



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 10:01 AM EDT

PDB ID : 3U3I / pdb_00003u3i
Title : A RNA binding protein from Crimean-Congo hemorrhagic fever virus
Authors : Guo, Y.; Wang, W.M.; Ji, W.; Deng, M.; Sun, Y.N.; Lou, Z.Y.; Rao, Z.H.
Deposited on : 2011-10-06
Resolution : 2.30 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

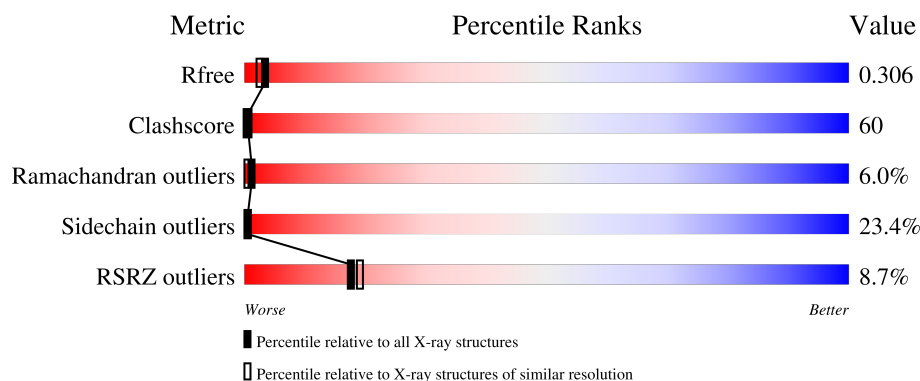
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	482	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3995 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3626	2308	615	685	18			

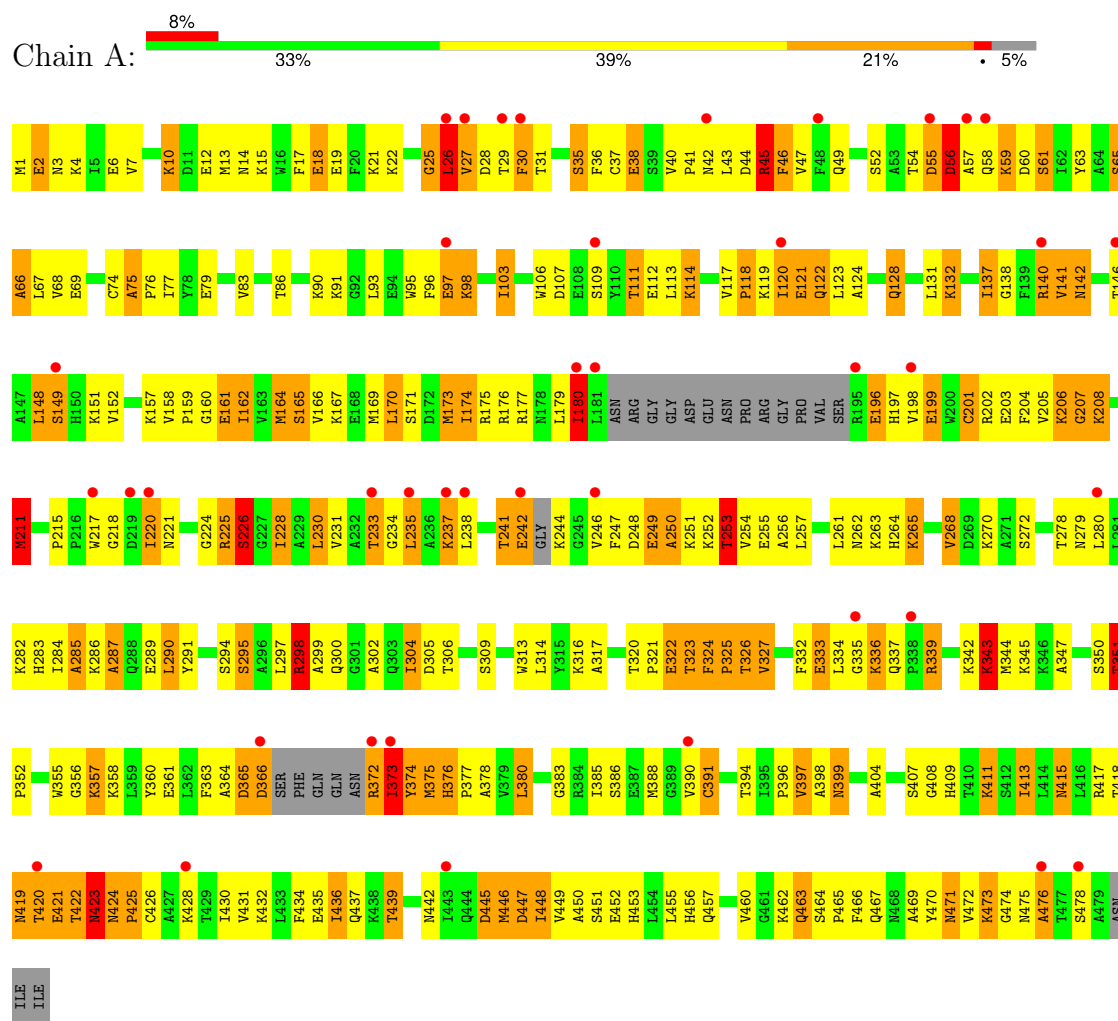
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	369	Total	O	0	0
			369	369		

3 Residue-property plots

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

• Molecule 1: Nucleocapsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.34Å 67.90Å 131.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.64 – 2.30 43.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.1 (43.64-2.30) 89.5 (43.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.88 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.6.1 _357	Depositor
R, R_{free}	0.224 , 0.257 0.260 , 0.306	Depositor DCC
R_{free} test set	1139 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3995	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 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.20	14/3699 (0.4%)	1.38	41/4989 (0.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	PHE	CA-C	8.55	1.62	1.52
1	A	464	SER	C-O	8.22	1.33	1.24
1	A	241	THR	CA-CB	6.17	1.62	1.53
1	A	124	ALA	CA-CB	6.11	1.63	1.53
1	A	404	ALA	CA-CB	6.10	1.64	1.53
1	A	298	ARG	N-CA	-5.92	1.40	1.46
1	A	287	ALA	CA-CB	-5.63	1.44	1.53
1	A	142	ASN	CA-C	-5.47	1.46	1.52
1	A	86	THR	CA-C	5.27	1.59	1.52
1	A	391	CYS	CA-CB	5.18	1.61	1.53
1	A	413	ILE	N-CA	-5.13	1.40	1.46
1	A	325	PRO	C-O	5.11	1.30	1.24
1	A	326	THR	C-O	-5.03	1.18	1.24
1	A	469	ALA	CA-C	5.01	1.60	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ASP	N-CA-C	-9.97	99.16	112.72
1	A	27	VAL	N-CA-C	-8.25	96.25	108.12
1	A	36	PHE	N-CA-C	-7.65	104.00	112.72
1	A	46	PHE	N-CA-C	7.53	119.57	111.36
1	A	253	THR	N-CA-C	-7.42	102.88	112.23
1	A	285	ALA	N-CA-C	-7.40	104.05	113.23
1	A	27	VAL	CB-CA-C	6.94	120.46	110.33
1	A	463	GLN	N-CA-C	-6.73	103.52	113.61
1	A	132	LYS	N-CA-C	-6.48	103.34	111.11
1	A	473	LYS	CA-C-N	-6.34	114.13	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	LYS	C-N-CA	-6.34	114.13	122.63
1	A	290	LEU	N-CA-C	6.33	118.70	111.11
1	A	298	ARG	N-CA-CB	-6.31	101.14	110.10
1	A	14	ASN	CA-C-N	6.31	129.25	120.29
1	A	14	ASN	C-N-CA	6.31	129.25	120.29
1	A	471	ASN	CA-C-N	-6.29	115.00	122.93
1	A	471	ASN	C-N-CA	-6.29	115.00	122.93
1	A	356	GLY	N-CA-C	6.16	120.10	112.64
1	A	295	SER	N-CA-C	-6.14	104.85	112.90
1	A	268	VAL	N-CA-C	5.86	117.19	108.46
1	A	65	SER	N-CA-C	5.82	117.43	111.14
1	A	457	GLN	N-CA-C	5.81	118.39	111.71
1	A	451	SER	N-CA-C	5.80	118.07	111.11
1	A	333	GLU	N-CA-C	-5.77	104.90	111.07
1	A	476	ALA	N-CA-C	-5.72	104.88	112.94
1	A	351	THR	N-CA-C	5.66	117.71	109.84
1	A	75	ALA	CA-C-N	5.64	126.89	119.84
1	A	75	ALA	C-N-CA	5.64	126.89	119.84
1	A	122	GLN	N-CA-C	-5.58	105.20	111.28
1	A	128	GLN	N-CA-C	-5.49	104.94	111.69
1	A	26	LEU	N-CA-C	5.38	118.99	109.96
1	A	118	PRO	CB-CA-C	-5.31	104.61	111.46
1	A	408	GLY	N-CA-C	5.31	125.76	113.18
1	A	103	ILE	CB-CA-C	-5.27	103.15	110.95
1	A	415	ASN	N-CA-C	-5.26	106.81	113.18
1	A	327	VAL	N-CA-C	5.23	115.44	110.53
1	A	343	LYS	N-CA-C	-5.22	105.67	111.36
1	A	208	LYS	N-CA-C	-5.21	101.47	109.76
1	A	66	ALA	CA-C-N	5.09	127.86	120.79
1	A	66	ALA	C-N-CA	5.09	127.86	120.79
1	A	25	GLY	N-CA-C	5.01	125.07	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3626	0	3614	434	0
2	A	369	0	0	21	0
All	All	3995	0	3614	434	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 60.

All (434) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:CG	1:A:420:THR:HG22	1.17	1.55
1:A:148:LEU:CA	1:A:149:SER:HB2	1.45	1.40
1:A:157:LYS:CG	1:A:420:THR:CG2	2.04	1.36
1:A:1:MET:HA	1:A:2:GLU:CB	1.44	1.35
1:A:29:THR:CG2	1:A:30:PHE:CE2	2.14	1.30
1:A:157:LYS:HG2	1:A:420:THR:CG2	1.60	1.27
1:A:148:LEU:HA	1:A:149:SER:CB	1.60	1.26
1:A:157:LYS:CB	1:A:420:THR:CG2	2.15	1.24
1:A:29:THR:HG21	1:A:30:PHE:CE2	1.70	1.23
1:A:4:LYS:HE2	1:A:398:ALA:O	1.40	1.18
1:A:1:MET:CA	1:A:2:GLU:HB2	1.75	1.16
1:A:1:MET:CA	1:A:2:GLU:CB	2.22	1.15
1:A:228:ILE:HG12	1:A:283:HIS:CE1	1.80	1.15
1:A:373:ILE:HG12	1:A:374:TYR:N	1.50	1.13
1:A:164:MET:HE3	1:A:164:MET:HA	1.31	1.13
1:A:424:ASN:OD1	1:A:428:LYS:HD2	1.49	1.12
1:A:373:ILE:CG1	1:A:374:TYR:H	1.56	1.12
1:A:58:GLN:HG2	1:A:61:SER:HB2	1.18	1.12
1:A:235:LEU:HD12	1:A:290:LEU:HB3	1.19	1.10
1:A:3:ASN:HA	1:A:397:VAL:HG13	1.27	1.10
1:A:157:LYS:HB3	1:A:420:THR:HG23	1.33	1.09
1:A:424:ASN:N	1:A:425:PRO:HD3	1.65	1.08
1:A:157:LYS:HB3	1:A:420:THR:CG2	1.78	1.07
1:A:235:LEU:CD1	1:A:290:LEU:HB3	1.83	1.07
1:A:58:GLN:N	1:A:59:LYS:HB2	1.69	1.07
1:A:1:MET:HA	1:A:2:GLU:HB2	1.30	1.07
1:A:58:GLN:HA	1:A:60:ASP:N	1.69	1.07
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.12	1.06
1:A:26:LEU:N	1:A:26:LEU:CD2	2.12	1.05
1:A:420:THR:O	1:A:421:GLU:HB2	1.55	1.05
1:A:58:GLN:HG2	1:A:61:SER:CB	1.88	1.03
1:A:1:MET:HA	1:A:2:GLU:HB3	1.09	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:HB3	1:A:4:LYS:NZ	1.74	1.02
1:A:225:ARG:O	1:A:226:SER:HB2	1.55	1.02
1:A:29:THR:HG21	1:A:30:PHE:HE2	1.19	1.01
1:A:29:THR:HG22	1:A:30:PHE:CD2	1.96	1.00
1:A:3:ASN:HA	1:A:397:VAL:CG1	1.92	1.00
1:A:29:THR:CG2	1:A:30:PHE:CD2	2.47	0.98
1:A:475:ASN:ND2	1:A:476:ALA:N	2.11	0.98
1:A:157:LYS:HG3	1:A:420:THR:HG22	1.41	0.98
1:A:475:ASN:CG	1:A:476:ALA:H	1.71	0.98
1:A:26:LEU:N	1:A:26:LEU:HD22	1.78	0.98
1:A:234:GLY:HA3	2:A:864:HOH:O	1.62	0.98
1:A:419:ASN:H	1:A:419:ASN:HD22	1.06	0.98
1:A:419:ASN:HD22	1:A:419:ASN:N	1.60	0.96
1:A:475:ASN:ND2	1:A:476:ALA:H	1.63	0.96
1:A:45:ARG:HG3	1:A:45:ARG:NH1	1.73	0.95
1:A:30:PHE:HD2	1:A:30:PHE:N	1.65	0.94
1:A:159:PRO:HD2	1:A:162:ILE:HD11	1.49	0.94
1:A:228:ILE:CG1	1:A:283:HIS:CE1	2.50	0.94
1:A:18:GLU:OE2	1:A:18:GLU:HA	1.68	0.93
1:A:58:GLN:HG3	1:A:61:SER:H	1.33	0.93
1:A:228:ILE:CG2	1:A:231:VAL:HG23	1.97	0.93
1:A:228:ILE:HG12	1:A:283:HIS:HE1	1.26	0.92
1:A:120:ILE:HG22	2:A:591:HOH:O	1.68	0.92
1:A:169:MET:O	1:A:173:MET:HG2	1.70	0.92
1:A:220:ILE:HG12	1:A:280:LEU:HD21	1.52	0.92
1:A:29:THR:HG22	1:A:30:PHE:CE2	2.02	0.91
1:A:58:GLN:HG3	1:A:61:SER:N	1.86	0.91
1:A:1:MET:N	1:A:2:GLU:HB2	1.84	0.91
1:A:373:ILE:HG12	1:A:374:TYR:H	0.76	0.91
1:A:424:ASN:N	1:A:425:PRO:CD	2.34	0.90
1:A:231:VAL:HG13	1:A:287:ALA:N	1.87	0.90
1:A:30:PHE:CD2	1:A:30:PHE:N	2.36	0.90
1:A:390:VAL:HG21	1:A:411:LYS:HB2	1.54	0.90
1:A:58:GLN:CG	1:A:61:SER:H	1.85	0.89
1:A:26:LEU:HD23	1:A:26:LEU:H	1.36	0.89
1:A:419:ASN:H	1:A:419:ASN:ND2	1.64	0.88
1:A:228:ILE:HG22	1:A:231:VAL:HG23	1.51	0.88
1:A:249:GLU:O	1:A:253:THR:HG23	1.72	0.88
1:A:45:ARG:HH11	1:A:45:ARG:CG	1.87	0.87
1:A:164:MET:HA	1:A:164:MET:CE	2.04	0.87
1:A:148:LEU:CB	1:A:149:SER:HB2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:CB	1:A:420:THR:HG22	1.89	0.87
1:A:164:MET:HE3	1:A:164:MET:CA	2.03	0.87
1:A:35:SER:HB3	1:A:37:CYS:H	1.41	0.86
1:A:262:ASN:O	1:A:265:LYS:HG2	1.76	0.86
1:A:339:ARG:HD3	1:A:339:ARG:N	1.89	0.86
1:A:2:GLU:HB3	1:A:4:LYS:HZ3	1.40	0.85
1:A:58:GLN:HA	1:A:60:ASP:H	1.37	0.85
1:A:423:ASN:C	1:A:425:PRO:HD3	2.02	0.85
1:A:385:ILE:HD13	1:A:388:MET:HE3	1.58	0.85
1:A:25:GLY:C	1:A:26:LEU:HD22	2.02	0.84
1:A:231:VAL:HG12	1:A:290:LEU:HD12	1.57	0.84
1:A:26:LEU:N	1:A:26:LEU:HD23	1.90	0.84
1:A:148:LEU:CA	1:A:149:SER:CB	2.30	0.83
1:A:238:LEU:HD23	1:A:246:VAL:HB	1.61	0.83
1:A:1:MET:H1	1:A:2:GLU:HB2	1.43	0.82
1:A:58:GLN:CA	1:A:59:LYS:HB2	2.10	0.81
1:A:228:ILE:HG22	1:A:231:VAL:H	1.44	0.81
1:A:238:LEU:HD22	1:A:247:PHE:CE2	2.16	0.81
1:A:58:GLN:N	1:A:59:LYS:CB	2.44	0.81
1:A:205:VAL:HG13	1:A:249:GLU:HB3	1.61	0.81
1:A:162:ILE:O	1:A:166:VAL:HG23	1.79	0.81
1:A:421:GLU:O	1:A:422:THR:OG1	1.98	0.80
1:A:29:THR:HB	1:A:30:PHE:CD2	2.16	0.80
1:A:201:CYS:O	1:A:205:VAL:HG23	1.83	0.79
1:A:57:ALA:C	1:A:59:LYS:HB2	2.08	0.78
1:A:235:LEU:HD12	1:A:290:LEU:CB	2.08	0.78
1:A:121:GLU:CD	1:A:121:GLU:H	1.88	0.78
1:A:157:LYS:HG2	1:A:420:THR:HG22	0.78	0.78
1:A:95:TRP:HZ2	1:A:132:LYS:HG2	1.49	0.78
1:A:29:THR:CB	1:A:30:PHE:CD2	2.68	0.77
1:A:103:ILE:HG23	1:A:106:TRP:CH2	2.18	0.77
1:A:298:ARG:HH11	1:A:298:ARG:CG	1.98	0.77
1:A:435:GLU:O	1:A:439:THR:HG22	1.84	0.77
1:A:220:ILE:CG1	1:A:280:LEU:HD21	2.15	0.77
1:A:385:ILE:CD1	1:A:388:MET:HE3	2.14	0.77
1:A:428:LYS:O	1:A:432:LYS:HG3	1.84	0.76
1:A:174:ILE:O	1:A:177:ARG:HB3	1.85	0.76
1:A:170:LEU:HA	1:A:173:MET:HG3	1.68	0.75
1:A:157:LYS:CB	1:A:420:THR:HG21	2.15	0.75
1:A:366:ASP:HB3	2:A:731:HOH:O	1.85	0.74
1:A:205:VAL:CG1	1:A:249:GLU:HB3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLN:HG2	1:A:470:TYR:CE1	2.23	0.74
1:A:103:ILE:HG22	1:A:107:ASP:HB2	1.69	0.74
1:A:90:LYS:HD3	2:A:785:HOH:O	1.87	0.73
1:A:202:ARG:HA	1:A:237:LYS:NZ	2.03	0.73
1:A:220:ILE:HG12	1:A:280:LEU:CD2	2.19	0.72
1:A:174:ILE:HG22	1:A:175:ARG:N	2.05	0.72
1:A:29:THR:CB	1:A:30:PHE:CE2	2.73	0.72
1:A:152:VAL:HG21	1:A:475:ASN:O	1.88	0.72
1:A:422:THR:HG23	2:A:589:HOH:O	1.87	0.72
1:A:142:ASN:O	1:A:146:THR:HG23	1.89	0.71
1:A:337:GLN:HB3	1:A:339:ARG:CD	2.20	0.71
1:A:339:ARG:HD3	1:A:339:ARG:H	1.53	0.71
1:A:55:ASP:C	1:A:57:ALA:H	1.99	0.70
1:A:35:SER:OG	1:A:74:CYS:HA	1.91	0.70
1:A:363:PHE:CE1	1:A:380:LEU:HD13	2.26	0.70
1:A:251:LYS:NZ	2:A:627:HOH:O	2.25	0.69
1:A:453:HIS:HB2	2:A:803:HOH:O	1.90	0.69
1:A:103:ILE:HG23	1:A:106:TRP:CZ2	2.25	0.69
1:A:119:LYS:HB2	1:A:122:GLN:HG3	1.74	0.69
1:A:235:LEU:HD23	1:A:235:LEU:O	1.91	0.69
1:A:380:LEU:HD21	1:A:388:MET:HE2	1.72	0.69
1:A:221:ASN:HD21	1:A:279:ASN:ND2	1.90	0.69
1:A:169:MET:HG2	1:A:434:PHE:CE2	2.28	0.68
1:A:306:THR:HG22	1:A:391:CYS:SG	2.33	0.68
1:A:29:THR:HB	1:A:30:PHE:HD2	1.54	0.68
1:A:234:GLY:C	1:A:238:LEU:HD12	2.17	0.68
1:A:339:ARG:HB3	1:A:343:LYS:HD3	1.75	0.68
1:A:30:PHE:HD2	1:A:30:PHE:H	1.39	0.68
1:A:148:LEU:HA	1:A:149:SER:HB2	0.72	0.68
1:A:375:MET:O	1:A:376:HIS:CB	2.42	0.68
1:A:335:GLY:HA3	1:A:407:SER:OG	1.94	0.67
1:A:228:ILE:CG2	1:A:230:LEU:HB3	2.24	0.67
1:A:334:LEU:HD11	1:A:344:MET:HG2	1.76	0.67
1:A:148:LEU:HB3	1:A:149:SER:CB	2.25	0.66
1:A:79:GLU:HB3	1:A:466:PHE:CD2	2.31	0.66
1:A:117:VAL:HG13	1:A:118:PRO:HD2	1.77	0.66
1:A:421:GLU:C	1:A:422:THR:HG1	1.97	0.66
1:A:238:LEU:HD22	1:A:247:PHE:CZ	2.31	0.65
1:A:169:MET:O	1:A:173:MET:CG	2.44	0.65
1:A:304:ILE:N	1:A:304:ILE:HD12	2.11	0.65
1:A:55:ASP:O	1:A:57:ALA:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HE3	1:A:455:LEU:HD22	1.78	0.65
1:A:2:GLU:HB3	1:A:4:LYS:HZ2	1.61	0.64
1:A:249:GLU:O	1:A:250:ALA:C	2.39	0.64
1:A:3:ASN:CA	1:A:397:VAL:HG13	2.17	0.64
1:A:111:THR:O	1:A:114:LYS:HB2	1.97	0.64
1:A:337:GLN:OE1	1:A:339:ARG:HG2	1.96	0.64
1:A:58:GLN:CG	1:A:61:SER:N	2.50	0.64
1:A:424:ASN:OD1	1:A:428:LYS:CD	2.38	0.64
1:A:18:GLU:OE2	1:A:21:LYS:HE3	1.97	0.63
1:A:58:GLN:HA	1:A:59:LYS:C	2.21	0.63
1:A:317:ALA:O	1:A:358:LYS:HD3	1.99	0.62
1:A:158:VAL:HG13	1:A:162:ILE:CD1	2.29	0.62
1:A:375:MET:O	1:A:376:HIS:HB2	2.00	0.62
1:A:202:ARG:HA	1:A:237:LYS:HZ2	1.61	0.62
1:A:95:TRP:CZ2	1:A:132:LYS:HG2	2.34	0.62
1:A:325:PRO:HB3	1:A:397:VAL:HG12	1.82	0.62
1:A:399:ASN:HB3	2:A:543:HOH:O	2.00	0.61
1:A:230:LEU:HD12	1:A:230:LEU:O	2.00	0.61
1:A:93:LEU:HD21	1:A:314:LEU:HB3	1.83	0.61
1:A:424:ASN:N	1:A:424:ASN:ND2	2.49	0.61
1:A:159:PRO:O	1:A:162:ILE:HD13	2.01	0.60
1:A:109:SER:O	1:A:113:LEU:HG	2.00	0.60
1:A:169:MET:HG2	1:A:434:PHE:CD2	2.37	0.60
1:A:372:ARG:O	1:A:373:ILE:C	2.43	0.60
1:A:159:PRO:HG3	1:A:424:ASN:HB3	1.82	0.60
1:A:29:THR:CB	1:A:30:PHE:HD2	2.12	0.60
1:A:164:MET:CE	1:A:164:MET:CA	2.72	0.60
1:A:220:ILE:CD1	1:A:280:LEU:HD21	2.32	0.60
1:A:230:LEU:HD21	1:A:280:LEU:CD2	2.32	0.60
1:A:148:LEU:HB3	1:A:149:SER:HB3	1.83	0.59
1:A:230:LEU:HD12	1:A:230:LEU:C	2.25	0.59
1:A:158:VAL:HG13	1:A:162:ILE:HD11	1.82	0.59
1:A:29:THR:CG2	1:A:30:PHE:HE2	1.81	0.59
1:A:109:SER:O	1:A:113:LEU:CG	2.51	0.59
1:A:159:PRO:HG3	1:A:424:ASN:CB	2.32	0.59
1:A:167:LYS:HA	1:A:170:LEU:HB2	1.83	0.59
1:A:109:SER:O	1:A:113:LEU:HB2	2.03	0.59
1:A:225:ARG:O	1:A:226:SER:CB	2.39	0.58
1:A:151:LYS:HG3	1:A:473:LYS:O	2.03	0.58
1:A:450:ALA:HA	2:A:803:HOH:O	2.02	0.58
1:A:29:THR:HB	1:A:30:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:O	1:A:421:GLU:CB	2.40	0.58
1:A:197:HIS:HB3	1:A:217:TRP:CZ3	2.39	0.58
1:A:333:GLU:HG2	2:A:608:HOH:O	2.03	0.58
1:A:449:VAL:HG12	1:A:452:GLU:H	1.67	0.57
1:A:238:LEU:CD2	1:A:247:PHE:CZ	2.87	0.57
1:A:298:ARG:HH11	1:A:298:ARG:HG3	1.68	0.57
1:A:363:PHE:HE1	1:A:380:LEU:CD1	2.18	0.57
1:A:148:LEU:CB	1:A:149:SER:CB	2.73	0.57
1:A:207:GLY:HA2	1:A:253:THR:HB	1.85	0.57
1:A:230:LEU:HD23	1:A:283:HIS:CD2	2.40	0.56
1:A:237:LYS:O	1:A:237:LYS:HG3	2.03	0.56
1:A:238:LEU:CD2	1:A:246:VAL:HB	2.32	0.56
1:A:30:PHE:HD1	1:A:40:VAL:HG23	1.70	0.56
1:A:411:LYS:HB3	1:A:465:PRO:HB3	1.87	0.56
1:A:30:PHE:CD1	1:A:40:VAL:HG23	2.41	0.56
1:A:235:LEU:C	1:A:235:LEU:CD2	2.78	0.56
1:A:423:ASN:C	1:A:425:PRO:CD	2.76	0.56
1:A:442:ASN:HB3	1:A:445:ASP:OD2	2.06	0.55
1:A:230:LEU:CD2	1:A:280:LEU:HD23	2.36	0.55
1:A:298:ARG:NH1	1:A:298:ARG:HG2	2.21	0.55
1:A:157:LYS:HD2	1:A:158:VAL:H	1.72	0.55
1:A:376:HIS:CE1	1:A:378:ALA:HB3	2.41	0.55
1:A:159:PRO:HD2	1:A:162:ILE:CD1	2.31	0.55
1:A:159:PRO:CD	1:A:162:ILE:HD11	2.30	0.55
1:A:180:ILE:HG23	1:A:180:ILE:O	2.06	0.55
1:A:235:LEU:HD23	1:A:235:LEU:C	2.31	0.55
1:A:238:LEU:HD23	1:A:242:GLU:O	2.07	0.55
1:A:282:LYS:HD2	2:A:791:HOH:O	2.07	0.55
1:A:103:ILE:CG2	1:A:107:ASP:HB2	2.37	0.54
1:A:177:ARG:NH2	1:A:475:ASN:ND2	2.56	0.54
1:A:49:GLN:O	1:A:52:SER:HB2	2.06	0.54
1:A:228:ILE:HG13	1:A:283:HIS:CE1	2.42	0.54
1:A:363:PHE:HE1	1:A:380:LEU:HD13	1.67	0.54
1:A:17:PHE:CE2	1:A:21:LYS:HD3	2.43	0.54
1:A:58:GLN:N	1:A:59:LYS:CG	2.71	0.54
1:A:58:GLN:HG3	1:A:60:ASP:HB2	1.89	0.53
1:A:58:GLN:HA	1:A:59:LYS:HB2	1.88	0.53
1:A:201:CYS:SG	1:A:233:THR:HB	2.48	0.53
1:A:228:ILE:HG21	1:A:283:HIS:ND1	2.24	0.53
1:A:55:ASP:C	1:A:57:ALA:N	2.65	0.53
1:A:253:THR:O	1:A:256:ALA:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HG21	1:A:411:LYS:CB	2.31	0.53
1:A:300:GLN:HG2	1:A:470:TYR:HE1	1.71	0.53
1:A:121:GLU:CD	1:A:121:GLU:N	2.62	0.53
1:A:215:PRO:HB2	1:A:218:GLY:O	2.09	0.53
1:A:96:PHE:C	1:A:98:LYS:H	2.17	0.53
1:A:228:ILE:CG1	1:A:283:HIS:HE1	2.02	0.53
1:A:475:ASN:HD22	1:A:476:ALA:N	2.03	0.53
1:A:332:PHE:CG	1:A:396:PRO:HG3	2.45	0.52
1:A:164:MET:HE3	1:A:164:MET:C	2.34	0.52
1:A:42:ASN:ND2	1:A:44:ASP:H	2.07	0.52
1:A:419:ASN:ND2	2:A:681:HOH:O	2.42	0.52
1:A:109:SER:O	1:A:113:LEU:CB	2.58	0.52
1:A:304:ILE:N	1:A:304:ILE:CD1	2.73	0.52
1:A:366:ASP:OD2	1:A:366:ASP:N	2.43	0.52
1:A:422:THR:O	1:A:423:ASN:C	2.53	0.52
1:A:43:LEU:CD2	1:A:69:GLU:HB3	2.39	0.52
1:A:305:ASP:HA	2:A:826:HOH:O	2.10	0.52
1:A:42:ASN:HD21	1:A:44:ASP:CG	2.18	0.52
1:A:157:LYS:HD2	1:A:158:VAL:N	2.24	0.52
1:A:79:GLU:HB3	1:A:466:PHE:HD2	1.73	0.51
1:A:448:ILE:HG23	1:A:449:VAL:N	2.24	0.51
1:A:299:ALA:O	1:A:302:ALA:HB3	2.11	0.51
1:A:205:VAL:HB	1:A:237:LYS:NZ	2.26	0.51
1:A:364:ALA:O	1:A:365:ASP:HB2	2.09	0.51
1:A:453:HIS:O	1:A:456:HIS:HB3	2.11	0.51
1:A:43:LEU:HD22	1:A:69:GLU:HB3	1.93	0.51
1:A:228:ILE:HG21	1:A:231:VAL:HG23	1.86	0.51
1:A:320:THR:HB	1:A:322:GLU:OE2	2.11	0.51
1:A:10:LYS:HB3	1:A:141:VAL:CG2	2.41	0.51
1:A:327:VAL:HG22	1:A:355:TRP:CE2	2.46	0.51
1:A:373:ILE:CG1	1:A:374:TYR:N	2.30	0.50
1:A:204:PHE:C	1:A:204:PHE:CD2	2.89	0.50
1:A:103:ILE:HG22	1:A:103:ILE:O	2.11	0.50
1:A:298:ARG:HH11	1:A:298:ARG:HG2	1.70	0.50
1:A:347:ALA:O	1:A:351:THR:HG22	2.10	0.50
1:A:424:ASN:ND2	1:A:424:ASN:H	2.09	0.50
1:A:58:GLN:CA	1:A:59:LYS:CB	2.74	0.50
1:A:120:ILE:O	1:A:123:LEU:HB2	2.11	0.50
1:A:138:GLY:C	1:A:140:ARG:H	2.19	0.50
1:A:337:GLN:HB3	1:A:339:ARG:HD3	1.93	0.50
1:A:44:ASP:O	1:A:45:ARG:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:O	1:A:57:ALA:C	2.54	0.50
1:A:58:GLN:CG	1:A:61:SER:CB	2.77	0.50
1:A:97:GLU:O	1:A:97:GLU:CG	2.58	0.50
1:A:205:VAL:HB	1:A:237:LYS:HZ1	1.77	0.50
1:A:1:MET:HB3	2:A:594:HOH:O	2.11	0.49
1:A:112:GLU:CD	1:A:112:GLU:H	2.20	0.49
1:A:42:ASN:HD22	1:A:43:LEU:N	2.10	0.49
1:A:138:GLY:C	1:A:140:ARG:N	2.70	0.49
1:A:238:LEU:O	1:A:242:GLU:HA	2.11	0.49
1:A:345:LYS:HE2	2:A:560:HOH:O	2.12	0.49
1:A:357:LYS:HD3	2:A:600:HOH:O	2.12	0.49
1:A:46:PHE:CE2	1:A:66:ALA:HA	2.46	0.49
1:A:152:VAL:HG12	1:A:474:GLY:HA3	1.93	0.49
1:A:321:PRO:O	1:A:323:THR:N	2.44	0.49
1:A:385:ILE:CD1	1:A:388:MET:CE	2.89	0.49
1:A:475:ASN:CG	1:A:476:ALA:N	2.44	0.49
1:A:43:LEU:HB3	1:A:46:PHE:HD2	1.77	0.49
1:A:230:LEU:O	1:A:233:THR:OG1	2.30	0.49
1:A:244:LYS:N	1:A:244:LYS:HD2	2.28	0.49
1:A:337:GLN:HB3	1:A:339:ARG:CG	2.42	0.49
1:A:27:VAL:C	1:A:29:THR:H	2.21	0.49
1:A:376:HIS:CG	1:A:377:PRO:HD2	2.48	0.49
1:A:35:SER:CB	1:A:37:CYS:H	2.18	0.49
1:A:332:PHE:CD2	1:A:396:PRO:HG3	2.48	0.49
1:A:339:ARG:N	1:A:339:ARG:CD	2.69	0.49
1:A:230:LEU:CD2	1:A:280:LEU:CD2	2.91	0.48
1:A:449:VAL:HG11	1:A:452:GLU:CD	2.38	0.48
1:A:205:VAL:HG21	1:A:237:LYS:CE	2.43	0.48
1:A:161:GLU:HG2	1:A:162:ILE:HG23	1.94	0.48
1:A:235:LEU:HD12	1:A:290:LEU:HD13	1.95	0.48
1:A:285:ALA:O	1:A:289:GLU:HG3	2.14	0.48
1:A:436:ILE:HG22	1:A:437:GLN:N	2.28	0.48
1:A:63:TYR:CE1	1:A:437:GLN:HG3	2.48	0.48
1:A:452:GLU:O	1:A:456:HIS:HB2	2.14	0.48
1:A:58:GLN:HG2	1:A:61:SER:H	1.72	0.48
1:A:131:LEU:O	1:A:132:LYS:C	2.55	0.48
1:A:337:GLN:HG2	1:A:339:ARG:HE	1.77	0.48
1:A:425:PRO:O	1:A:426:CYS:C	2.57	0.48
1:A:158:VAL:HG13	1:A:162:ILE:HG12	1.96	0.48
1:A:203:GLU:HB3	1:A:211:MET:SD	2.54	0.48
1:A:305:ASP:C	1:A:305:ASP:OD2	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HA	1:A:38:GLU:OE1	2.14	0.48
1:A:58:GLN:H	1:A:59:LYS:CG	2.27	0.47
1:A:337:GLN:HB3	1:A:339:ARG:NE	2.29	0.47
1:A:157:LYS:HB2	1:A:420:THR:HG21	1.94	0.47
1:A:238:LEU:HD21	1:A:247:PHE:CD1	2.50	0.47
1:A:49:GLN:O	1:A:52:SER:CB	2.63	0.47
1:A:97:GLU:O	1:A:97:GLU:HG3	2.15	0.47
1:A:337:GLN:CG	1:A:339:ARG:HE	2.27	0.47
1:A:322:GLU:CD	1:A:322:GLU:H	2.23	0.47
1:A:152:VAL:HG11	1:A:475:ASN:N	2.30	0.47
1:A:176:ARG:NH1	1:A:446:MET:O	2.43	0.47
1:A:205:VAL:O	1:A:249:GLU:CG	2.63	0.47
1:A:238:LEU:HD22	1:A:247:PHE:CD2	2.49	0.47
1:A:383:GLY:CA	2:A:626:HOH:O	2.62	0.47
1:A:199:GLU:O	1:A:202:ARG:N	2.47	0.47
1:A:205:VAL:CG1	1:A:249:GLU:CB	2.92	0.47
1:A:220:ILE:HD11	1:A:280:LEU:HD21	1.97	0.47
1:A:248:ASP:O	1:A:251:LYS:HB2	2.14	0.47
1:A:29:THR:CB	1:A:30:PHE:HE2	2.24	0.46
1:A:394:THR:HG22	1:A:409:HIS:HD2	1.80	0.46
1:A:1:MET:HA	1:A:4:LYS:NZ	2.31	0.46
1:A:12:GLU:O	1:A:13:MET:C	2.54	0.46
1:A:351:THR:HA	1:A:352:PRO:HD3	1.79	0.46
1:A:202:ARG:HA	1:A:237:LYS:HZ3	1.78	0.46
1:A:203:GLU:CB	1:A:211:MET:SD	3.04	0.46
1:A:164:MET:HE3	1:A:164:MET:O	2.16	0.46
1:A:205:VAL:O	1:A:249:GLU:HG2	2.15	0.46
1:A:383:GLY:HA2	2:A:626:HOH:O	2.15	0.45
1:A:7:VAL:HG12	2:A:546:HOH:O	2.16	0.45
1:A:98:LYS:HE3	1:A:98:LYS:HB3	1.52	0.45
1:A:234:GLY:O	1:A:238:LEU:HD12	2.17	0.45
1:A:231:VAL:HG11	1:A:286:LYS:HG3	1.98	0.45
1:A:231:VAL:CG1	1:A:287:ALA:N	2.69	0.45
1:A:249:GLU:O	1:A:252:LYS:N	2.49	0.45
1:A:385:ILE:HD13	1:A:388:MET:CE	2.37	0.45
1:A:385:ILE:HD13	1:A:385:ILE:HA	1.75	0.45
1:A:43:LEU:O	1:A:44:ASP:C	2.60	0.45
1:A:298:ARG:HB3	1:A:299:ALA:H	1.59	0.45
1:A:336:LYS:HB3	1:A:336:LYS:HE2	1.41	0.45
1:A:15:LYS:HD3	2:A:743:HOH:O	2.15	0.45
1:A:250:ALA:O	1:A:254:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ALA:O	1:A:351:THR:CG2	2.65	0.45
1:A:257:LEU:HG	1:A:261:LEU:HD11	1.99	0.44
1:A:244:LYS:N	1:A:244:LYS:CD	2.81	0.44
1:A:294:SER:O	1:A:298:ARG:HB2	2.18	0.44
1:A:205:VAL:O	1:A:206:LYS:C	2.61	0.44
1:A:228:ILE:HG22	1:A:228:ILE:O	2.17	0.44
1:A:40:VAL:O	1:A:41:PRO:C	2.61	0.44
1:A:386:SER:O	1:A:390:VAL:HG23	2.17	0.44
1:A:173:MET:HB3	1:A:173:MET:HE3	1.72	0.44
1:A:431:VAL:O	1:A:432:LYS:C	2.60	0.43
1:A:173:MET:HG2	1:A:173:MET:H	1.50	0.43
1:A:231:VAL:HG13	1:A:287:ALA:H	1.80	0.43
1:A:230:LEU:HD21	1:A:280:LEU:HD22	1.99	0.43
1:A:45:ARG:NH2	1:A:69:GLU:OE1	2.52	0.43
1:A:65:SER:O	1:A:68:VAL:HB	2.19	0.43
1:A:18:GLU:O	1:A:19:GLU:C	2.62	0.43
1:A:106:TRP:CD1	1:A:106:TRP:N	2.87	0.43
1:A:31:THR:HA	1:A:415:ASN:O	2.18	0.43
1:A:316:LYS:HD2	1:A:316:LYS:HA	1.77	0.43
1:A:462:LYS:HA	1:A:467:GLN:OE1	2.18	0.43
1:A:375:MET:HE3	1:A:375:MET:HB2	1.88	0.43
1:A:206:LYS:HE2	1:A:208:LYS:HE3	2.01	0.43
1:A:251:LYS:O	1:A:255:GLU:HG3	2.19	0.43
1:A:313:TRP:CH2	1:A:380:LEU:HD23	2.54	0.43
1:A:140:ARG:H	1:A:140:ARG:HG3	1.46	0.42
1:A:333:GLU:C	1:A:335:GLY:N	2.74	0.42
1:A:29:THR:C	1:A:30:PHE:CD2	2.95	0.42
1:A:30:PHE:HA	1:A:417:ARG:HD2	2.00	0.42
1:A:158:VAL:HG13	1:A:162:ILE:CG1	2.49	0.42
1:A:1:MET:O	1:A:1:MET:CG	2.67	0.42
1:A:196:GLU:H	1:A:196:GLU:HG3	1.64	0.42
1:A:25:GLY:C	1:A:26:LEU:CD2	2.74	0.42
1:A:75:ALA:HA	1:A:76:PRO:HD3	1.66	0.42
1:A:91:LYS:HB3	1:A:137:ILE:HG22	2.01	0.42
1:A:424:ASN:H	1:A:425:PRO:HD3	1.69	0.42
1:A:18:GLU:OE2	1:A:18:GLU:CA	2.49	0.42
1:A:205:VAL:HG12	1:A:249:GLU:HB3	1.99	0.42
1:A:63:TYR:HE1	1:A:437:GLN:HG3	1.85	0.42
1:A:321:PRO:O	1:A:322:GLU:C	2.63	0.42
1:A:333:GLU:C	1:A:335:GLY:H	2.27	0.42
1:A:90:LYS:O	1:A:91:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:O	1:A:165:SER:C	2.63	0.41
1:A:235:LEU:HG	1:A:291:TYR:N	2.35	0.41
1:A:419:ASN:HB2	1:A:423:ASN:ND2	2.36	0.41
1:A:83:VAL:O	1:A:83:VAL:HG12	2.20	0.41
1:A:174:ILE:O	1:A:175:ARG:C	2.63	0.41
1:A:447:ASP:OD1	1:A:447:ASP:N	2.53	0.41
1:A:418:THR:HG22	1:A:426:CYS:HB3	2.02	0.41
1:A:448:ILE:HD12	1:A:448:ILE:HA	1.89	0.41
1:A:174:ILE:O	1:A:177:ARG:N	2.53	0.41
1:A:230:LEU:HD21	1:A:280:LEU:HD23	1.98	0.41
1:A:321:PRO:C	1:A:323:THR:N	2.79	0.41
1:A:374:TYR:O	1:A:375:MET:C	2.62	0.41
1:A:119:LYS:N	1:A:122:GLN:OE1	2.50	0.41
1:A:449:VAL:HG11	1:A:452:GLU:OE2	2.20	0.41
1:A:148:LEU:C	1:A:472:VAL:HG23	2.46	0.41
1:A:159:PRO:HG2	1:A:162:ILE:HD12	2.02	0.41
1:A:324:PHE:O	1:A:327:VAL:N	2.52	0.41
1:A:360:TYR:O	1:A:363:PHE:HB2	2.20	0.41
1:A:120:ILE:H	1:A:120:ILE:HG13	1.39	0.41
1:A:152:VAL:HG23	1:A:460:VAL:HA	2.02	0.41
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.75	0.41
1:A:31:THR:OG1	1:A:35:SER:HB2	2.20	0.41
1:A:449:VAL:HG12	1:A:449:VAL:O	2.22	0.40
1:A:137:ILE:H	1:A:137:ILE:HG12	1.79	0.40
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.86	0.40
1:A:426:CYS:O	1:A:430:ILE:HG13	2.21	0.40
1:A:254:VAL:HG21	1:A:284:ILE:HD11	2.03	0.40
1:A:294:SER:HA	1:A:297:LEU:HB2	2.04	0.40
1:A:419:ASN:HB2	1:A:423:ASN:HD22	1.87	0.40
1:A:453:HIS:CB	2:A:803:HOH:O	2.60	0.40
1:A:419:ASN:N	1:A:419:ASN:ND2	2.30	0.40
1:A:103:ILE:HG21	1:A:103:ILE:HD13	1.73	0.40
1:A:169:MET:CE	1:A:455:LEU:HD22	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	452/482 (94%)	360 (80%)	65 (14%)	27 (6%)	1 0

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	149	SER
1	A	180	ILE
1	A	322	GLU
1	A	365	ASP
1	A	373	ILE
1	A	374	TYR
1	A	376	HIS
1	A	56	ASP
1	A	165	SER
1	A	226	SER
1	A	421	GLU
1	A	423	ASN
1	A	478	SER
1	A	164	MET
1	A	211	MET
1	A	45	ARG
1	A	47	VAL
1	A	250	ALA
1	A	425	PRO
1	A	471	ASN
1	A	6	GLU
1	A	59	LYS
1	A	160	GLY
1	A	422	THR
1	A	207	GLY
1	A	224	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	389/408 (95%)	298 (77%)	91 (23%)	0 0

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	18	GLU
1	A	22	LYS
1	A	26	LEU
1	A	30	PHE
1	A	35	SER
1	A	38	GLU
1	A	45	ARG
1	A	54	THR
1	A	55	ASP
1	A	56	ASP
1	A	61	SER
1	A	67	LEU
1	A	77	ILE
1	A	97	GLU
1	A	98	LYS
1	A	111	THR
1	A	114	LYS
1	A	120	ILE
1	A	121	GLU
1	A	128	GLN
1	A	137	ILE
1	A	140	ARG
1	A	141	VAL
1	A	148	LEU
1	A	161	GLU
1	A	162	ILE
1	A	170	LEU
1	A	171	SER
1	A	173	MET

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Mol	Chain	Res	Type
1	A	174	ILE
1	A	180	ILE
1	A	196	GLU
1	A	198	VAL
1	A	199	GLU
1	A	201	CYS
1	A	206	LYS
1	A	211	MET
1	A	220	ILE
1	A	225	ARG
1	A	226	SER
1	A	228	ILE
1	A	230	LEU
1	A	233	THR
1	A	235	LEU
1	A	237	LYS
1	A	241	THR
1	A	242	GLU
1	A	249	GLU
1	A	253	THR
1	A	263	LYS
1	A	264	HIS
1	A	265	LYS
1	A	268	VAL
1	A	270	LYS
1	A	272	SER
1	A	278	THR
1	A	295	SER
1	A	298	ARG
1	A	304	ILE
1	A	309	SER
1	A	323	THR
1	A	326	THR
1	A	336	LYS
1	A	339	ARG
1	A	342	LYS
1	A	343	LYS
1	A	350	SER
1	A	351	THR
1	A	357	LYS
1	A	361	GLU
1	A	366	ASP

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Mol	Chain	Res	Type
1	A	372	ARG
1	A	373	ILE
1	A	375	MET
1	A	380	LEU
1	A	397	VAL
1	A	399	ASN
1	A	411	LYS
1	A	413	ILE
1	A	419	ASN
1	A	420	THR
1	A	423	ASN
1	A	424	ASN
1	A	436	ILE
1	A	439	THR
1	A	445	ASP
1	A	446	MET
1	A	447	ASP
1	A	448	ILE
1	A	463	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	42	ASN
1	A	279	ASN
1	A	283	HIS
1	A	399	ASN
1	A	409	HIS
1	A	419	ASN
1	A	423	ASN
1	A	453	HIS
1	A	475	ASN

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	460/482 (95%)	0.71	40 (8%) 17 19	25, 46, 82, 151	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	VAL	7.0
1	A	140	ARG	4.9
1	A	58	GLN	4.1
1	A	476	ALA	3.8
1	A	338	PRO	3.8
1	A	242	GLU	3.8
1	A	149	SER	3.7
1	A	57	ALA	3.7
1	A	372	ARG	3.6
1	A	280	LEU	3.6
1	A	29	THR	3.4
1	A	220	ILE	3.3
1	A	443	ILE	3.2
1	A	97	GLU	3.0
1	A	120	ILE	3.0
1	A	233	THR	2.9
1	A	26	LEU	2.9
1	A	146	THR	2.8
1	A	217	TRP	2.8
1	A	420	THR	2.7
1	A	373	ILE	2.7
1	A	55	ASP	2.7
1	A	235	LEU	2.6
1	A	366	ASP	2.6
1	A	428	LYS	2.5
1	A	30	PHE	2.5
1	A	246	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	390	VAL	2.5
1	A	181	LEU	2.4
1	A	180	ILE	2.4
1	A	109	SER	2.3
1	A	198	VAL	2.3
1	A	237	LYS	2.3
1	A	238	LEU	2.3
1	A	195	ARG	2.3
1	A	42	ASN	2.2
1	A	478	SER	2.1
1	A	48	PHE	2.0
1	A	219	ASP	2.0
1	A	335	GLY	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.