



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:03 AM EDT

PDB ID : 2QMR / pdb_00002qmr
Title : Karyopherin beta2/transportin
Authors : Cansizoglu, A.E.; Chook, Y.M.
Deposited on : 2007-07-16
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

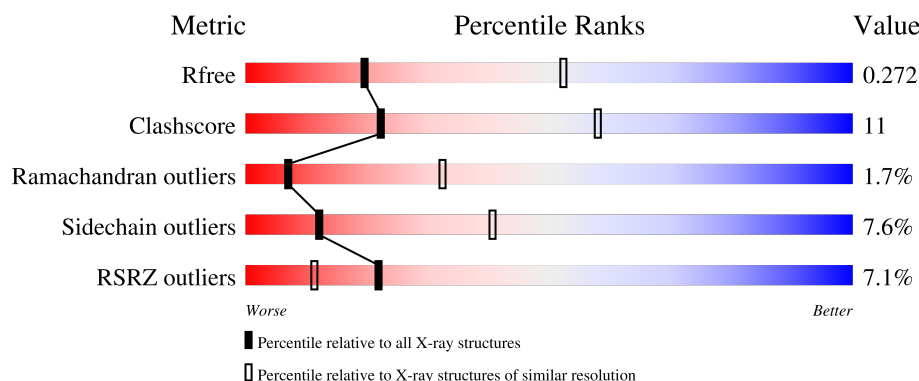
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	890	 6% 69% 21% • 6%
1	B	890	 5% 69% 19% • 10%
1	C	890	 7% 70% 20% • 7%
1	D	890	 7% 69% 22% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25774 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.

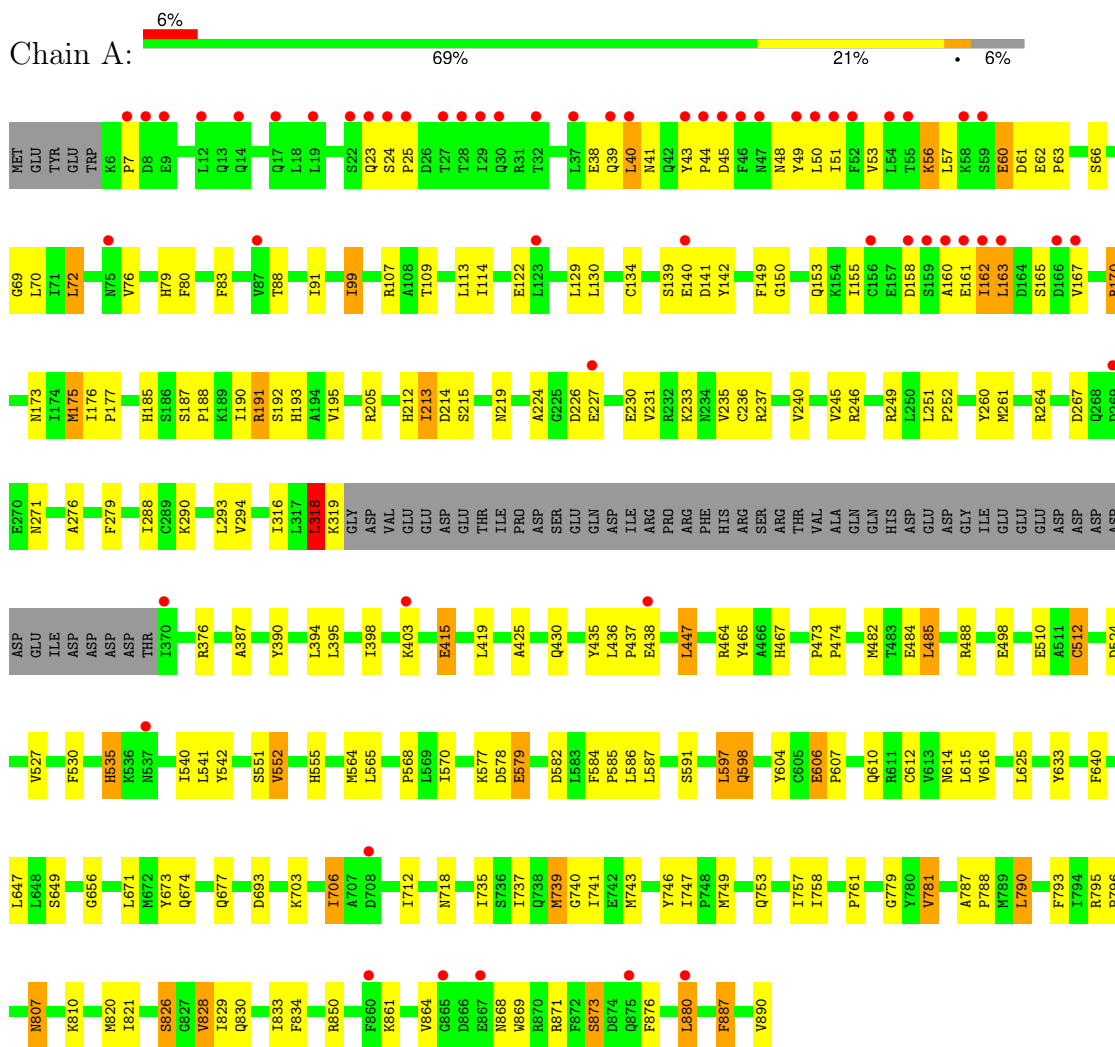
- Molecule 1 is a protein called Transportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6523	4183	1090	1199	51			
1	B	801	Total	C	N	O	S	0	0	0
			6308	4054	1051	1152	51			
1	C	824	Total	C	N	O	S	0	0	0
			6422	4122	1073	1176	51			
1	D	835	Total	C	N	O	S	0	0	0
			6521	4182	1089	1199	51			

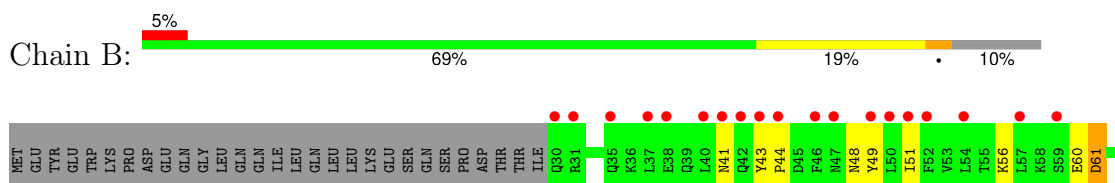
3 Residue-property plots

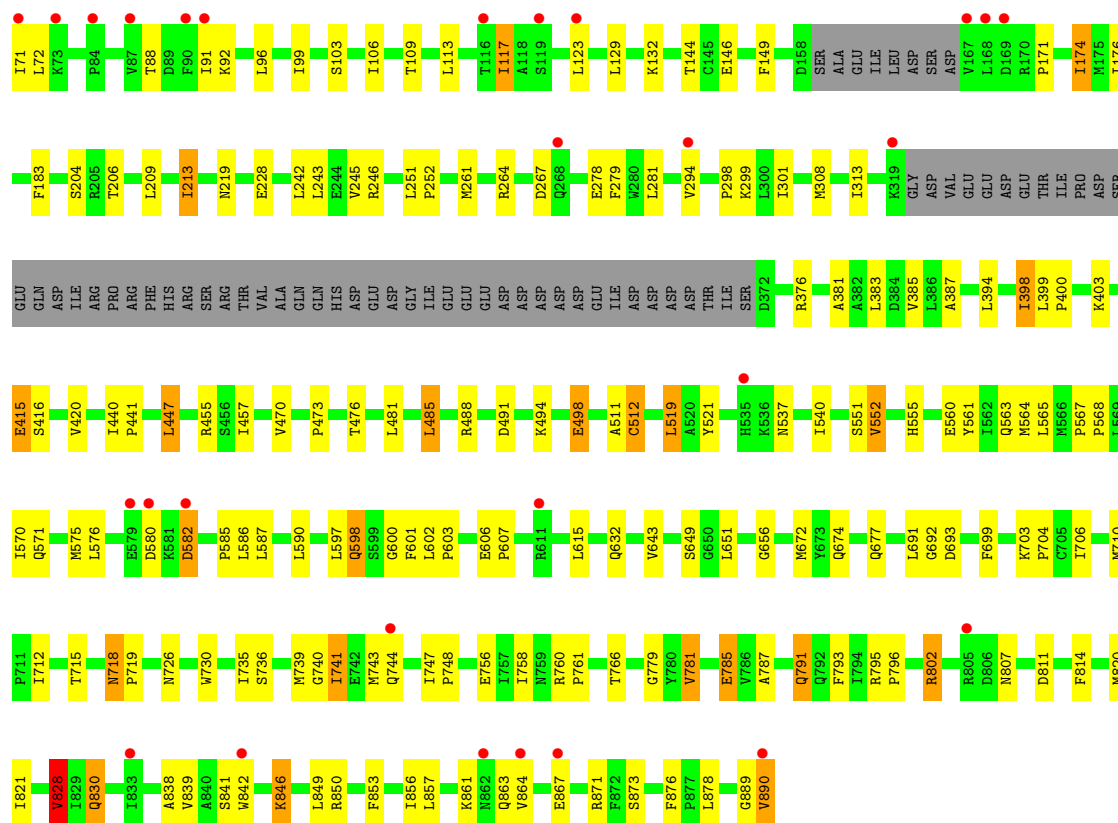
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transportin-1

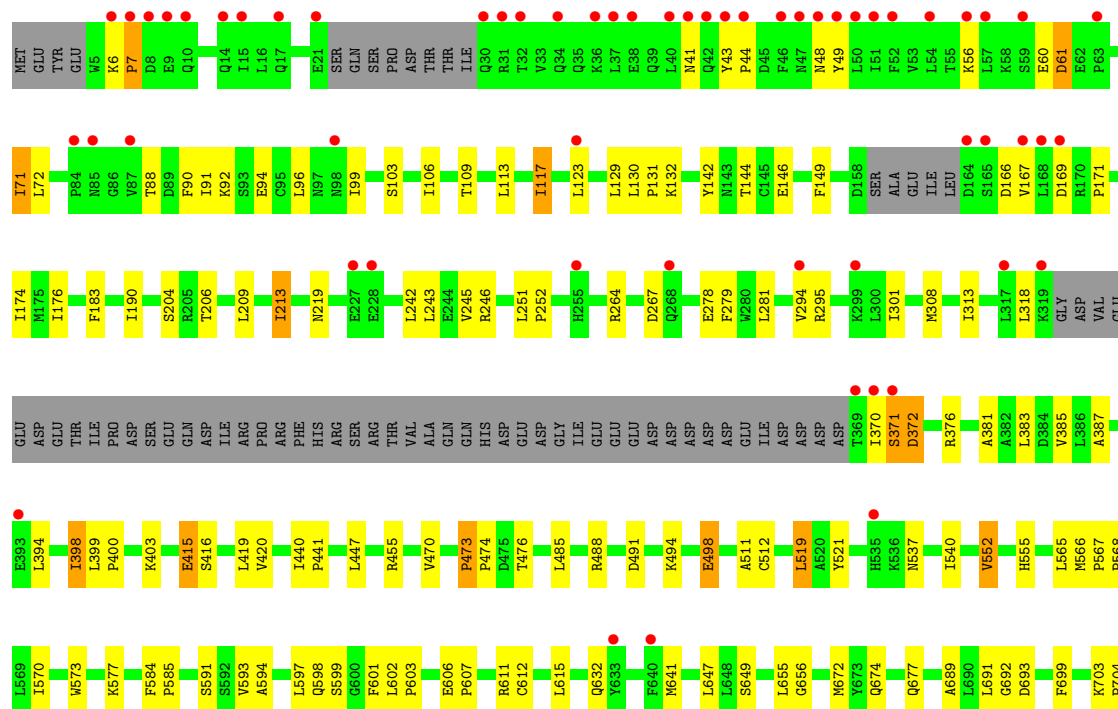


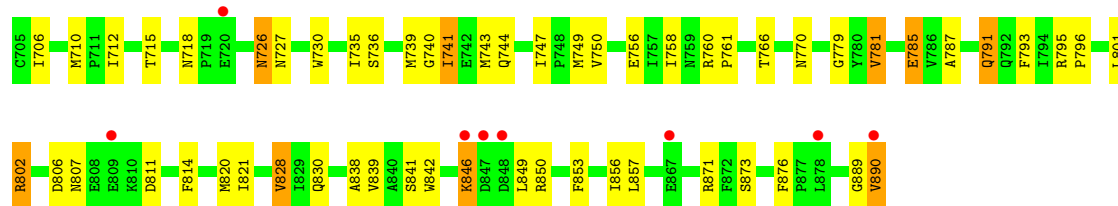
• Molecule 1: Transportin-1



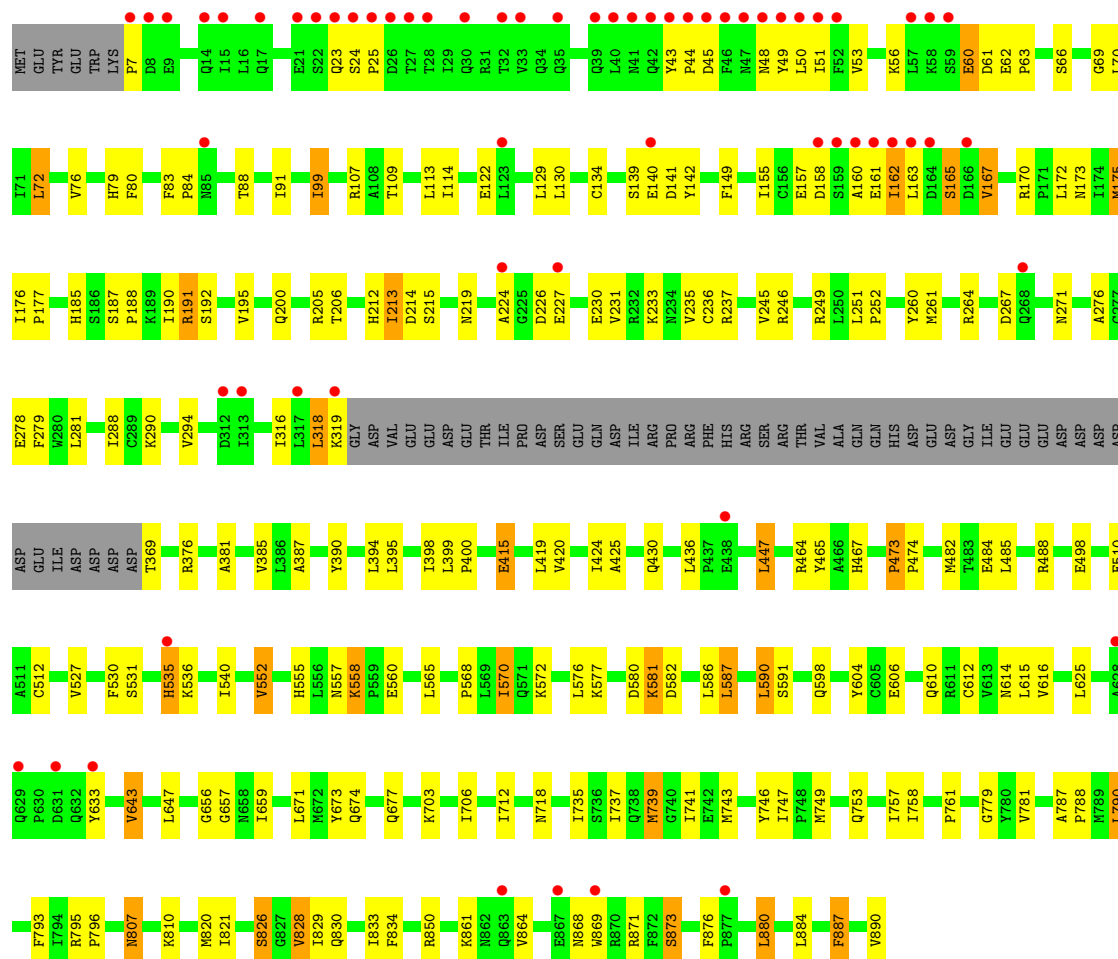


- Molecule 1: Transportin-1





● Molecule 1: Transportin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.34Å 168.89Å 140.96Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.00) 99.9 (50.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.286 0.247 , 0.272	Depositor DCC
R_{free} test set	6088 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25774	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	1/6662 (0.0%)	0.91	5/9060 (0.1%)
1	B	0.48	0/6446	0.91	8/8762 (0.1%)
1	C	0.50	0/6559	0.91	5/8918 (0.1%)
1	D	0.51	0/6660	0.92	8/9056 (0.1%)
All	All	0.50	1/26327 (0.0%)	0.91	26/35796 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	LEU	CA-C	5.40	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	PRO	N-CA-CB	6.99	110.58	102.76
1	D	7	PRO	N-CA-CB	6.85	110.53	103.00
1	C	7	PRO	N-CA-CB	6.75	110.33	103.25
1	A	718	ASN	CA-C-N	6.58	126.28	119.56
1	A	718	ASN	C-N-CA	6.58	126.28	119.56
1	B	718	ASN	CA-C-N	6.48	126.41	119.28
1	B	718	ASN	C-N-CA	6.48	126.41	119.28
1	C	718	ASN	CA-C-N	6.35	126.27	119.28
1	C	718	ASN	C-N-CA	6.35	126.27	119.28
1	D	25	PRO	N-CA-CB	6.32	110.52	103.44
1	D	718	ASN	CA-C-N	6.23	125.91	119.56
1	D	718	ASN	C-N-CA	6.23	125.91	119.56
1	A	25	PRO	N-CA-CB	6.19	110.38	103.44
1	B	473	PRO	CA-C-N	5.95	125.63	119.56
1	B	473	PRO	C-N-CA	5.95	125.63	119.56
1	B	600	GLY	N-CA-C	-5.86	107.39	114.66
1	B	228	GLU	CA-C-N	5.64	125.11	119.24
1	B	228	GLU	C-N-CA	5.64	125.11	119.24
1	B	828	VAL	CB-CA-C	-5.56	106.17	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	473	PRO	CA-C-N	5.41	125.74	119.47
1	D	473	PRO	C-N-CA	5.41	125.74	119.47
1	D	512	CYS	CB-CA-C	-5.24	110.55	116.63
1	C	473	PRO	CA-C-N	5.21	125.51	119.47
1	C	473	PRO	C-N-CA	5.21	125.51	119.47
1	D	167	VAL	N-CA-C	-5.09	106.62	112.98
1	A	512	CYS	CB-CA-C	-5.00	110.83	116.63

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	6523	0	6459	156	0
1	B	6308	0	6296	119	0
1	C	6422	0	6345	125	0
1	D	6521	0	6462	150	0
All	All	25774	0	25562	544	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 11.

All (544) 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:60:GLU:CG	1:A:61:ASP:H	1.73	1.01
1:C:56:LYS:O	1:C:60:GLU:HB3	1.61	1.01
1:D:60:GLU:CG	1:D:61:ASP:H	1.71	1.01
1:B:56:LYS:O	1:B:60:GLU:HB3	1.64	0.98
1:D:188:PRO:HA	1:D:191:ARG:NH1	1.82	0.95
1:D:793:PHE:HZ	1:D:820:MET:HE1	1.29	0.94
1:A:188:PRO:HA	1:A:191:ARG:NH1	1.82	0.94
1:A:793:PHE:HZ	1:A:820:MET:HE1	1.31	0.93
1:D:177:PRO:HG3	1:D:212:HIS:CE1	2.03	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:LEU:HD22	1:D:643:VAL:HG12	1.50	0.92
1:A:177:PRO:HG3	1:A:212:HIS:CE1	2.05	0.92
1:C:873:SER:HA	1:C:876:PHE:CD2	2.04	0.91
1:B:873:SER:HA	1:B:876:PHE:CD2	2.05	0.90
1:C:736:SER:HA	1:C:743:MET:HE3	1.53	0.89
1:A:821:ILE:HG12	1:A:828:VAL:HG21	1.56	0.85
1:A:49:TYR:CE1	1:A:91:ILE:HG12	2.11	0.85
1:D:49:TYR:CE1	1:D:91:ILE:HG12	2.11	0.85
1:C:584:PHE:HB3	1:C:585:PRO:HD3	1.56	0.84
1:D:60:GLU:HG2	1:D:61:ASP:H	1.42	0.84
1:C:873:SER:HA	1:C:876:PHE:HD2	1.41	0.83
1:C:735:ILE:HG22	1:C:743:MET:HE1	1.61	0.82
1:A:60:GLU:HG2	1:A:61:ASP:H	1.44	0.80
1:D:134:CYS:HB3	1:D:175:MET:HE2	1.61	0.80
1:D:793:PHE:CZ	1:D:820:MET:HE1	2.16	0.80
1:D:213:ILE:CD1	1:D:246:ARG:HH21	1.95	0.80
1:B:873:SER:HA	1:B:876:PHE:HD2	1.44	0.79
1:D:60:GLU:HG3	1:D:61:ASP:H	1.47	0.79
1:B:308:MET:HE1	1:B:383:LEU:HD22	1.64	0.79
1:D:60:GLU:CG	1:D:61:ASP:N	2.45	0.79
1:D:425:ALA:HB2	1:D:465:TYR:HE1	1.46	0.78
1:C:793:PHE:HZ	1:C:820:MET:HE1	1.49	0.78
1:B:839:VAL:HG11	1:B:853:PHE:CE2	2.19	0.78
1:A:213:ILE:CD1	1:A:246:ARG:HH21	1.97	0.77
1:B:793:PHE:HZ	1:B:820:MET:HE1	1.48	0.77
1:A:60:GLU:HG3	1:A:61:ASP:H	1.48	0.77
1:A:793:PHE:CZ	1:A:820:MET:HE1	2.18	0.77
1:B:736:SER:HA	1:B:743:MET:HE3	1.64	0.77
1:D:821:ILE:HG12	1:D:828:VAL:HG21	1.65	0.76
1:A:60:GLU:CG	1:A:61:ASP:N	2.47	0.76
1:C:839:VAL:HG11	1:C:853:PHE:CE2	2.20	0.76
1:C:814:PHE:HZ	1:C:853:PHE:HD2	1.33	0.76
1:C:785:GLU:OE1	1:C:785:GLU:HA	1.87	0.75
1:D:793:PHE:HZ	1:D:820:MET:CE	2.00	0.75
1:A:162:ILE:HG22	1:A:163:LEU:N	2.02	0.75
1:B:498:GLU:HG3	1:B:537:ASN:ND2	2.03	0.74
1:B:814:PHE:HZ	1:B:853:PHE:HD2	1.33	0.74
1:B:793:PHE:CZ	1:B:820:MET:HE1	2.22	0.74
1:C:793:PHE:CZ	1:C:820:MET:HE1	2.22	0.74
1:C:814:PHE:HZ	1:C:853:PHE:CD2	2.06	0.74
1:A:425:ALA:HB2	1:A:465:TYR:HE1	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:PHE:HZ	1:B:853:PHE:CD2	2.05	0.73
1:D:191:ARG:CG	1:D:191:ARG:HH11	2.02	0.73
1:D:570:ILE:HD11	1:D:604:TYR:HB3	1.71	0.73
1:A:821:ILE:HG12	1:A:828:VAL:CG2	2.20	0.71
1:C:649:SER:HB2	1:C:693:ASP:OD2	1.89	0.71
1:C:308:MET:HE1	1:C:383:LEU:HD22	1.73	0.71
1:C:470:VAL:HG22	1:C:511:ALA:HB2	1.71	0.71
1:A:793:PHE:HZ	1:A:820:MET:CE	2.04	0.71
1:A:49:TYR:CE1	1:A:72:LEU:HD21	2.26	0.70
1:B:649:SER:HB2	1:B:693:ASP:OD2	1.90	0.70
1:D:162:ILE:HG22	1:D:163:LEU:H	1.56	0.70
1:A:134:CYS:HB3	1:A:175:MET:CE	2.22	0.70
1:D:233:LYS:HE3	1:D:237:ARG:NH1	2.07	0.70
1:B:470:VAL:HG22	1:B:511:ALA:HB2	1.74	0.69
1:A:807:ASN:ND2	1:A:810:LYS:H	1.91	0.69
1:B:735:ILE:HG22	1:B:743:MET:HE1	1.76	0.68
1:D:49:TYR:CE1	1:D:72:LEU:HD21	2.29	0.68
1:B:567:PRO:HB2	1:B:568:PRO:HD3	1.75	0.68
1:A:49:TYR:CZ	1:A:72:LEU:HD21	2.28	0.68
1:A:673:TYR:OH	1:A:712:ILE:HD11	1.94	0.68
1:B:740:GLY:HA2	1:B:781:VAL:HG22	1.74	0.68
1:A:191:ARG:HH11	1:A:191:ARG:CG	2.07	0.68
1:C:599:SER:HA	1:C:655:LEU:HD23	1.75	0.67
1:C:740:GLY:HA2	1:C:781:VAL:HG22	1.75	0.67
1:A:612:CYS:O	1:A:616:VAL:HG23	1.94	0.67
1:D:673:TYR:OH	1:D:712:ILE:HD11	1.95	0.67
1:C:498:GLU:HG3	1:C:537:ASN:ND2	2.09	0.66
1:D:162:ILE:HG22	1:D:163:LEU:N	2.11	0.66
1:D:807:ASN:ND2	1:D:810:LYS:H	1.94	0.66
1:A:233:LYS:HE3	1:A:237:ARG:NH1	2.10	0.65
1:B:785:GLU:OE1	1:B:785:GLU:HA	1.94	0.65
1:A:188:PRO:CA	1:A:191:ARG:NH1	2.58	0.65
1:C:313:ILE:H	1:C:313:ILE:HD12	1.62	0.65
1:D:49:TYR:CZ	1:D:72:LEU:HD21	2.32	0.65
1:D:185:HIS:HD2	1:D:187:SER:H	1.44	0.65
1:D:188:PRO:HA	1:D:191:ARG:HH12	1.62	0.65
1:B:447:LEU:O	1:B:488:ARG:HD2	1.96	0.65
1:D:612:CYS:O	1:D:616:VAL:HG23	1.96	0.65
1:C:470:VAL:CG2	1:C:511:ALA:HB2	2.28	0.64
1:D:674:GLN:HA	1:D:677:GLN:HE21	1.63	0.64
1:A:162:ILE:HG22	1:A:163:LEU:H	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ILE:CD1	1:D:604:TYR:HB3	2.28	0.64
1:A:674:GLN:HA	1:A:677:GLN:HE21	1.62	0.64
1:D:395:LEU:HA	1:D:398:ILE:HG22	1.80	0.64
1:A:236:CYS:SG	1:A:261:MET:HE1	2.38	0.64
1:C:447:LEU:O	1:C:488:ARG:HD2	1.98	0.64
1:A:134:CYS:SG	1:A:175:MET:HE3	2.38	0.63
1:A:746:TYR:HA	1:A:749:MET:HE3	1.80	0.63
1:D:188:PRO:HA	1:D:191:ARG:HH11	1.62	0.63
1:D:821:ILE:HG12	1:D:828:VAL:CG2	2.27	0.63
1:A:552:VAL:HG13	1:A:555:HIS:HB2	1.80	0.63
1:D:264:ARG:HB3	1:D:276:ALA:HB2	1.80	0.63
1:B:376:ARG:NH2	1:B:415:GLU:OE2	2.32	0.63
1:D:552:VAL:HG13	1:D:555:HIS:HB2	1.81	0.62
1:A:264:ARG:NH1	1:A:267:ASP:OD2	2.33	0.62
1:D:425:ALA:CB	1:D:465:TYR:HE1	2.11	0.62
1:B:601:PHE:CE2	1:B:651:LEU:HD11	2.34	0.62
1:C:566:MET:HE1	1:C:593:VAL:HG11	1.80	0.62
1:D:191:ARG:HH11	1:D:191:ARG:HG2	1.62	0.62
1:C:308:MET:HE1	1:C:383:LEU:CD2	2.28	0.62
1:A:188:PRO:HA	1:A:191:ARG:HH12	1.64	0.62
1:B:814:PHE:CZ	1:B:853:PHE:HD2	2.15	0.62
1:D:188:PRO:CA	1:D:191:ARG:NH1	2.61	0.62
1:C:814:PHE:CZ	1:C:853:PHE:HD2	2.15	0.62
1:B:455:ARG:NH1	1:B:491:ASP:OD2	2.31	0.62
1:A:188:PRO:CA	1:A:191:ARG:HH12	2.13	0.61
1:A:264:ARG:HB3	1:A:276:ALA:HB2	1.81	0.61
1:D:236:CYS:SG	1:D:261:MET:HE1	2.40	0.61
1:A:173:ASN:ND2	1:C:521:TYR:OH	2.33	0.61
1:B:308:MET:HE1	1:B:383:LEU:CD2	2.29	0.61
1:A:192:SER:OG	1:A:230:GLU:HG3	2.01	0.61
1:B:313:ILE:HD12	1:B:313:ILE:H	1.65	0.61
1:D:795:ARG:HB2	1:D:796:PRO:HD3	1.81	0.60
1:A:185:HIS:HD2	1:A:187:SER:H	1.48	0.60
1:B:213:ILE:HD13	1:B:246:ARG:HE	1.65	0.60
1:C:400:PRO:HA	1:C:403:LYS:HE3	1.83	0.60
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.83	0.60
1:C:821:ILE:HG23	1:C:828:VAL:HG21	1.83	0.60
1:D:80:PHE:O	1:D:83:PHE:HB2	2.01	0.60
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.65	0.60
1:B:470:VAL:CG2	1:B:511:ALA:HB2	2.31	0.60
1:C:455:ARG:NH1	1:C:491:ASP:OD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ILE:HD11	1:A:604:TYR:HB3	1.84	0.60
1:B:740:GLY:HA2	1:B:781:VAL:CG2	2.32	0.60
1:D:192:SER:OG	1:D:230:GLU:HG3	2.01	0.59
1:B:521:TYR:OH	1:D:173:ASN:ND2	2.35	0.59
1:D:213:ILE:HD11	1:D:246:ARG:HH21	1.67	0.59
1:A:261:MET:HE2	1:A:261:MET:HA	1.83	0.59
1:A:290:LYS:O	1:A:294:VAL:HG23	2.02	0.59
1:A:425:ALA:CB	1:A:465:TYR:HE1	2.15	0.59
1:C:567:PRO:HB2	1:C:568:PRO:HD3	1.85	0.59
1:D:142:TYR:HE1	1:D:190:ILE:HD12	1.67	0.59
1:A:231:VAL:O	1:A:235:VAL:HG23	2.02	0.59
1:A:80:PHE:O	1:A:83:PHE:HB2	2.03	0.59
1:D:861:LYS:HD2	1:D:890:VAL:HG13	1.83	0.59
1:B:821:ILE:HG23	1:B:828:VAL:HG21	1.83	0.59
1:A:188:PRO:HA	1:A:191:ARG:HH11	1.62	0.59
1:B:873:SER:HA	1:B:876:PHE:CE2	2.36	0.59
1:D:62:GLU:N	1:D:63:PRO:HD2	2.17	0.59
1:C:873:SER:HA	1:C:876:PHE:CE2	2.37	0.59
1:D:188:PRO:CA	1:D:191:ARG:HH12	2.15	0.59
1:B:565:LEU:O	1:B:568:PRO:HD2	2.03	0.58
1:D:213:ILE:HD12	1:D:249:ARG:HG3	1.84	0.58
1:C:49:TYR:CE2	1:C:72:LEU:HD21	2.38	0.58
1:A:142:TYR:CE1	1:A:190:ILE:HD12	2.38	0.58
1:D:290:LYS:O	1:D:294:VAL:HG23	2.03	0.58
1:A:864:VAL:HG22	1:A:868:ASN:CB	2.34	0.58
1:B:793:PHE:HZ	1:B:820:MET:CE	2.15	0.58
1:C:91:ILE:HG23	1:C:92:LYS:N	2.19	0.58
1:A:793:PHE:O	1:A:796:PRO:HD2	2.03	0.58
1:B:49:TYR:CE2	1:B:72:LEU:HD21	2.39	0.58
1:B:213:ILE:HG21	1:B:246:ARG:HD3	1.86	0.57
1:C:740:GLY:HA2	1:C:781:VAL:CG2	2.34	0.57
1:D:436:LEU:HD21	1:D:465:TYR:CE2	2.38	0.57
1:B:91:ILE:HG23	1:B:92:LYS:N	2.18	0.57
1:D:587:LEU:HD22	1:D:643:VAL:CG1	2.30	0.57
1:C:103:SER:HB3	1:C:106:ILE:HD12	1.86	0.57
1:B:576:LEU:HD11	1:B:586:LEU:HD23	1.87	0.57
1:D:735:ILE:HG22	1:D:743:MET:HE1	1.87	0.57
1:C:213:ILE:HG21	1:C:246:ARG:HD3	1.85	0.57
1:C:381:ALA:O	1:C:385:VAL:HG23	2.05	0.57
1:C:519:LEU:HD11	1:C:552:VAL:HG21	1.85	0.57
1:D:251:LEU:HB3	1:D:252:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:MET:HA	1:D:261:MET:HE2	1.85	0.57
1:C:243:LEU:HD22	1:C:279:PHE:CE1	2.40	0.57
1:C:793:PHE:HZ	1:C:820:MET:CE	2.16	0.57
1:A:170:ARG:HD2	1:A:175:MET:HE2	1.87	0.57
1:B:779:GLY:HA3	1:B:820:MET:SD	2.45	0.56
1:B:597:LEU:O	1:B:598:GLN:C	2.48	0.56
1:C:213:ILE:HD13	1:C:246:ARG:HE	1.71	0.56
1:D:134:CYS:HB3	1:D:175:MET:CE	2.34	0.56
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.87	0.56
1:B:802:ARG:HA	1:B:842:TRP:CD1	2.40	0.56
1:D:746:TYR:HA	1:D:749:MET:HE3	1.88	0.56
1:C:96:LEU:HD13	1:C:132:LYS:HG2	1.87	0.56
1:C:376:ARG:NH2	1:C:415:GLU:OE2	2.39	0.56
1:A:60:GLU:HG3	1:A:61:ASP:N	2.18	0.56
1:B:400:PRO:HA	1:B:403:LYS:HE3	1.87	0.56
1:A:150:GLY:HA2	1:A:193:HIS:CE1	2.41	0.56
1:C:48:ASN:HD22	1:C:72:LEU:HD13	1.71	0.56
1:A:214:ASP:OD1	1:A:249:ARG:HD2	2.06	0.56
1:C:552:VAL:HG13	1:C:555:HIS:HB2	1.88	0.56
1:C:802:ARG:HA	1:C:842:TRP:CD1	2.40	0.56
1:A:62:GLU:N	1:A:63:PRO:HD2	2.20	0.56
1:A:735:ILE:HG22	1:A:743:MET:HE1	1.88	0.56
1:A:527:VAL:O	1:A:530:PHE:HB2	2.07	0.55
1:A:795:ARG:HB2	1:A:796:PRO:HD3	1.86	0.55
1:B:552:VAL:HG13	1:B:555:HIS:HB2	1.87	0.55
1:D:165:SER:C	1:D:167:VAL:H	2.15	0.55
1:A:861:LYS:HD2	1:A:890:VAL:HG13	1.89	0.55
1:B:787:ALA:HA	1:B:820:MET:HE3	1.89	0.55
1:A:49:TYR:OH	1:A:91:ILE:HG23	2.07	0.55
1:B:103:SER:HB3	1:B:106:ILE:HD12	1.89	0.55
1:D:464:ARG:C	1:D:465:TYR:HD1	2.15	0.54
1:A:45:ASP:HA	1:A:48:ASN:HB2	1.89	0.54
1:A:864:VAL:HG22	1:A:868:ASN:HB2	1.89	0.54
1:B:49:TYR:CZ	1:B:72:LEU:HD21	2.43	0.54
1:D:758:ILE:HG12	1:D:796:PRO:HB2	1.89	0.54
1:D:864:VAL:HG22	1:D:868:ASN:CB	2.37	0.54
1:A:215:SER:O	1:A:219:ASN:ND2	2.40	0.54
1:A:779:GLY:HA3	1:A:820:MET:SD	2.48	0.54
1:A:142:TYR:HE1	1:A:190:ILE:HD12	1.72	0.54
1:D:49:TYR:OH	1:D:91:ILE:HG23	2.07	0.54
1:A:153:GLN:OE1	1:A:193:HIS:ND1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:779:GLY:HA3	1:C:820:MET:SD	2.48	0.54
1:A:464:ARG:C	1:A:465:TYR:HD1	2.16	0.53
1:A:582:ASP:O	1:A:585:PRO:HD2	2.08	0.53
1:D:134:CYS:CB	1:D:175:MET:HE2	2.33	0.53
1:D:264:ARG:NH1	1:D:267:ASP:OD2	2.38	0.53
1:A:130:LEU:HD21	1:A:155:ILE:HG21	1.90	0.53
1:C:264:ARG:NH1	1:C:267:ASP:OD2	2.41	0.53
1:C:594:ALA:HA	1:C:601:PHE:CD1	2.43	0.53
1:D:425:ALA:CB	1:D:465:TYR:CE1	2.90	0.53
1:D:557:ASN:C	1:D:558:LYS:HG2	2.33	0.53
1:C:853:PHE:HE1	1:C:857:LEU:HD11	1.73	0.53
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.89	0.53
1:A:826:SER:HA	1:A:829:ILE:HD12	1.90	0.53
1:A:625:LEU:HB3	1:A:633:TYR:CD1	2.43	0.53
1:C:584:PHE:HB3	1:C:585:PRO:CD	2.35	0.53
1:D:214:ASP:OD1	1:D:249:ARG:HD2	2.09	0.53
1:A:134:CYS:HB3	1:A:175:MET:HE2	1.91	0.53
1:A:703:LYS:HE3	1:A:739:MET:HE1	1.91	0.53
1:B:498:GLU:HG3	1:B:537:ASN:HD22	1.72	0.53
1:B:519:LEU:HD11	1:B:552:VAL:HG21	1.89	0.53
1:C:606:GLU:HB3	1:C:607:PRO:HD3	1.91	0.53
1:D:703:LYS:HE3	1:D:739:MET:HE1	1.91	0.53
1:C:183:PHE:HD1	1:C:219:ASN:HB3	1.74	0.52
1:C:735:ILE:HG22	1:C:743:MET:CE	2.35	0.52
1:D:447:LEU:O	1:D:488:ARG:HD2	2.09	0.52
1:D:45:ASP:HA	1:D:48:ASN:HB2	1.90	0.52
1:D:790:LEU:HD13	1:D:820:MET:HE2	1.92	0.52
1:B:601:PHE:HE2	1:B:651:LEU:HD11	1.74	0.52
1:C:674:GLN:HA	1:C:677:GLN:HE21	1.74	0.52
1:D:264:ARG:O	1:D:267:ASP:HB2	2.09	0.52
1:B:183:PHE:HD1	1:B:219:ASN:HB3	1.75	0.52
1:B:853:PHE:HE1	1:B:857:LEU:HD11	1.75	0.52
1:C:49:TYR:CZ	1:C:72:LEU:HD21	2.44	0.52
1:C:308:MET:HE1	1:C:383:LEU:CB	2.39	0.52
1:A:447:LEU:HD23	1:A:484:GLU:HB3	1.92	0.51
1:C:308:MET:HE1	1:C:383:LEU:HB2	1.91	0.51
1:C:318:LEU:HD21	1:C:370:ILE:HB	1.91	0.51
1:D:793:PHE:O	1:D:796:PRO:HD2	2.09	0.51
1:B:674:GLN:HA	1:B:677:GLN:HE21	1.76	0.51
1:D:130:LEU:HD21	1:D:155:ILE:HG21	1.91	0.51
1:D:245:VAL:HG12	1:D:246:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD21	1:A:465:TYR:CE2	2.44	0.51
1:A:318:LEU:O	1:A:319:LYS:HB2	2.11	0.51
1:B:96:LEU:HD13	1:B:132:LYS:HG2	1.92	0.51
1:B:243:LEU:HD22	1:B:279:PHE:CE1	2.45	0.51
1:C:573:TRP:HZ2	1:C:611:ARG:HB3	1.76	0.51
1:D:60:GLU:HG3	1:D:61:ASP:N	2.17	0.51
1:D:625:LEU:HB3	1:D:633:TYR:CD1	2.45	0.51
1:D:826:SER:HA	1:D:829:ILE:HD12	1.91	0.51
1:D:60:GLU:HG2	1:D:61:ASP:N	2.18	0.51
1:A:403:LYS:HE3	1:B:299:LYS:HE3	1.92	0.51
1:A:425:ALA:CB	1:A:465:TYR:CE1	2.94	0.51
1:D:376:ARG:NH2	1:D:415:GLU:OE2	2.43	0.51
1:A:790:LEU:HD13	1:A:820:MET:HE2	1.92	0.51
1:B:838:ALA:O	1:B:842:TRP:HB2	2.10	0.51
1:B:91:ILE:CG2	1:B:92:LYS:N	2.75	0.50
1:C:251:LEU:HB3	1:C:252:PRO:HD3	1.92	0.50
1:A:577:LYS:O	1:A:579:GLU:N	2.44	0.50
1:C:91:ILE:CG2	1:C:92:LYS:N	2.74	0.50
1:C:440:ILE:HB	1:C:441:PRO:HD3	1.92	0.50
1:A:597:LEU:O	1:A:598:GLN:C	2.55	0.50
1:B:301:ILE:HG21	1:B:398:ILE:HG12	1.92	0.50
1:C:88:THR:O	1:C:91:ILE:HG22	2.12	0.50
1:D:318:LEU:O	1:D:319:LYS:HB2	2.11	0.50
1:D:753:GLN:O	1:D:757:ILE:HG13	2.12	0.50
1:A:69:GLY:HA2	1:A:72:LEU:HD23	1.93	0.50
1:A:213:ILE:HD12	1:A:249:ARG:HG3	1.92	0.50
1:D:69:GLY:HA2	1:D:72:LEU:HD23	1.93	0.50
1:A:264:ARG:O	1:A:267:ASP:HB2	2.12	0.50
1:C:498:GLU:HG3	1:C:537:ASN:HD22	1.74	0.50
1:B:113:LEU:O	1:B:117:ILE:HD12	2.12	0.50
1:A:565:LEU:O	1:A:568:PRO:HD2	2.12	0.50
1:A:758:ILE:HG12	1:A:796:PRO:HB2	1.93	0.49
1:A:162:ILE:CG2	1:A:163:LEU:N	2.73	0.49
1:B:381:ALA:O	1:B:385:VAL:HG23	2.12	0.49
1:B:699:PHE:CE1	1:B:706:ILE:HD11	2.47	0.49
1:C:60:GLU:O	1:C:61:ASP:C	2.55	0.49
1:D:779:GLY:HA3	1:D:820:MET:SD	2.52	0.49
1:B:60:GLU:O	1:B:61:ASP:C	2.55	0.49
1:B:440:ILE:HB	1:B:441:PRO:HD3	1.93	0.49
1:B:560:GLU:O	1:B:564:MET:HG2	2.12	0.49
1:B:176:ILE:HD13	1:B:209:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:GLU:HB3	1:B:607:PRO:HD3	1.93	0.49
1:D:436:LEU:HD21	1:D:465:TYR:CD2	2.47	0.49
1:D:577:LYS:O	1:D:580:ASP:HB2	2.13	0.49
1:A:213:ILE:HD11	1:A:246:ARG:HH21	1.73	0.49
1:B:846:LYS:O	1:B:850:ARG:HB2	2.11	0.49
1:D:591:SER:HA	1:D:647:LEU:HD13	1.95	0.49
1:A:795:ARG:HD3	1:A:834:PHE:HE2	1.78	0.49
1:C:176:ILE:HD13	1:C:209:LEU:HB2	1.95	0.49
1:A:447:LEU:O	1:A:488:ARG:HD2	2.12	0.49
1:B:48:ASN:HD22	1:B:72:LEU:HD13	1.77	0.49
1:C:183:PHE:CD1	1:C:219:ASN:HB3	2.48	0.49
1:A:438:GLU:OE1	1:B:299:LYS:NZ	2.36	0.48
1:A:376:ARG:NH2	1:A:415:GLU:OE2	2.45	0.48
1:B:692:GLY:HA3	1:B:730:TRP:CZ3	2.47	0.48
1:D:498:GLU:HG2	1:D:540:ILE:HD12	1.95	0.48
1:B:43:TYR:N	1:B:44:PRO:CD	2.77	0.48
1:B:264:ARG:NH1	1:B:267:ASP:OD2	2.44	0.48
1:A:524:ASP:OD1	1:A:564:MET:HE1	2.13	0.48
1:D:565:LEU:O	1:D:568:PRO:HD2	2.14	0.48
1:C:806:ASP:HB3	1:C:846:LYS:HE3	1.94	0.48
1:A:224:ALA:HB1	1:A:260:TYR:CE1	2.49	0.48
1:A:753:GLN:O	1:A:757:ILE:HG13	2.13	0.48
1:C:43:TYR:N	1:C:44:PRO:CD	2.76	0.48
1:A:498:GLU:HG2	1:A:540:ILE:HD12	1.96	0.48
1:D:99:ILE:HG13	1:D:114:ILE:CD1	2.44	0.48
1:D:864:VAL:HG22	1:D:868:ASN:HB2	1.96	0.48
1:B:183:PHE:CD1	1:B:219:ASN:HB3	2.48	0.48
1:A:850:ARG:HH11	1:A:887:PHE:HE2	1.61	0.47
1:D:807:ASN:HD22	1:D:810:LYS:H	1.62	0.47
1:D:586:LEU:O	1:D:590:LEU:HB2	2.14	0.47
1:A:435:TYR:CE2	1:B:298:PRO:HG2	2.49	0.47
1:B:251:LEU:HB3	1:B:252:PRO:HD3	1.95	0.47
1:B:795:ARG:HB2	1:B:796:PRO:HD3	1.95	0.47
1:C:570:ILE:O	1:C:573:TRP:HB3	2.14	0.47
1:D:376:ARG:NH2	1:D:419:LEU:HD22	2.30	0.47
1:C:113:LEU:O	1:C:117:ILE:HD12	2.15	0.47
1:B:387:ALA:HA	1:B:394:LEU:HD22	1.97	0.47
1:B:582:ASP:O	1:B:585:PRO:HD2	2.14	0.47
1:D:213:ILE:HD13	1:D:246:ARG:HE	1.80	0.47
1:C:699:PHE:CE1	1:C:706:ILE:HD11	2.49	0.47
1:C:787:ALA:HA	1:C:820:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ALA:HA	1:C:394:LEU:HD22	1.96	0.47
1:A:376:ARG:NH2	1:A:419:LEU:HD22	2.29	0.47
1:C:736:SER:CA	1:C:743:MET:HE3	2.37	0.47
1:D:795:ARG:HD3	1:D:834:PHE:HE2	1.80	0.47
1:A:38:GLU:C	1:A:40:LEU:H	2.23	0.46
1:C:49:TYR:CZ	1:C:91:ILE:HG13	2.50	0.46
1:C:692:GLY:HA3	1:C:730:TRP:CZ3	2.50	0.46
1:C:873:SER:CA	1:C:876:PHE:HD2	2.20	0.46
1:D:482:MET:HB3	1:D:482:MET:HE2	1.54	0.46
1:A:530:PHE:HD2	1:A:568:PRO:HB2	1.80	0.46
1:C:264:ARG:O	1:C:267:ASP:HB2	2.14	0.46
1:C:795:ARG:HB2	1:C:796:PRO:HD3	1.96	0.46
1:C:846:LYS:O	1:C:850:ARG:HB2	2.14	0.46
1:C:889:GLY:O	1:C:890:VAL:HG23	2.16	0.46
1:D:215:SER:O	1:D:219:ASN:ND2	2.46	0.46
1:A:70:LEU:HG	1:A:109:THR:HG23	1.98	0.46
1:A:99:ILE:HG13	1:A:114:ILE:CD1	2.45	0.46
1:D:231:VAL:O	1:D:235:VAL:HG23	2.16	0.46
1:B:488:ARG:HA	1:B:488:ARG:NE	2.31	0.46
1:D:43:TYR:N	1:D:44:PRO:CD	2.79	0.46
1:A:60:GLU:O	1:A:61:ASP:HB3	2.16	0.45
1:C:488:ARG:HA	1:C:488:ARG:NE	2.30	0.45
1:A:49:TYR:CE1	1:A:72:LEU:CD2	2.97	0.45
1:A:587:LEU:HD23	1:A:647:LEU:HD23	1.99	0.45
1:B:88:THR:O	1:B:91:ILE:HG22	2.15	0.45
1:C:602:LEU:HB3	1:C:603:PRO:HD3	1.98	0.45
1:A:76:VAL:O	1:A:80:PHE:HB2	2.16	0.45
1:B:416:SER:O	1:B:420:VAL:HG23	2.16	0.45
1:D:142:TYR:CE1	1:D:190:ILE:CD1	2.99	0.45
1:D:224:ALA:HB1	1:D:260:TYR:CE1	2.51	0.45
1:A:213:ILE:H	1:A:213:ILE:HG12	1.57	0.45
1:B:587:LEU:HD13	1:B:643:VAL:HG12	1.98	0.45
1:C:741:ILE:H	1:C:741:ILE:HG13	1.34	0.45
1:A:584:PHE:HB2	1:A:640:PHE:HE1	1.82	0.45
1:C:597:LEU:O	1:C:599:SER:N	2.50	0.45
1:D:467:HIS:HA	1:D:510:GLU:HG2	1.97	0.45
1:C:591:SER:HA	1:C:647:LEU:HD13	1.98	0.45
1:D:233:LYS:HE3	1:D:237:ARG:HH12	1.78	0.45
1:D:581:LYS:HD2	1:D:581:LYS:HA	1.77	0.45
1:A:60:GLU:HG2	1:A:61:ASP:N	2.19	0.45
1:C:308:MET:CE	1:C:383:LEU:HD22	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:HA	1:A:319:LYS:HE3	1.99	0.45
1:A:387:ALA:HA	1:A:394:LEU:HD22	1.99	0.45
1:B:308:MET:HE1	1:B:383:LEU:CB	2.47	0.45
1:C:760:ARG:HA	1:C:761:PRO:HD3	1.82	0.45
1:A:165:SER:C	1:A:167:VAL:H	2.25	0.45
1:B:699:PHE:HE1	1:B:706:ILE:HD11	1.81	0.45
1:C:301:ILE:HG21	1:C:398:ILE:HG12	1.99	0.44
1:C:498:GLU:HG2	1:C:540:ILE:HD12	1.99	0.44
1:D:230:GLU:OE2	1:D:233:LYS:NZ	2.34	0.44
1:C:672:MET:HE1	1:C:691:LEU:HA	1.98	0.44
1:D:527:VAL:O	1:D:530:PHE:HB2	2.17	0.44
1:A:542:TYR:HE1	1:A:586:LEU:HB2	1.82	0.44
1:B:498:GLU:HG2	1:B:540:ILE:HD12	2.00	0.44
1:D:213:ILE:H	1:D:213:ILE:HG12	1.61	0.44
1:A:57:LEU:HA	1:A:60:GLU:HB2	1.99	0.44
1:A:649:SER:HB2	1:A:693:ASP:OD2	2.16	0.44
1:A:861:LYS:HG3	1:A:869:TRP:CG	2.53	0.44
1:C:838:ALA:O	1:C:842:TRP:HB2	2.16	0.44
1:D:60:GLU:O	1:D:61:ASP:HB3	2.16	0.44
1:B:741:ILE:H	1:B:741:ILE:HG13	1.35	0.44
1:A:467:HIS:HA	1:A:510:GLU:HG2	1.98	0.44
1:B:672:MET:HE1	1:B:691:LEU:HA	1.98	0.44
1:B:735:ILE:HG22	1:B:743:MET:CE	2.44	0.44
1:B:873:SER:CA	1:B:876:PHE:HD2	2.22	0.44
1:D:657:GLY:H	1:D:659:ILE:HG22	1.82	0.44
1:A:43:TYR:N	1:A:44:PRO:CD	2.81	0.44
1:C:791:GLN:H	1:C:791:GLN:HG3	1.56	0.44
1:A:134:CYS:CB	1:A:175:MET:CE	2.95	0.44
1:D:70:LEU:HG	1:D:109:THR:HG23	1.99	0.44
1:D:294:VAL:HG22	1:D:390:TYR:HE2	1.83	0.44
1:D:316:ILE:HA	1:D:319:LYS:HE3	1.99	0.44
1:A:191:ARG:O	1:A:195:VAL:HG23	2.18	0.43
1:A:293:LEU:O	1:A:294:VAL:C	2.61	0.43
1:B:308:MET:HE1	1:B:383:LEU:HB2	2.00	0.43
1:D:173:ASN:OD1	1:D:173:ASN:O	2.36	0.43
1:D:807:ASN:HD22	1:D:807:ASN:C	2.26	0.43
1:B:602:LEU:HB3	1:B:603:PRO:HD3	1.99	0.43
1:D:530:PHE:CD2	1:D:568:PRO:HB2	2.53	0.43
1:A:482:MET:HE2	1:A:482:MET:HB3	1.62	0.43
1:B:48:ASN:HA	1:B:51:ILE:HD12	2.01	0.43
1:B:174:ILE:H	1:B:174:ILE:HG13	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:CYS:HB3	1:B:551:SER:O	2.18	0.43
1:C:473:PRO:HA	1:C:474:PRO:HD3	1.82	0.43
1:B:739:MET:HG3	1:B:743:MET:HE2	2.00	0.43
1:C:399:LEU:O	1:C:403:LYS:HG2	2.19	0.43
1:C:749:MET:HG3	1:C:750:VAL:HG23	2.00	0.43
1:D:157:GLU:HG3	1:D:200:GLN:NE2	2.32	0.43
1:B:567:PRO:CB	1:B:568:PRO:HD3	2.47	0.43
1:D:88:THR:O	1:D:91:ILE:HB	2.19	0.43
1:D:850:ARG:HH11	1:D:887:PHE:HE2	1.65	0.43
1:C:242:LEU:O	1:C:245:VAL:O	2.36	0.43
1:D:376:ARG:CZ	1:D:419:LEU:HD22	2.49	0.43
1:D:572:LYS:O	1:D:576:LEU:HG	2.18	0.43
1:A:49:TYR:CZ	1:A:91:ILE:HG23	2.53	0.43
1:A:213:ILE:HD13	1:A:246:ARG:HE	1.83	0.43
1:B:519:LEU:HD23	1:B:561:TYR:CE1	2.53	0.43
1:A:236:CYS:O	1:A:240:VAL:HG23	2.19	0.43
1:A:706:ILE:HD12	1:A:706:ILE:HA	1.94	0.43
1:B:242:LEU:O	1:B:245:VAL:O	2.37	0.43
1:B:703:LYS:HB3	1:B:704:PRO:HD3	2.01	0.43
1:C:593:VAL:O	1:C:593:VAL:HG12	2.19	0.43
1:C:699:PHE:HE1	1:C:706:ILE:HD11	1.83	0.43
1:D:205:ARG:HG2	1:D:245:VAL:HG13	2.00	0.43
1:D:861:LYS:HG3	1:D:869:TRP:CG	2.53	0.43
1:D:876:PHE:HB3	1:D:880:LEU:HB3	2.00	0.43
1:C:758:ILE:HG12	1:C:796:PRO:HB2	2.01	0.43
1:D:172:LEU:HD13	1:D:206:THR:HG21	2.01	0.43
1:D:399:LEU:N	1:D:400:PRO:HD2	2.34	0.43
1:D:625:LEU:HD22	1:D:633:TYR:CE1	2.53	0.43
1:A:530:PHE:HD1	1:A:541:LEU:HD21	1.83	0.43
1:B:49:TYR:CZ	1:B:91:ILE:HG13	2.54	0.43
1:B:457:ILE:HD12	1:B:457:ILE:HA	1.91	0.42
1:B:744:GLN:HA	1:B:747:ILE:HD12	2.01	0.42
1:C:416:SER:O	1:C:420:VAL:HG23	2.19	0.42
1:A:56:LYS:O	1:A:60:GLU:HA	2.19	0.42
1:A:205:ARG:HG2	1:A:245:VAL:HG13	2.00	0.42
1:C:130:LEU:HB2	1:C:131:PRO:HD3	2.01	0.42
1:C:744:GLN:HA	1:C:747:ILE:HD12	2.01	0.42
1:A:876:PHE:HB3	1:A:880:LEU:HB3	2.01	0.42
1:C:295:ARG:H	1:C:295:ARG:HG2	1.52	0.42
1:D:49:TYR:CZ	1:D:91:ILE:HG23	2.55	0.42
1:D:191:ARG:NH1	1:D:191:ARG:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:MET:HE2	1:A:743:MET:HA	2.02	0.42
1:C:49:TYR:OH	1:C:91:ILE:HG13	2.19	0.42
1:C:565:LEU:O	1:C:568:PRO:HD2	2.20	0.42
1:A:436:LEU:N	1:A:437:PRO:CD	2.83	0.42
1:B:718:ASN:HA	1:B:719:PRO:HD3	1.78	0.42
1:D:873:SER:HA	1:D:876:PHE:CD1	2.55	0.42
1:C:739:MET:HG3	1:C:743:MET:HE2	2.02	0.42
1:D:425:ALA:HB2	1:D:465:TYR:CE1	2.37	0.42
1:D:473:PRO:HA	1:D:474:PRO:HD3	1.87	0.42
1:B:861:LYS:O	1:B:864:VAL:HG12	2.20	0.42
1:D:76:VAL:O	1:D:80:PHE:HB2	2.19	0.42
1:A:48:ASN:HA	1:A:51:ILE:HD12	2.00	0.42
1:B:264:ARG:O	1:B:267:ASP:HB2	2.20	0.42
1:B:399:LEU:O	1:B:403:LYS:HG2	2.19	0.42
1:B:481:LEU:O	1:B:485:LEU:HB2	2.20	0.42
1:B:889:GLY:O	1:B:890:VAL:HG23	2.19	0.42
1:D:191:ARG:O	1:D:195:VAL:HG23	2.19	0.42
1:A:294:VAL:HG22	1:A:390:TYR:HE2	1.85	0.42
1:C:376:ARG:NH2	1:C:419:LEU:HD22	2.35	0.42
1:B:567:PRO:HB2	1:B:568:PRO:CD	2.47	0.42
1:D:387:ALA:HA	1:D:394:LEU:HD22	2.01	0.42
1:A:88:THR:O	1:A:91:ILE:HB	2.19	0.41
1:A:512:CYS:HA	1:A:551:SER:HB3	2.02	0.41
1:B:760:ARG:HA	1:B:761:PRO:HD3	1.83	0.41
1:C:726:ASN:HD21	1:C:770:ASN:HD22	1.68	0.41
1:B:706:ILE:HG23	1:B:710:MET:HG2	2.01	0.41
1:B:811:ASP:OD2	1:B:849:LEU:HD11	2.20	0.41
1:C:371:SER:O	1:C:372:ASP:C	2.63	0.41
1:C:811:ASP:OD2	1:C:849:LEU:HD11	2.20	0.41
1:D:673:TYR:CZ	1:D:712:ILE:HD11	2.55	0.41
1:A:473:PRO:HA	1:A:474:PRO:HD3	1.85	0.41
1:A:606:GLU:HB3	1:A:607:PRO:HD3	2.02	0.41
1:A:673:TYR:CZ	1:A:712:ILE:HD11	2.55	0.41
1:B:791:GLN:H	1:B:791:GLN:HG3	1.59	0.41
1:A:591:SER:HA	1:A:647:LEU:HD13	2.02	0.41
1:A:787:ALA:HB3	1:A:788:PRO:HD3	2.02	0.41
1:C:90:PHE:CE1	1:C:94:GLU:HG3	2.55	0.41
1:C:706:ILE:HG23	1:C:710:MET:HG2	2.03	0.41
1:B:519:LEU:HD21	1:B:552:VAL:HG11	2.03	0.41
1:C:71:ILE:H	1:C:71:ILE:HG13	1.76	0.41
1:D:142:TYR:CE1	1:D:190:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:VAL:O	1:D:424:ILE:HG12	2.20	0.41
1:A:807:ASN:C	1:A:807:ASN:HD22	2.27	0.41
1:B:498:GLU:HG3	1:B:537:ASN:HD21	1.83	0.41
1:B:830:GLN:HA	1:B:830:GLN:HE21	1.84	0.41
1:C:573:TRP:CZ2	1:C:611:ARG:HB3	2.54	0.41
1:A:173:ASN:OD1	1:A:173:ASN:O	2.39	0.41
1:A:276:ALA:O	1:A:279:PHE:HB3	2.21	0.41
1:A:807:ASN:HD21	1:A:810:LYS:H	1.68	0.41
1:D:134:CYS:SG	1:D:175:MET:HE2	2.60	0.41
1:D:276:ALA:O	1:D:279:PHE:HB3	2.20	0.41
1:B:261:MET:HE3	1:B:279:PHE:HB2	2.02	0.41
1:B:758:ILE:HG12	1:B:796:PRO:HB2	2.03	0.41
1:C:142:TYR:CE1	1:C:190:ILE:HD12	2.55	0.41
1:C:726:ASN:HD22	1:C:726:ASN:HA	1.76	0.41
1:D:48:ASN:HA	1:D:51:ILE:HD12	2.02	0.41
1:D:83:PHE:HA	1:D:84:PRO:HD3	1.96	0.41
1:D:447:LEU:HD23	1:D:484:GLU:HB3	2.03	0.41
1:A:864:VAL:HG22	1:A:868:ASN:HB3	2.02	0.41
1:A:873:SER:HA	1:A:876:PHE:CD1	2.56	0.41
1:B:521:TYR:CZ	1:D:173:ASN:ND2	2.89	0.41
1:B:747:ILE:N	1:B:748:PRO:CD	2.84	0.41
1:C:703:LYS:HB3	1:C:704:PRO:HD3	2.03	0.41
1:D:185:HIS:HD2	1:D:187:SER:N	2.13	0.41
1:D:436:LEU:CD2	1:D:465:TYR:CD2	3.04	0.40
1:D:787:ALA:HB3	1:D:788:PRO:HD3	2.03	0.40
1:D:864:VAL:HG22	1:D:868:ASN:HB3	2.02	0.40
1:A:787:ALA:O	1:A:790:LEU:HB2	2.22	0.40
1:C:567:PRO:CB	1:C:568:PRO:HD3	2.50	0.40
1:A:376:ARG:CZ	1:A:419:LEU:HD22	2.50	0.40
1:A:740:GLY:HA2	1:A:781:VAL:HG22	2.04	0.40
1:B:736:SER:CA	1:B:743:MET:HE3	2.45	0.40
1:C:90:PHE:HE1	1:C:94:GLU:HG3	1.87	0.40
1:C:689:ALA:HB2	1:C:727:ASN:ND2	2.36	0.40
1:D:739:MET:HG3	1:D:743:MET:CE	2.51	0.40
1:A:233:LYS:HE2	1:A:233:LYS:HB3	1.94	0.40
1:A:861:LYS:HE3	1:A:869:TRP:CD1	2.56	0.40
1:C:447:LEU:O	1:C:455:ARG:HG2	2.22	0.40
1:D:185:HIS:CD2	1:D:187:SER:H	2.32	0.40
1:D:381:ALA:O	1:D:385:VAL:HG23	2.21	0.40
1:A:173:ASN:OD1	1:A:173:ASN:C	2.64	0.40
1:A:485:LEU:HD12	1:A:485:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:801:LEU:C	1:C:842:TRP:HD1	2.29	0.40
1:C:821:ILE:HG12	1:C:828:VAL:HG21	2.04	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	831/890 (93%)	758 (91%)	56 (7%)	17 (2%)	6	28
1	B	795/890 (89%)	736 (93%)	49 (6%)	10 (1%)	9	38
1	C	816/890 (92%)	739 (91%)	63 (8%)	14 (2%)	7	32
1	D	831/890 (93%)	766 (92%)	50 (6%)	15 (2%)	6	31
All	All	3273/3560 (92%)	2999 (92%)	218 (7%)	56 (2%)	7	32

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	SER
1	A	60	GLU
1	A	122	GLU
1	A	535	HIS
1	A	578	ASP
1	A	598	GLN
1	B	580	ASP
1	C	7	PRO
1	C	372	ASP
1	C	598	GLN
1	D	23	GLN
1	D	24	SER

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Mol	Chain	Res	Type
1	D	60	GLU
1	D	122	GLU
1	D	535	HIS
1	A	41	ASN
1	A	158	ASP
1	A	160	ALA
1	A	656	GLY
1	B	123	LEU
1	B	294	VAL
1	B	575	MET
1	B	598	GLN
1	B	656	GLY
1	C	171	PRO
1	C	656	GLY
1	D	160	ALA
1	D	162	ILE
1	D	598	GLN
1	D	656	GLY
1	A	140	GLU
1	A	761	PRO
1	B	41	ASN
1	B	61	ASP
1	B	171	PRO
1	C	41	ASN
1	C	61	ASP
1	C	123	LEU
1	C	169	ASP
1	D	158	ASP
1	D	165	SER
1	A	56	LYS
1	A	162	ILE
1	C	166	ASP
1	C	512	CYS
1	D	56	LYS
1	D	140	GLU
1	D	761	PRO
1	A	39	GLN
1	A	139	SER
1	D	139	SER
1	B	512	CYS
1	C	294	VAL
1	C	167	VAL

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Mol	Chain	Res	Type
1	C	6	LYS

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	712/802 (89%)	659 (93%)	53 (7%)	13	42
1	B	696/802 (87%)	645 (93%)	51 (7%)	13	42
1	C	697/802 (87%)	651 (93%)	46 (7%)	15	46
1	D	712/802 (89%)	649 (91%)	63 (9%)	9	35
All	All	2817/3208 (88%)	2604 (92%)	213 (8%)	12	41

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	50	LEU
1	A	53	VAL
1	A	66	SER
1	A	72	LEU
1	A	79	HIS
1	A	99	ILE
1	A	107	ARG
1	A	113	LEU
1	A	129	LEU
1	A	141	ASP
1	A	149	PHE
1	A	161	GLU
1	A	163	LEU
1	A	170	ARG
1	A	175	MET
1	A	176	ILE
1	A	191	ARG
1	A	213	ILE
1	A	226	ASP

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Mol	Chain	Res	Type
1	A	227	GLU
1	A	271	ASN
1	A	288	ILE
1	A	318	LEU
1	A	415	GLU
1	A	430	GLN
1	A	447	LEU
1	A	485	LEU
1	A	535	HIS
1	A	552	VAL
1	A	579	GLU
1	A	597	LEU
1	A	606	GLU
1	A	610	GLN
1	A	614	ASN
1	A	615	LEU
1	A	671	LEU
1	A	706	ILE
1	A	737	ILE
1	A	739	MET
1	A	741	ILE
1	A	747	ILE
1	A	781	VAL
1	A	790	LEU
1	A	807	ASN
1	A	826	SER
1	A	828	VAL
1	A	830	GLN
1	A	833	ILE
1	A	871	ARG
1	A	873	SER
1	A	880	LEU
1	A	887	PHE
1	B	71	ILE
1	B	99	ILE
1	B	109	THR
1	B	117	ILE
1	B	129	LEU
1	B	144	THR
1	B	146	GLU
1	B	149	PHE
1	B	174	ILE

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Mol	Chain	Res	Type
1	B	204	SER
1	B	206	THR
1	B	213	ILE
1	B	278	GLU
1	B	281	LEU
1	B	398	ILE
1	B	415	GLU
1	B	447	LEU
1	B	476	THR
1	B	485	LEU
1	B	494	LYS
1	B	498	GLU
1	B	519	LEU
1	B	552	VAL
1	B	563	GLN
1	B	570	ILE
1	B	571	GLN
1	B	582	ASP
1	B	590	LEU
1	B	615	LEU
1	B	632	GLN
1	B	712	ILE
1	B	715	THR
1	B	726	ASN
1	B	741	ILE
1	B	756	GLU
1	B	766	THR
1	B	781	VAL
1	B	785	GLU
1	B	791	GLN
1	B	802	ARG
1	B	807	ASN
1	B	828	VAL
1	B	830	GLN
1	B	841	SER
1	B	846	LYS
1	B	856	ILE
1	B	863	GLN
1	B	867	GLU
1	B	871	ARG
1	B	878	LEU
1	B	890	VAL

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Mol	Chain	Res	Type
1	C	71	ILE
1	C	99	ILE
1	C	109	THR
1	C	117	ILE
1	C	129	LEU
1	C	144	THR
1	C	146	GLU
1	C	149	PHE
1	C	174	ILE
1	C	204	SER
1	C	206	THR
1	C	213	ILE
1	C	278	GLU
1	C	281	LEU
1	C	371	SER
1	C	398	ILE
1	C	415	GLU
1	C	476	THR
1	C	485	LEU
1	C	494	LYS
1	C	498	GLU
1	C	519	LEU
1	C	552	VAL
1	C	577	LYS
1	C	612	CYS
1	C	615	LEU
1	C	632	GLN
1	C	641	MET
1	C	712	ILE
1	C	715	THR
1	C	726	ASN
1	C	741	ILE
1	C	756	GLU
1	C	766	THR
1	C	781	VAL
1	C	785	GLU
1	C	791	GLN
1	C	802	ARG
1	C	807	ASN
1	C	828	VAL
1	C	830	GLN
1	C	841	SER

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Mol	Chain	Res	Type
1	C	846	LYS
1	C	856	ILE
1	C	871	ARG
1	C	890	VAL
1	D	50	LEU
1	D	53	VAL
1	D	66	SER
1	D	72	LEU
1	D	79	HIS
1	D	99	ILE
1	D	107	ARG
1	D	113	LEU
1	D	129	LEU
1	D	141	ASP
1	D	149	PHE
1	D	161	GLU
1	D	170	ARG
1	D	175	MET
1	D	176	ILE
1	D	191	ARG
1	D	213	ILE
1	D	226	ASP
1	D	227	GLU
1	D	271	ASN
1	D	278	GLU
1	D	281	LEU
1	D	288	ILE
1	D	318	LEU
1	D	369	THR
1	D	415	GLU
1	D	430	GLN
1	D	447	LEU
1	D	485	LEU
1	D	531	SER
1	D	535	HIS
1	D	536	LYS
1	D	552	VAL
1	D	558	LYS
1	D	560	GLU
1	D	570	ILE
1	D	581	LYS
1	D	582	ASP

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Mol	Chain	Res	Type
1	D	587	LEU
1	D	590	LEU
1	D	606	GLU
1	D	610	GLN
1	D	614	ASN
1	D	615	LEU
1	D	643	VAL
1	D	671	LEU
1	D	706	ILE
1	D	737	ILE
1	D	739	MET
1	D	741	ILE
1	D	747	ILE
1	D	781	VAL
1	D	790	LEU
1	D	807	ASN
1	D	826	SER
1	D	828	VAL
1	D	830	GLN
1	D	833	ILE
1	D	871	ARG
1	D	873	SER
1	D	880	LEU
1	D	884	LEU
1	D	887	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	173	ASN
1	A	185	HIS
1	A	212	HIS
1	A	253	HIS
1	A	271	ASN
1	A	554	HIS
1	A	617	GLN
1	A	626	ASN
1	A	677	GLN
1	A	685	GLN
1	A	792	GLN
1	A	807	ASN

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Mol	Chain	Res	Type
1	A	824	ASN
1	B	47	ASN
1	B	48	ASN
1	B	234	ASN
1	B	397	HIS
1	B	442	HIS
1	B	535	HIS
1	B	537	ASN
1	B	617	GLN
1	B	626	ASN
1	B	629	GLN
1	B	677	GLN
1	B	726	ASN
1	B	762	ASN
1	B	824	ASN
1	B	830	GLN
1	C	47	ASN
1	C	48	ASN
1	C	234	ASN
1	C	442	HIS
1	C	535	HIS
1	C	537	ASN
1	C	617	GLN
1	C	626	ASN
1	C	629	GLN
1	C	677	GLN
1	C	726	ASN
1	C	762	ASN
1	C	824	ASN
1	C	830	GLN
1	C	863	GLN
1	D	173	ASN
1	D	185	HIS
1	D	200	GLN
1	D	212	HIS
1	D	253	HIS
1	D	617	GLN
1	D	626	ASN
1	D	677	GLN
1	D	685	GLN
1	D	792	GLN
1	D	807	ASN

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Mol	Chain	Res	Type
1	D	824	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 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	835/890 (93%)	0.40	57 (6%) 23 12	41, 67, 117, 128	0
1	B	801/890 (90%)	0.44	47 (5%) 28 14	37, 69, 122, 161	0
1	C	824/890 (92%)	0.60	66 (8%) 18 9	44, 76, 149, 163	0
1	D	835/890 (93%)	0.38	63 (7%) 20 10	41, 64, 101, 116	0
All	All	3295/3560 (92%)	0.45	233 (7%) 22 11	37, 69, 121, 163	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	LEU	6.6
1	A	28	THR	6.3
1	C	370	ILE	6.3
1	D	7	PRO	6.0
1	D	46	PHE	5.2
1	A	46	PHE	5.2
1	D	159	SER	5.1
1	A	162	ILE	4.8
1	D	162	ILE	4.8
1	C	7	PRO	4.7
1	D	22	SER	4.5
1	A	163	LEU	4.5
1	C	294	VAL	4.4
1	C	46	PHE	4.3
1	C	37	LEU	4.3
1	A	22	SER	4.3
1	D	49	TYR	4.2
1	A	160	ALA	4.2
1	C	41	ASN	4.1
1	B	51	ILE	4.1
1	B	46	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	21	GLU	4.1
1	B	42	GLN	4.1
1	A	7	PRO	4.0
1	C	50	LEU	4.0
1	C	42	GLN	4.0
1	C	59	SER	4.0
1	B	59	SER	3.9
1	C	371	SER	3.9
1	D	40	LEU	3.9
1	B	319	LYS	3.8
1	C	44	PRO	3.8
1	C	87	VAL	3.8
1	B	294	VAL	3.8
1	C	167	VAL	3.8
1	A	8	ASP	3.8
1	A	159	SER	3.7
1	D	28	THR	3.7
1	A	9	GLU	3.7
1	C	8	ASP	3.7
1	A	49	TYR	3.6
1	D	21	GLU	3.6
1	A	123	LEU	3.6
1	C	164	ASP	3.6
1	A	40	LEU	3.6
1	A	865	GLY	3.5
1	C	168	LEU	3.5
1	D	41	ASN	3.5
1	D	160	ALA	3.4
1	C	51	ILE	3.4
1	B	123	LEU	3.4
1	C	85	ASN	3.4
1	D	30	GLN	3.4
1	D	58	LYS	3.3
1	D	319	LYS	3.3
1	D	32	THR	3.3
1	D	50	LEU	3.3
1	C	54	LEU	3.2
1	A	860	PHE	3.2
1	C	49	TYR	3.2
1	D	123	LEU	3.2
1	D	26	ASP	3.2
1	D	23	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	25	PRO	3.2
1	B	867	GLU	3.1
1	B	890	VAL	3.1
1	A	12	LEU	3.1
1	D	47	ASN	3.1
1	B	168	LEU	3.1
1	D	161	GLU	3.1
1	C	47	ASN	3.1
1	B	119	SER	3.1
1	A	55	THR	3.0
1	A	140	GLU	3.0
1	B	44	PRO	3.0
1	B	37	LEU	2.9
1	D	140	GLU	2.9
1	D	8	ASP	2.9
1	D	166	ASP	2.9
1	A	47	ASN	2.9
1	C	720	GLU	2.9
1	D	48	ASN	2.9
1	A	50	LEU	2.9
1	A	43	TYR	2.9
1	B	73	LYS	2.8
1	B	91	ILE	2.8
1	C	57	LEU	2.8
1	A	24	SER	2.8
1	B	31	ARG	2.8
1	A	880	LEU	2.8
1	C	15	ILE	2.8
1	C	393	GLU	2.8
1	A	44	PRO	2.8
1	B	71	ILE	2.8
1	D	863	GLN	2.8
1	B	57	LEU	2.8
1	C	123	LEU	2.8
1	A	52	PHE	2.7
1	A	370	ILE	2.7
1	C	165	SER	2.7
1	C	867	GLU	2.7
1	C	14	GLN	2.7
1	D	27	THR	2.7
1	A	403	LYS	2.7
1	B	41	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	640	PHE	2.7
1	B	52	PHE	2.7
1	B	805	ARG	2.7
1	A	227	GLU	2.7
1	C	319	LYS	2.6
1	D	438	GLU	2.6
1	A	14	GLN	2.6
1	C	268	GLN	2.6
1	D	52	PHE	2.6
1	D	85	ASN	2.6
1	B	87	VAL	2.6
1	D	43	TYR	2.6
1	A	875	GLN	2.6
1	B	862	ASN	2.6
1	C	10	GLN	2.6
1	B	49	TYR	2.6
1	B	90	PHE	2.6
1	C	56	LYS	2.6
1	D	15	ILE	2.6
1	B	54	LEU	2.6
1	C	809	GLU	2.6
1	D	25	PRO	2.5
1	D	535	HIS	2.5
1	A	156	CYS	2.5
1	A	23	GLN	2.5
1	D	628	ALA	2.5
1	D	24	SER	2.5
1	D	39	GLN	2.5
1	C	890	VAL	2.5
1	A	17	GLN	2.5
1	D	313	ILE	2.5
1	C	878	LEU	2.5
1	C	255	HIS	2.5
1	D	14	GLN	2.5
1	A	867	GLU	2.4
1	C	63	PRO	2.4
1	B	38	GLU	2.4
1	B	116	THR	2.4
1	D	869	TRP	2.4
1	A	51	ILE	2.4
1	D	629	GLN	2.4
1	C	317	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	877	PRO	2.4
1	C	848	ASP	2.4
1	D	45	ASP	2.4
1	A	29	ILE	2.4
1	D	224	ALA	2.4
1	D	867	GLU	2.4
1	A	59	SER	2.4
1	C	52	PHE	2.4
1	A	54	LEU	2.4
1	C	40	LEU	2.4
1	D	57	LEU	2.4
1	C	43	TYR	2.3
1	C	847	ASP	2.3
1	B	744	GLN	2.3
1	D	163	LEU	2.3
1	B	84	PRO	2.3
1	C	84	PRO	2.3
1	C	846	LYS	2.3
1	C	38	GLU	2.3
1	A	19	LEU	2.3
1	D	631	ASP	2.3
1	C	34	GLN	2.3
1	D	9	GLU	2.3
1	B	167	VAL	2.3
1	D	44	PRO	2.3
1	D	59	SER	2.3
1	B	582	ASP	2.3
1	D	164	ASP	2.3
1	D	268	GLN	2.3
1	A	167	VAL	2.3
1	C	228	GLU	2.3
1	C	535	HIS	2.3
1	A	39	GLN	2.3
1	B	268	GLN	2.3
1	D	633	TYR	2.2
1	C	48	ASN	2.2
1	B	579	GLU	2.2
1	A	37	LEU	2.2
1	B	535	HIS	2.2
1	B	47	ASN	2.2
1	C	169	ASP	2.2
1	C	31	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	VAL	2.2
1	B	30	GLN	2.2
1	D	42	GLN	2.2
1	A	58	LYS	2.2
1	C	36	LYS	2.2
1	A	269	ASP	2.2
1	D	312	ASP	2.2
1	A	27	THR	2.1
1	C	32	THR	2.1
1	C	633	TYR	2.1
1	C	17	GLN	2.1
1	C	6	LYS	2.1
1	B	580	ASP	2.1
1	D	158	ASP	2.1
1	C	299	LYS	2.1
1	D	35	GLN	2.1
1	A	438	GLU	2.1
1	D	317	LEU	2.1
1	B	35	GLN	2.1
1	A	161	GLU	2.1
1	D	227	GLU	2.1
1	B	864	VAL	2.1
1	B	833	ILE	2.1
1	C	30	GLN	2.1
1	D	33	VAL	2.1
1	A	45	ASP	2.1
1	A	166	ASP	2.1
1	A	708	ASP	2.1
1	A	32	THR	2.1
1	B	43	TYR	2.1
1	A	30	GLN	2.1
1	D	17	GLN	2.1
1	C	9	GLU	2.1
1	A	537	ASN	2.0
1	B	611	ARG	2.0
1	A	158	ASP	2.0
1	B	169	ASP	2.0
1	C	227	GLU	2.0
1	B	40	LEU	2.0
1	A	75	ASN	2.0
1	C	98	ASN	2.0
1	B	842	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	369	THR	2.0
1	D	51	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.