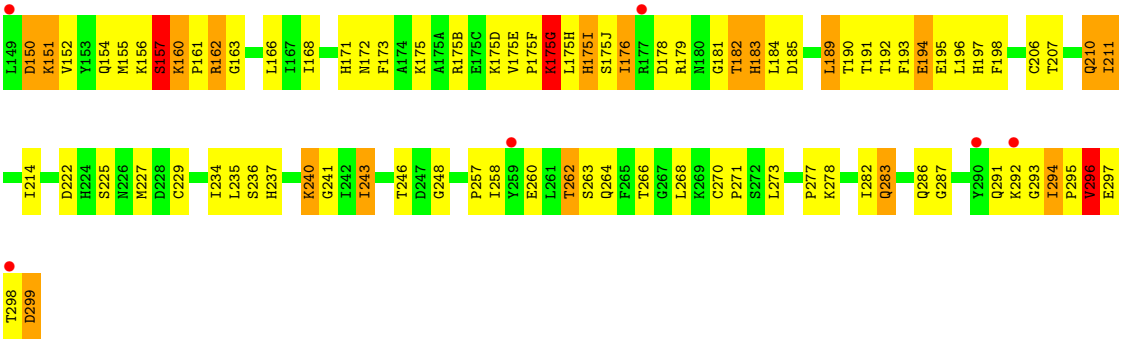
- Molecule 1: CASPASE-8 ALPHA-CHAIN

Chain G:



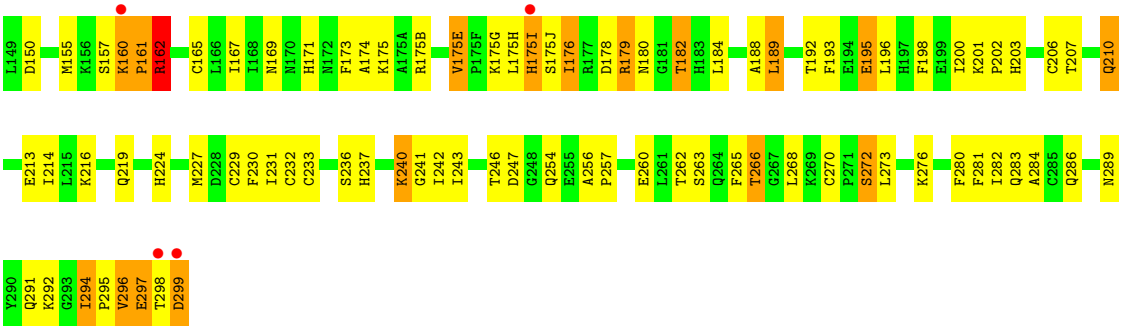
- Molecule 1: CASPASE-8 ALPHA-CHAIN

Chain I:



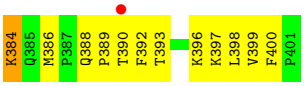
- Molecule 1: CASPASE-8 ALPHA-CHAIN

Chain K:



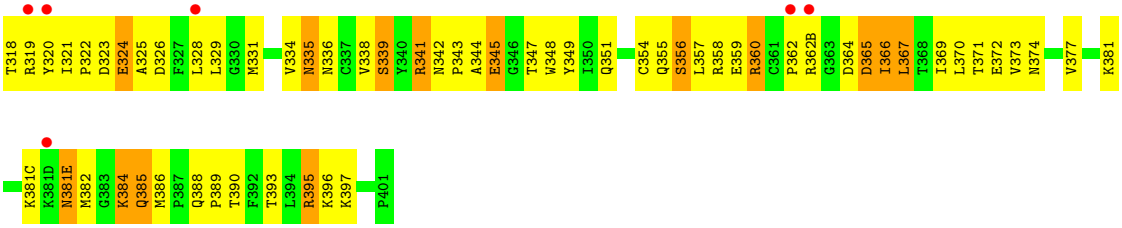
- Molecule 2: CASPASE-8 BETA-CHAIN

Chain B:



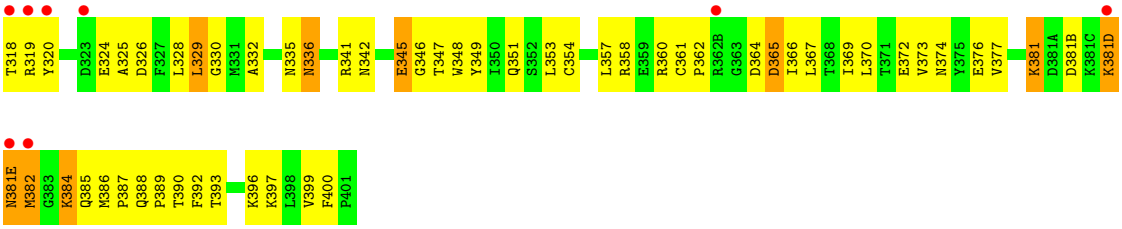
• Molecule 2: CASPASE-8 BETA-CHAIN

Chain D:



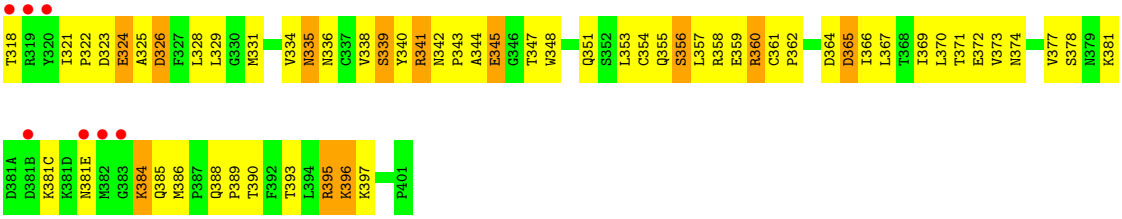
• Molecule 2: CASPASE-8 BETA-CHAIN

Chain F:



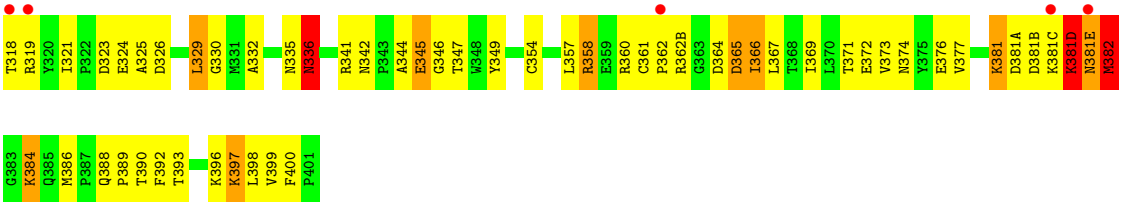
• Molecule 2: CASPASE-8 BETA-CHAIN

Chain H:



• Molecule 2: CASPASE-8 BETA-CHAIN

Chain J:



• Molecule 2: CASPASE-8 BETA-CHAIN

Chain L: 7% 35% 51% 14%

T318 R319 Y320 I321 P322 D323 E324 A325 D326 L329 G330 M331 V334 N335 N336 C337 V338 S339 Y340 R341 N342 P343 A344 E345 G346 T347 Q351 C354 Q355 S356 L357 R358 E359 R360 C361 P362 R362B D365 I366 L367 T368 I369 L370 T371 E372 V373 N374 V377 K381C K381D N381E M382 G383

K384 Q385 M386 P387 Q388 P389 T390 F392 T393 L394 R395 K396 K397 P401

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

Chain T: 60% 40%

PHQ4100 E4101 V4102 D4103 OQE4104

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

Chain U: 60% 20% 20%

PHQ4200 E4201 V4202 D4203 OQE4204

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

Chain V: 60% 20% 20%

PHQ4300 E4301 V4302 D4303 OQE4304

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

Chain W: 40% 20% 40%

PHQ4400 E4401 V4402 D4403 OQE4404

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

Chain X: 60% 40%

PHQ4500 E4501 V4502 D4503 OQE4504

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

Chain Y: 40% 40% 20%

PHQ4600
E4601
V4602
D4603
OQE4604

4 Data and refinement statistics (i)

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 29.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (100.00-2.80) 84.9 (29.39-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.302 0.237 , (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 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PHQ, 0QE

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	0.55	0/1248	0.70	0/1682
1	C	0.53	0/1248	0.67	0/1682
1	E	0.53	0/1248	0.69	0/1682
1	G	0.51	0/1248	0.66	0/1682
1	I	0.53	0/1248	0.69	0/1682
1	K	0.51	0/1248	0.66	0/1682
2	B	0.50	0/726	0.69	0/981
2	D	0.49	0/726	0.70	0/981
2	F	0.47	0/726	0.69	0/981
2	H	0.48	0/726	0.66	0/981
2	J	0.47	0/726	0.69	0/981
2	L	0.50	0/726	0.66	0/981
3	T	2.18	1/23 (4.3%)	2.82	2/30 (6.7%)
3	U	2.28	1/23 (4.3%)	2.73	2/30 (6.7%)
3	V	2.25	1/23 (4.3%)	2.65	2/30 (6.7%)
3	W	2.25	1/23 (4.3%)	2.68	2/30 (6.7%)
3	X	2.27	1/23 (4.3%)	2.72	2/30 (6.7%)
3	Y	2.26	1/23 (4.3%)	2.63	2/30 (6.7%)
All	All	0.56	6/11982 (0.1%)	0.74	12/16158 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	4201	GLU	CD-OE2	7.75	1.34	1.25
3	T	4101	GLU	CD-OE2	7.55	1.33	1.25
3	Y	4601	GLU	CD-OE2	7.48	1.33	1.25
3	V	4301	GLU	CD-OE2	7.35	1.33	1.25
3	X	4501	GLU	CD-OE2	7.25	1.33	1.25
3	W	4401	GLU	CD-OE2	7.24	1.33	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	4103	ASP	CB-CG-OD1	9.56	126.91	118.30
3	U	4203	ASP	CB-CG-OD1	9.22	126.60	118.30
3	T	4103	ASP	CB-CG-OD2	-9.01	110.19	118.30
3	U	4203	ASP	CB-CG-OD2	-8.96	110.23	118.30
3	X	4503	ASP	CB-CG-OD2	-8.92	110.27	118.30
3	V	4303	ASP	CB-CG-OD1	8.84	126.25	118.30
3	X	4503	ASP	CB-CG-OD1	8.81	126.23	118.30
3	W	4403	ASP	CB-CG-OD1	8.74	126.17	118.30
3	Y	4603	ASP	CB-CG-OD1	8.66	126.10	118.30
3	W	4403	ASP	CB-CG-OD2	-8.54	110.61	118.30
3	Y	4603	ASP	CB-CG-OD2	-8.22	110.90	118.30
3	V	4303	ASP	CB-CG-OD2	-7.95	111.14	118.30

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	107	0
1	C	1220	0	1198	102	0
1	E	1220	0	1198	99	0
1	G	1220	0	1198	114	0
1	I	1220	0	1198	99	0
1	K	1220	0	1198	107	0
2	B	712	0	707	77	0
2	D	712	0	707	75	0
2	F	712	0	707	73	0
2	H	712	0	707	73	0
2	J	712	0	707	71	0
2	L	712	0	707	76	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	906	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 39.

All (906) 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:H:360:ARG:HH11	2:H:360:ARG:HB3	1.34	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:295:PRO:O	1:A:296:VAL:HG13	1.83	0.78
2:B:381(E):ASN:ND2	2:B:381(E):ASN:H	1.81	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:J:388:GLN:HE21	2:L:390:THR:HG21	1.50	0.77
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
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
1:A:234:ILE:C	1:A:235:LEU:HD23	2.08	0.74
2:D:325:ALA:HA	2:D:393:THR:HG21	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:396:LYS:NZ	1:K:299:ASP:HA	2.04	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
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
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:B:329:LEU:HD12	2:B:330:GLY:N	2.07	0.70
2:F:386:MET:CE	2:H:393:THR:HG23	2.22	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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:396:LYS:HZ3	1:G:299:ASP:HA	1.58	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
1:C:260:GLU:HA	1:C:260:GLU:OE1	1.95	0.66
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:A:155:MET:HE3	1:A:162:ARG:HD3	1.79	0.65
1:K:175(E):VAL:HG11	1:K:175(H):LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:234:ILE:C	1:E:235:LEU:HD23	2.16	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:E:175(B):ARG:HH22	1:E:178:ASP:CG	2.01	0.63
2:H:325:ALA:HA	2:H:393:THR:CG2	2.29	0.63
1:I:155:MET:HE3	1:I:162:ARG:HD3	1.81	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
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
1:A:155:MET:HE3	1:A:162:ARG:CD	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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:C:155:MET:HE3	1:C:162:ARG:HD2	1.83	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
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:F:393:THR:HG23	2:H:386:MET:CE	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:GLN:HE21	2:J:347:THR:CB	2.16	0.59
1:K:231:ILE:C	4:K:126:HOH:O	2.41	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
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: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
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
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
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
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
2:B:396:LYS:HZ3	1:C:299:ASP:HA	1.69	0.57
1:K:155:MET:HE3	1:K:162:ARG:CD	2.34	0.57
1:A:207:THR:N	1:A:210:GLN:NE2	2.38	0.57
1:G:282:ILE:N	1:G:282:ILE:HD12	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:155:MET:HE3	1:C:162:ARG:CD	2.35	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
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
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: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:E:234:ILE:O	1:E:235:LEU:HD23	2.05	0.56
2:D:355:GLN:NE2	4:D:41:HOH:O	2.37	0.56
2:J:396:LYS:HZ1	1:K:299:ASP:HA	1.70	0.56
1:A:262:THR:HG22	1:A:263:SER:N	2.21	0.56
2:B:393:THR:HG23	2:D:386:MET:CE	2.36	0.56
1:E:182:THR:O	1:E:185:ASP:N	2.38	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: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:C:289:ASN:O	2:D:338:VAL:HG13	2.05	0.55
1:G:185:ASP:OD2	2:H:347:THR:HG23	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:381(E):ASN:O	2:B:382:MET:C	2.45	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: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
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: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:I:182:THR:O	1:I:183:HIS:C	2.46	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: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:E:182:THR:O	1:E:183:HIS:C	2.46	0.54
1:A:192:THR:HG21	2:B:354:CYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:393:THR:O	2:L:393:THR:CG2	2.56	0.54
1:E:295:PRO:C	1:E:296:VAL:HG22	2.28	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:G:155:MET:HE3	1:G:162:ARG:HD2	1.91	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:381(E):ASN:O	2:J:382:MET:C	2.45	0.53
2:J:389:PRO:HG3	4:J:94:HOH:O	2.06	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: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:242:ILE:C	1:C:242:ILE:HD12	2.28	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
2:J:396:LYS:HZ3	1:K:299:ASP:HA	1.72	0.53
1:C:171:HIS:C	1:C:171:HIS:CD2	2.82	0.53
1:G:157:SER:O	1:G:162:ARG:NH1	2.41	0.53
1:G:171:HIS:C	1:G:171:HIS:CD2	2.82	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
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
1:E:283:GLN:CD	4:E:93:HOH:O	2.48	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:155:MET:HE3	1:K:162:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:388:GLN:HE21	2:D:390:THR:CG2	2.21	0.52
1:C:173:PHE:HB3	1:C:176:ILE:HD13	1.91	0.52
1:C:175(G):LYS:C	1:C:175(H):LEU:HD23	2.30	0.52
1:C:192:THR:HA	1:C:195:GLU:HG3	1.90	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
2:F:329:LEU:HD12	2:F:329:LEU:C	2.28	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:A:182:THR:O	1:A:183:HIS:C	2.47	0.52
1:E:190:THR:HG22	1:E:191:THR:N	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:381(D):LYS:C	2:F:382:MET:H	2.13	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
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:291:GLN:HE22	2:D:324:GLU:HB2	1.75	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
2:J:381(D):LYS:C	2:J:382:MET:H	2.13	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:I:295:PRO:C	1:I:296:VAL:HG22	2.31	0.51
1:C:157:SER:OG	1:C:162:ARG:HA	2.11	0.51
1:G:175(G):LYS:C	1:G:175(H):LEU:HD23	2.31	0.51
1:I:234:ILE:C	1:I:235:LEU:HD23	2.31	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:340:TYR:HA	3:W:4401:GLU:O	2.11	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:K:281:PHE:C	1:K:282:ILE:HD12	2.32	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: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
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:G:155:MET:HE3	1:G:162:ARG:CD	2.42	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(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:360:ARG:HH11	2:F:364:ASP:CG	2.16	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
2:F:396:LYS:HZ1	1:G:299:ASP:HA	1.74	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:I:179:ARG:HH12	1:I:182:THR:HG23	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:341:ARG:HA	2:L:347:THR:HA	1.95	0.49
1:A:163:GLY:HA3	1:A:229:CYS:O	2.12	0.49
2:B:381(B):ASP:O	2:B:381(B):ASP:CG	2.51	0.49
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
1:I:291:GLN:HE22	2:L:324:GLU:HB2	1.77	0.49
1:K:171:HIS:CD2	1:K:171:HIS:C	2.86	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:A:240:LYS:HG3	1:A:240:LYS:O	2.13	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:L:342:ASN:C	2:L:344:ALA:H	2.15	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
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:D:342:ASN:C	2:D:344:ALA:H	2.17	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
2:B:381(D):LYS:C	2:B:382:MET:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:GLN:HG2	2:B:388:GLN:O	2.12	0.47
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
1:G:234:ILE:C	1:G:235:LEU:HD23	2.34	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:K:283:GLN:C	1:K:283:GLN:HE21	2.18	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
1:E:150:ASP:OD1	1:E:150:ASP:N	2.46	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:B:354:CYS:O	2:B:358:ARG:HG3	2.15	0.47
1:E:262:THR:CG2	1:E:263:SER:N	2.78	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
1:C:294:ILE:O	1:C:294:ILE:HG12	2.14	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
2:D:381(E):ASN:C	2:D:382:MET:HG2	2.34	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
1:E:283:GLN:HE21	2:F:347:THR:CB	2.28	0.47
2:F:381(E):ASN:O	2:F:382:MET:C	2.52	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
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
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: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: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:207:THR:HG23	1:A:210:GLN:NE2	2.30	0.46
1:C:157:SER:O	1:C:160:LYS:C	2.53	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: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
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:175(D):LYS:O	1:E:175(E):VAL:C	2.54	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
1:A:239:ASP:O	1:A:240:LYS:C	2.53	0.46
2:B:375:TYR:HA	2:D:395:ARG:HG2	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:ILE:C	1:G:242:ILE:HD12	2.36	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
1:A:171:HIS:C	1:A:171:HIS:CD2	2.89	0.46
2:D:342:ASN:ND2	2:D:345:GLU:HG2	2.31	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:K:155:MET:HE3	1:K:162:ARG:HD3	1.98	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
2:B:381(B):ASP:O	2:B:381(C):LYS:C	2.54	0.45
1:I:270:CYS:SG	1:I:270:CYS:O	2.74	0.45
2:J:386:MET:HE1	2:L:393:THR:HG23	1.98	0.45
2:J:392:PHE:O	2:L:389:PRO:HD2	2.16	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:204:HIS:O	1:G:205:ASP:C	2.54	0.45
1:K:294:ILE:HG12	1:K:294:ILE:O	2.17	0.45
1:A:179:ARG:HA	2:B:341:ARG:CZ	2.46	0.45
1:E:155:MET:HE3	1:E:162:ARG:HD3	1.98	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
2:F:381(B):ASP:O	2:F:381(B):ASP:CG	2.52	0.45
1:A:162:ARG:HG3	1:A:197:HIS:O	2.16	0.45
1:A:270:CYS:O	1:A:270:CYS:SG	2.75	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
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:K:242:ILE:HD12	1:K:242:ILE:C	2.37	0.45
1:E:168:ILE:CD1	1:E:211:ILE:HG23	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:PRO:HG3	4:G:82:HOH:O	2.17	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:A:175(B):ARG:HH22	1:A:178:ASP:CG	2.20	0.45
1:C:153:TYR:OH	2:D:326:ASP:OD1	2.27	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
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: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
2:H:328:LEU:HD12	2:H:328:LEU:C	2.37	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
1:A:161:PRO:O	1:A:162:ARG:HB2	2.16	0.44
1:A:295:PRO:C	1:A:296:VAL:HG22	2.37	0.44
1:C:169:ASN:OD1	1:C:169:ASN:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:169:ASN:OD1	1:K:169:ASN:C	2.57	0.44
2:H:341:ARG:NH1	3:W:4403:ASP:OD1	2.51	0.44
2:H:342:ASN:C	2:H:344:ALA:H	2.21	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:155:MET:HE3	1:A:162:ARG:HD2	1.99	0.43
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
2:F:353:LEU:HD12	2:F:353:LEU:C	2.38	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: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
2:D:367:LEU:HD12	2:D:367:LEU:HA	1.70	0.43
1:G:161:PRO:O	1:G:162:ARG:C	2.56	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:C:184:LEU:HD12	1:C:184:LEU:H	1.82	0.43
1:E:229:CYS:SG	1:E:230:PHE:N	2.92	0.43
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
2:F:328:LEU:HD12	2:F:329:LEU:N	2.33	0.43
1:K:175(E):VAL:HG22	1:K:175(H):LEU:HG	1.99	0.43
1:C:155:MET:CE	1:C:162:ARG:HD2	2.49	0.43
1:E:171:HIS:C	1:E:171:HIS:CD2	2.91	0.43
1:K:207:THR:CG2	1:K:210:GLN:HE22	2.31	0.43
1:C:282:ILE:HD12	1:C:282:ILE:N	2.33	0.43
2:J:342:ASN:HD21	2:J:344:ALA:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:I:206:CYS:HA	1:I:210:GLN:NE2	2.33	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
2:L:342:ASN:HD22	2:L:345:GLU:CG	2.32	0.42
2:L:354:CYS:O	2:L:355:GLN:C	2.56	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: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
2:L:381(C):LYS:O	2:L:381(D):LYS:C	2.55	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
2:J:329:LEU:HD12	2:J:329:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:161:PRO:O	1:K:162:ARG:C	2.57	0.42
1:C:282:ILE:HD13	2:D:329:LEU:CD1	2.49	0.42
1:G:175(F):PRO:C	1:G:175(H):LEU:H	2.22	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
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:157:SER:O	1:K:160:LYS:C	2.58	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:393:THR:HG23	2:L:386:MET:CE	2.50	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
1:G:234:ILE:O	1:G:235:LEU:HD23	2.20	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: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
2:H:354:CYS:O	2:H:355:GLN:C	2.58	0.41
1:I:287:GLY:HA3	2:J:336:ASN:HA	2.02	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:I:171:HIS:CD2	1:I:171:HIS:C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:175(F):PRO:C	1:E:175(H):LEU:H	2.23	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
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
2:L:342:ASN:C	2:L:344:ALA:N	2.73	0.41
1:C:175(C):GLU:O	1:C:175(C):GLU:HG2	2.20	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:A:287:GLY:HA3	2:B:336:ASN:C	2.41	0.41
2:B:323:ASP:HB2	1:C:292:LYS:O	2.21	0.41
1:G:299:ASP:CB	4:H:122:HOH:O	2.68	0.41
1:I:175(F):PRO:C	1:I:175(H):LEU:N	2.74	0.41
1:K:262:THR:HA	1:K:280:PHE:CZ	2.56	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:204:HIS:O	1:C:205:ASP:C	2.59	0.41
2:D:349:TYR:N	4:D:50:HOH:O	2.23	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:161:PRO:O	1:C:162:ARG:C	2.59	0.41
1:C:243:ILE:H	1:C:243:ILE:HG13	1.62	0.41
2:D:342:ASN:C	2:D:344:ALA:N	2.74	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:E:271:PRO:C	1:E:273:LEU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:169:ASN:C	1:G:169:ASN:OD1	2.60	0.40
1:I:155:MET:HE3	1:I:162:ARG:CD	2.48	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:175(F):PRO:C	1:E:175(H):LEU:N	2.74	0.40
1:E:179:ARG:HG2	1:E:237:HIS:CE1	2.56	0.40
1:E:239:ASP:O	1:E:240:LYS:C	2.59	0.40
2:H:378:SER:O	2:H:384:LYS:HE2	2.22	0.40
1:I:179:ARG:HA	2:J:341:ARG:CZ	2.51	0.40
2:J:381(B):ASP:O	2:J:381(B):ASP:CG	2.58	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
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%)	3	9
1	C	151/153 (99%)	121 (80%)	23 (15%)	7 (5%)	2	7
1	E	151/153 (99%)	125 (83%)	21 (14%)	5 (3%)	4	13
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	7
1	K	151/153 (99%)	125 (83%)	19 (13%)	7 (5%)	2	7
2	B	86/88 (98%)	74 (86%)	8 (9%)	4 (5%)	2	7
2	D	86/88 (98%)	70 (81%)	15 (17%)	1 (1%)	13	39
2	F	86/88 (98%)	76 (88%)	8 (9%)	2 (2%)	6	21
2	H	86/88 (98%)	70 (81%)	15 (17%)	1 (1%)	13	39
2	J	86/88 (98%)	76 (88%)	6 (7%)	4 (5%)	2	7
2	L	86/88 (98%)	71 (83%)	14 (16%)	1 (1%)	13	39
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%)	3	10

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

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Mol	Chain	Res	Type
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
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 (i)

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%)	114 (84%)	21 (16%)	2	8
1	C	135/135 (100%)	118 (87%)	17 (13%)	4	14
1	E	135/135 (100%)	115 (85%)	20 (15%)	3	9
1	G	135/135 (100%)	115 (85%)	20 (15%)	3	9
1	I	135/135 (100%)	110 (82%)	25 (18%)	1	5
1	K	135/135 (100%)	116 (86%)	19 (14%)	3	10
2	B	81/81 (100%)	67 (83%)	14 (17%)	2	6
2	D	81/81 (100%)	64 (79%)	17 (21%)	1	3
2	F	81/81 (100%)	69 (85%)	12 (15%)	3	9
2	H	81/81 (100%)	66 (82%)	15 (18%)	1	5
2	J	81/81 (100%)	65 (80%)	16 (20%)	1	4
2	L	81/81 (100%)	65 (80%)	16 (20%)	1	4
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%)	1102 (84%)	212 (16%)	2	7

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ASP
1	A	151	LYS
1	A	156	LYS
1	A	160	LYS
1	A	166	LEU
1	A	175	LYS

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Mol	Chain	Res	Type
1	A	175(G)	LYS
1	A	176	ILE
1	A	182	THR
1	A	183	HIS
1	A	189	LEU
1	A	211	ILE
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	365	ASP
2	B	366	ILE
2	B	367	LEU
2	B	381	LYS
2	B	381(A)	ASP
2	B	381(C)	LYS
2	B	381(E)	ASN
2	B	382	MET
2	B	384	LYS
1	C	150	ASP
1	C	157	SER
1	C	162	ARG
1	C	175(G)	LYS
1	C	179	ARG
1	C	182	THR
1	C	195	GLU
1	C	210	GLN
1	C	213	GLU
1	C	216	LYS
1	C	219	GLN
1	C	246	THR
1	C	272	SER

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Mol	Chain	Res	Type
1	C	294	ILE
1	C	297	GLU
1	C	298	THR
1	C	299	ASP
2	D	324	GLU
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	362(B)	ARG
2	D	365	ASP
2	D	366	ILE
2	D	367	LEU
2	D	381(C)	LYS
2	D	381(E)	ASN
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	162	ARG
1	E	175(G)	LYS
1	E	176	ILE
1	E	182	THR
1	E	183	HIS
1	E	189	LEU
1	E	190	THR
1	E	211	ILE
1	E	243	ILE
1	E	246	THR
1	E	262	THR
1	E	264	GLN
1	E	283	GLN
1	E	294	ILE
1	E	296	VAL
1	E	299	ASP
2	F	326	ASP

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Mol	Chain	Res	Type
2	F	329	LEU
2	F	335	ASN
2	F	336	ASN
2	F	345	GLU
2	F	365	ASP
2	F	366	ILE
2	F	367	LEU
2	F	381	LYS
2	F	381(E)	ASN
2	F	382	MET
2	F	384	LYS
1	G	150	ASP
1	G	157	SER
1	G	162	ARG
1	G	175(G)	LYS
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	216	LYS
1	G	219	GLN
1	G	246	THR
1	G	272	SER
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	356	SER
2	H	358	ARG
2	H	360	ARG
2	H	365	ASP
2	H	366	ILE
2	H	367	LEU

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Mol	Chain	Res	Type
2	H	381(E)	ASN
2	H	384	LYS
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	162	ARG
1	I	175	LYS
1	I	175(G)	LYS
1	I	176	ILE
1	I	182	THR
1	I	183	HIS
1	I	184	LEU
1	I	189	LEU
1	I	194	GLU
1	I	210	GLN
1	I	211	ILE
1	I	243	ILE
1	I	246	THR
1	I	262	THR
1	I	264	GLN
1	I	283	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(D)	LYS
2	J	381(E)	ASN

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Mol	Chain	Res	Type
2	J	382	MET
2	J	384	LYS
2	J	397	LYS
1	K	150	ASP
1	K	162	ARG
1	K	175(E)	VAL
1	K	175(G)	LYS
1	K	176	ILE
1	K	179	ARG
1	K	182	THR
1	K	189	LEU
1	K	195	GLU
1	K	210	GLN
1	K	213	GLU
1	K	216	LYS
1	K	219	GLN
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	335	ASN
2	L	339	SER
2	L	341	ARG
2	L	356	SER
2	L	358	ARG
2	L	360	ARG
2	L	362(B)	ARG
2	L	365	ASP
2	L	366	ILE
2	L	367	LEU
2	L	381(E)	ASN
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	210	GLN
1	A	286	GLN
1	A	291	GLN
2	B	381(E)	ASN
1	C	169	ASN
1	C	175(I)	HIS
1	C	203	HIS
1	C	210	GLN
1	C	283	GLN
1	C	286	GLN
1	C	291	GLN
2	D	335	ASN
2	D	336	ASN
1	E	154	GLN
1	E	171	HIS
1	E	210	GLN
1	E	286	GLN
1	E	291	GLN
2	F	381(E)	ASN
2	F	388	GLN
1	G	169	ASN
1	G	210	GLN
1	G	219	GLN
1	G	283	GLN
1	G	286	GLN
1	G	291	GLN
2	H	335	ASN
2	H	336	ASN
1	I	154	GLN
1	I	171	HIS
1	I	180	ASN
1	I	210	GLN
1	I	286	GLN
1	I	291	GLN
2	J	381(E)	ASN
1	K	169	ASN
1	K	210	GLN
1	K	219	GLN
1	K	264	GLN
1	K	283	GLN
1	K	286	GLN

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Mol	Chain	Res	Type
1	K	291	GLN
2	L	335	ASN
2	L	336	ASN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.13	2 (1%)	77	72	19, 38, 80, 100	0
1	C	153/153 (100%)	0.12	4 (2%)	56	46	21, 45, 77, 100	0
1	E	153/153 (100%)	0.08	5 (3%)	46	36	23, 42, 86, 100	0
1	G	153/153 (100%)	0.27	10 (6%)	18	11	21, 49, 89, 100	0
1	I	153/153 (100%)	0.09	6 (3%)	39	29	18, 45, 81, 100	0
1	K	153/153 (100%)	-0.09	4 (2%)	56	46	22, 44, 85, 100	0
2	B	88/88 (100%)	0.07	3 (3%)	45	35	21, 39, 72, 100	0
2	D	88/88 (100%)	0.33	6 (6%)	17	10	26, 41, 79, 100	0
2	F	88/88 (100%)	0.34	8 (9%)	9	5	20, 48, 82, 100	0
2	H	88/88 (100%)	0.46	7 (7%)	12	6	20, 51, 94, 100	0
2	J	88/88 (100%)	0.46	5 (5%)	23	15	25, 46, 82, 98	0
2	L	88/88 (100%)	0.33	6 (6%)	17	10	22, 47, 94, 100	0
3	T	3/5 (60%)	0.13	0	100	100	51, 51, 54, 64	0
3	U	3/5 (60%)	0.19	0	100	100	51, 51, 60, 70	0
3	V	3/5 (60%)	-0.13	0	100	100	58, 58, 60, 67	0
3	W	3/5 (60%)	-0.07	0	100	100	57, 57, 67, 74	0
3	X	3/5 (60%)	0.40	0	100	100	61, 61, 64, 70	0
3	Y	3/5 (60%)	-0.21	0	100	100	53, 53, 58, 60	0
All	All	1464/1476 (99%)	0.16	66 (4%)	33	23	18, 45, 86, 100	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	298	THR	10.0
1	G	298	THR	8.6
1	E	298	THR	7.8

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Mol	Chain	Res	Type	RSRZ
1	I	298	THR	7.3
1	K	298	THR	5.9
1	G	299	ASP	5.8
1	E	149	LEU	4.9
1	G	292	LYS	4.7
2	H	381(E)	ASN	4.3
2	L	319	ARG	4.3
2	F	319	ARG	4.0
2	F	318	THR	3.9
1	G	149	LEU	3.8
2	D	362(B)	ARG	3.7
2	B	319	ARG	3.6
1	G	175(I)	HIS	3.6
1	C	297	GLU	3.5
2	J	381(E)	ASN	3.4
2	H	382	MET	3.4
1	A	149	LEU	3.3
1	C	299	ASP	3.2
1	K	160	LYS	3.1
2	F	320	TYR	3.1
2	J	319	ARG	3.1
1	E	299	ASP	3.1
2	J	318	THR	3.1
1	K	175(I)	HIS	3.1
1	E	175(I)	HIS	3.0
1	I	149	LEU	3.0
1	C	160	LYS	3.0
1	I	292	LYS	2.9
2	H	319	ARG	2.9
2	D	362	PRO	2.9
1	K	299	ASP	2.8
2	F	381(E)	ASN	2.8
1	G	175(F)	PRO	2.8
2	L	381(E)	ASN	2.8
1	I	290	TYR	2.8
2	F	381(D)	LYS	2.7
2	H	320	TYR	2.7
2	L	382	MET	2.7
1	G	290	TYR	2.6
1	G	160	LYS	2.6
1	G	297	GLU	2.5
2	J	362	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	381(D)	LYS	2.5
1	G	293	GLY	2.4
2	J	381(C)	LYS	2.4
2	H	318	THR	2.4
2	F	382	MET	2.3
1	E	160	LYS	2.3
2	B	336	ASN	2.2
2	B	390	THR	2.2
2	D	320	TYR	2.2
2	L	381(D)	LYS	2.2
2	H	381(B)	ASP	2.1
1	A	298	THR	2.1
2	D	328	LEU	2.1
2	F	362(B)	ARG	2.1
2	F	323	ASP	2.1
1	I	177	ARG	2.1
2	H	383	GLY	2.0
2	L	381(C)	LYS	2.0
2	L	330	GLY	2.0
1	I	259	TYR	2.0
2	D	319	ARG	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 monosaccharides 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.