



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:13 PM UTC

PDB ID : 3MI6 / pdb_00003mi6
Title : Crystal structure of the alpha-galactosidase from Lactobacillus brevis, Northeast Structural Genomics Consortium Target LbR11.
Authors : Vorobiev, S.; Chen, Y.; Seetharaman, J.; Belote, R.; Sahdev, S.; Xiao, R.; Acton, T.B.; Everett, J.K.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-04-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

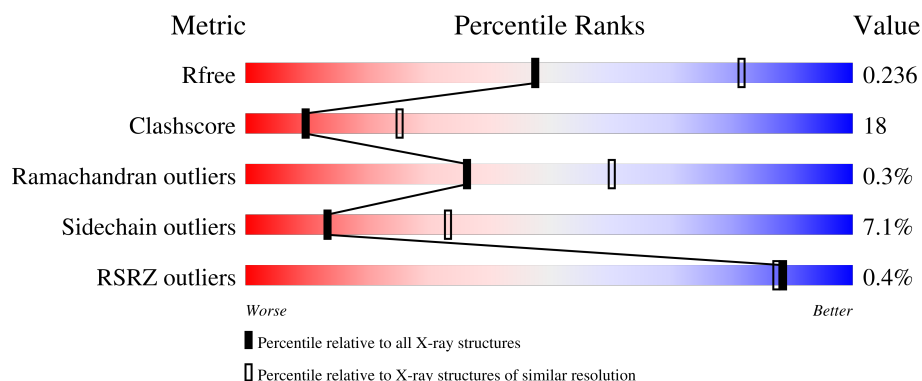
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	745	 63% 32% .
1	B	745	 70% 25% . .
1	C	745	 63% 32% . .
1	D	745	 70% 25% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24417 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 Alpha-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	Se	0	0	0
			6007	3822	1022	1137	2	24			
1	B	736	Total	C	N	O	S	Se	0	0	0
			5947	3786	1008	1127	2	24			
1	C	737	Total	C	N	O	S	Se	0	0	0
			5946	3782	1008	1130	2	24			
1	D	743	Total	C	N	O	S	Se	0	0	0
			6018	3829	1027	1136	2	24			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	738	LEU	-	expression tag	UNP Q03PP7
A	739	GLU	-	expression tag	UNP Q03PP7
A	740	HIS	-	expression tag	UNP Q03PP7
A	741	HIS	-	expression tag	UNP Q03PP7
A	742	HIS	-	expression tag	UNP Q03PP7
A	743	HIS	-	expression tag	UNP Q03PP7
A	744	HIS	-	expression tag	UNP Q03PP7
A	745	HIS	-	expression tag	UNP Q03PP7
B	738	LEU	-	expression tag	UNP Q03PP7
B	739	GLU	-	expression tag	UNP Q03PP7
B	740	HIS	-	expression tag	UNP Q03PP7
B	741	HIS	-	expression tag	UNP Q03PP7
B	742	HIS	-	expression tag	UNP Q03PP7
B	743	HIS	-	expression tag	UNP Q03PP7
B	744	HIS	-	expression tag	UNP Q03PP7
B	745	HIS	-	expression tag	UNP Q03PP7
C	738	LEU	-	expression tag	UNP Q03PP7
C	739	GLU	-	expression tag	UNP Q03PP7
C	740	HIS	-	expression tag	UNP Q03PP7
C	741	HIS	-	expression tag	UNP Q03PP7
C	742	HIS	-	expression tag	UNP Q03PP7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	743	HIS	-	expression tag	UNP Q03PP7
C	744	HIS	-	expression tag	UNP Q03PP7
C	745	HIS	-	expression tag	UNP Q03PP7
D	738	LEU	-	expression tag	UNP Q03PP7
D	739	GLU	-	expression tag	UNP Q03PP7
D	740	HIS	-	expression tag	UNP Q03PP7
D	741	HIS	-	expression tag	UNP Q03PP7
D	742	HIS	-	expression tag	UNP Q03PP7
D	743	HIS	-	expression tag	UNP Q03PP7
D	744	HIS	-	expression tag	UNP Q03PP7
D	745	HIS	-	expression tag	UNP Q03PP7

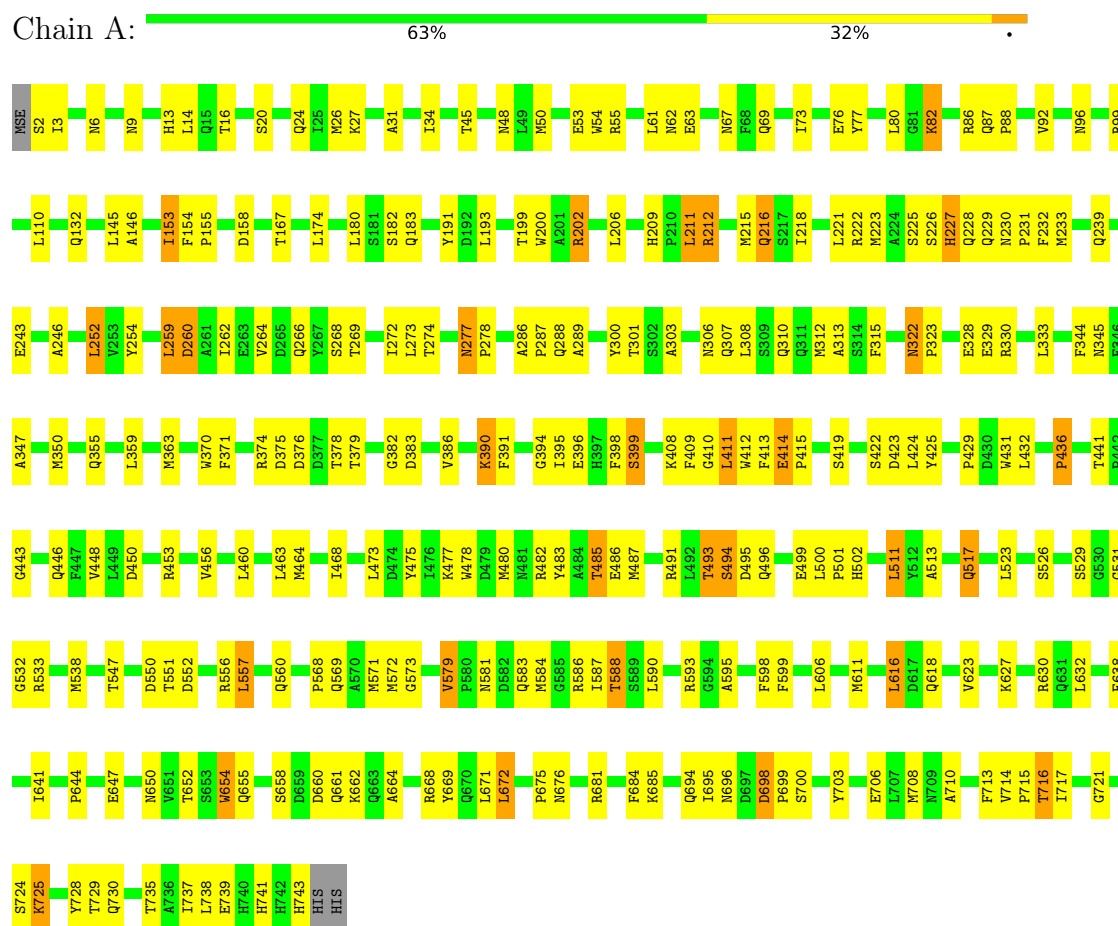
- Molecule 2 is water.

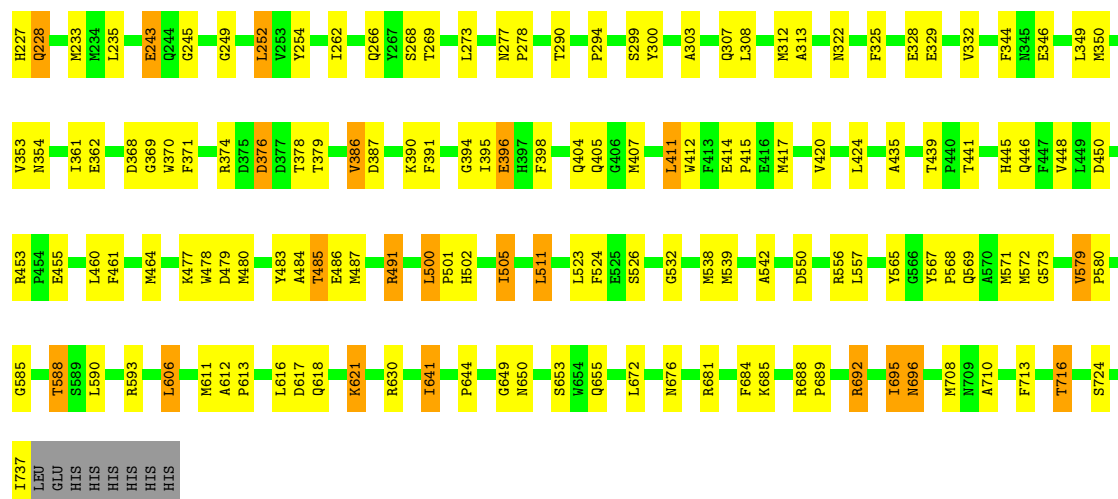
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	117	Total 117	O 117	0	0
2	B	179	Total 179	O 179	0	0
2	C	84	Total 84	O 84	0	0
2	D	119	Total 119	O 119	0	0

3 Residue-property plots

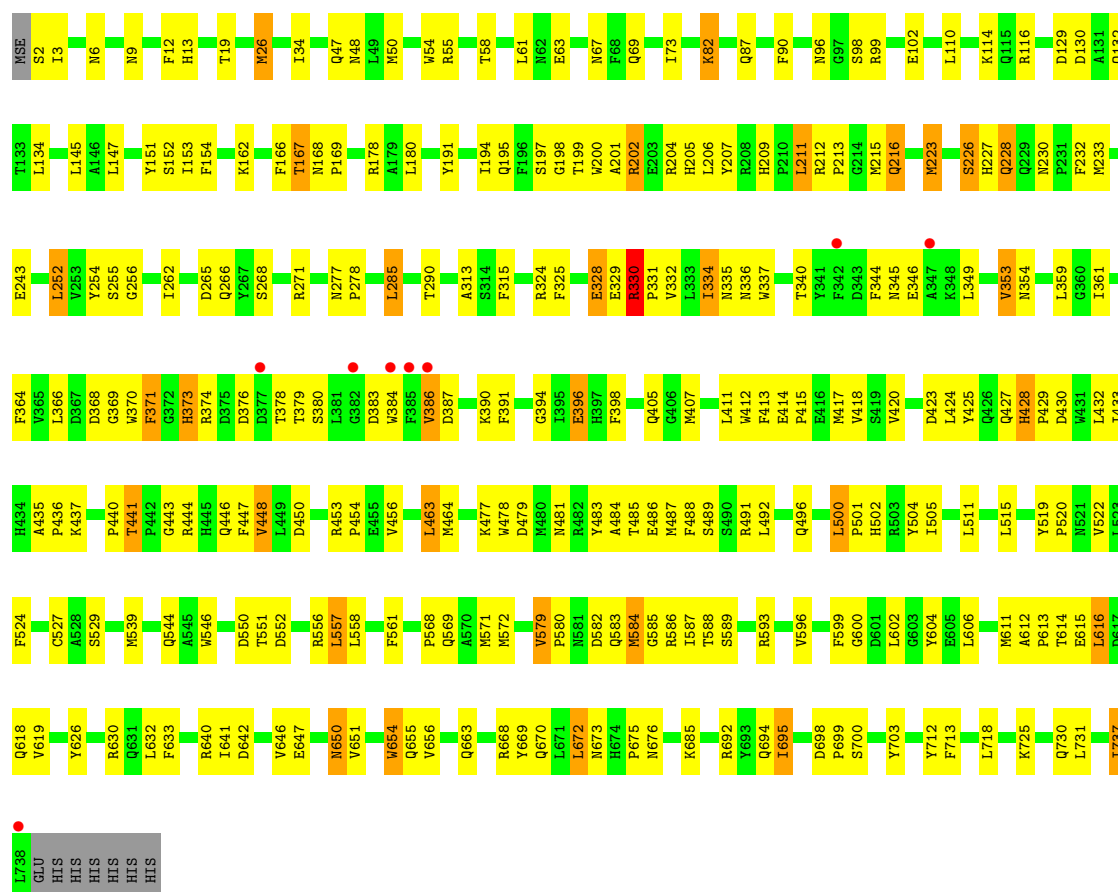
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: Alpha-galactosidase



• Molecule 1: Alpha-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.94Å 158.82Å 166.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.03 – 2.70 40.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.03-2.70) 99.6 (40.03-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.11 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2), CNS	Depositor
R, R_{free}	0.173 , 0.241 0.173 , 0.236	Depositor DCC
R_{free} test set	4195 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24417	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.57	1/6150 (0.0%)	0.91	18/8319 (0.2%)
1	B	0.60	0/6086	0.93	10/8232 (0.1%)
1	C	0.55	0/6083	0.91	19/8227 (0.2%)
1	D	0.58	1/6163 (0.0%)	0.92	18/8336 (0.2%)
All	All	0.58	2/24482 (0.0%)	0.92	65/33114 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ASP	C-N	-7.25	1.22	1.33
1	D	696	ASN	C-O	-5.33	1.18	1.24

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	695	ILE	N-CA-C	9.92	124.26	106.61
1	B	695	ILE	CB-CA-C	-9.32	100.75	111.09
1	C	695	ILE	N-CA-C	8.74	120.30	107.37
1	A	695	ILE	CB-CA-C	-8.57	100.54	110.73
1	D	225	SER	N-CA-C	-8.57	97.81	110.23
1	D	695	ILE	CB-CA-C	-8.27	100.89	110.73
1	C	695	ILE	CB-CA-C	-8.23	99.75	111.19
1	D	414	GLU	CA-C-N	8.07	127.64	119.24
1	D	414	GLU	C-N-CA	8.07	127.64	119.24
1	C	226	SER	N-CA-C	8.06	122.36	109.79
1	B	225	SER	N-CA-C	-7.88	99.14	110.24
1	C	647	GLU	CB-CA-C	-7.33	106.22	115.89
1	D	321	VAL	CB-CA-C	7.26	121.30	111.28
1	D	245	GLY	N-CA-C	6.94	120.07	112.29
1	A	647	GLU	CB-CA-C	-6.83	106.78	116.34
1	A	227	HIS	N-CA-C	-6.75	103.99	111.82
1	A	698	ASP	CA-C-N	6.64	126.42	119.05
1	A	698	ASP	C-N-CA	6.64	126.42	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	GLU	CA-C-N	6.51	126.74	119.32
1	A	414	GLU	C-N-CA	6.51	126.74	119.32
1	A	696	ASN	CB-CA-C	-6.47	107.28	116.34
1	B	435	ALA	CA-C-N	6.47	127.93	119.84
1	B	435	ALA	C-N-CA	6.47	127.93	119.84
1	B	322	ASN	CA-C-N	6.43	126.06	119.56
1	B	322	ASN	C-N-CA	6.43	126.06	119.56
1	C	646	VAL	N-CA-C	6.25	116.86	108.11
1	C	435	ALA	CA-C-N	6.15	127.52	119.84
1	C	435	ALA	C-N-CA	6.15	127.52	119.84
1	D	698	ASP	CA-C-N	6.14	125.84	119.64
1	D	698	ASP	C-N-CA	6.14	125.84	119.64
1	B	245	GLY	N-CA-C	6.07	119.67	111.72
1	A	322	ASN	CA-C-N	6.07	125.95	119.28
1	A	322	ASN	C-N-CA	6.07	125.95	119.28
1	C	330	ARG	CA-C-N	5.86	125.88	119.90
1	C	330	ARG	C-N-CA	5.86	125.88	119.90
1	A	375	ASP	N-CA-C	-5.85	105.90	114.39
1	A	573	GLY	N-CA-C	-5.85	104.59	112.14
1	D	654	TRP	N-CA-C	5.83	116.78	108.74
1	A	259	LEU	O-C-N	-5.73	116.61	123.31
1	B	226	SER	N-CA-C	5.67	118.18	110.35
1	A	259	LEU	CA-C-N	5.63	131.11	123.11
1	A	259	LEU	C-N-CA	5.63	131.11	123.11
1	D	646	VAL	N-CA-C	-5.61	100.20	108.85
1	C	646	VAL	CB-CA-C	-5.59	102.35	110.63
1	A	695	ILE	N-CA-C	5.58	116.62	107.24
1	D	186	LEU	CA-C-N	5.57	125.27	119.64
1	D	186	LEU	C-N-CA	5.57	125.27	119.64
1	D	487	MSE	N-CA-C	5.54	117.74	109.59
1	C	481	ASN	N-CA-C	5.52	119.55	112.26
1	C	204	ARG	N-CA-C	5.35	118.81	111.54
1	C	371	PHE	N-CA-C	5.34	118.13	109.06
1	B	696	ASN	N-CA-C	-5.25	99.61	110.80
1	D	322	ASN	CA-C-N	5.25	124.91	119.56
1	D	322	ASN	C-N-CA	5.25	124.91	119.56
1	D	481	ASN	N-CA-C	5.24	119.64	112.88
1	C	391	PHE	CA-C-N	5.24	124.42	118.97
1	C	391	PHE	C-N-CA	5.24	124.42	118.97
1	D	375	ASP	N-CA-C	-5.16	107.01	113.72
1	C	26	MSE	N-CA-C	5.11	117.04	109.69
1	A	277	ASN	CA-C-N	5.10	125.39	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASN	C-N-CA	5.10	125.39	119.47
1	C	371	PHE	CB-CA-C	-5.07	99.09	109.38
1	C	58	THR	CA-C-N	5.06	124.99	119.78
1	C	58	THR	C-N-CA	5.06	124.99	119.78
1	D	386	VAL	N-CA-C	5.04	116.89	109.63

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	6007	0	5701	235	0
1	B	5947	0	5654	197	0
1	C	5946	0	5650	239	0
1	D	6018	0	5706	193	0
2	A	117	0	0	9	0
2	B	179	0	0	13	0
2	C	84	0	0	4	0
2	D	119	0	0	10	0
All	All	24417	0	22711	817	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (817) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:MSE:HE1	1:A:262:ILE:HD11	1.27	1.11
1:B:299:SER:HB3	1:B:312:MSE:HE2	1.10	1.05
1:C:584:MSE:HE1	1:C:586:ARG:HB2	1.41	1.00
1:D:226:SER:HB2	1:D:228:GLN:NE2	1.80	0.97
1:C:167:THR:HG23	1:C:290:THR:HG22	1.47	0.96
1:A:513:ALA:O	1:A:517:GLN:HG2	1.64	0.96
1:D:223:MSE:HE3	1:D:487:MSE:SE	2.16	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:MSE:HE1	1:D:262:ILE:HD11	1.49	0.94
1:A:87:GLN:HG3	1:A:215:MSE:HE1	1.46	0.94
1:A:48:ASN:HD21	1:B:713:PHE:H	0.96	0.94
1:A:650:ASN:HD21	1:A:672:LEU:H	1.11	0.93
1:B:299:SER:CB	1:B:312:MSE:HE2	2.00	0.92
1:B:87:GLN:HG3	1:B:215:MSE:HE1	1.49	0.91
1:A:441:THR:HB	1:A:485:THR:HG21	1.54	0.90
1:A:371:PHE:CZ	1:A:374:ARG:HD3	2.08	0.89
1:C:226:SER:HB2	1:C:228:GLN:NE2	1.87	0.89
1:B:411:LEU:HD13	2:B:1017:HOH:O	1.73	0.88
1:B:485:THR:HG23	1:B:486:GLU:OE1	1.73	0.88
1:D:87:GLN:HG3	1:D:215:MSE:HE1	1.56	0.88
1:C:313:ALA:HB1	1:C:568:PRO:HG3	1.57	0.87
1:A:493:THR:HG22	1:A:495:ASP:H	1.40	0.86
1:B:329:GLU:HB3	1:B:630:ARG:HD3	1.55	0.86
1:D:230:ASN:HD22	1:D:232:PHE:H	1.21	0.86
1:C:212:ARG:H	1:C:216:GLN:HE22	1.16	0.86
1:B:550:ASP:O	1:B:556:ARG:HD3	1.76	0.86
1:D:153:ILE:HG22	1:D:155:PRO:HD3	1.57	0.86
1:B:233:MSE:HE1	1:B:262:ILE:HD11	1.55	0.84
1:D:48:ASN:HB3	2:D:1173:HOH:O	1.77	0.84
1:C:369:GLY:HA2	1:C:374:ARG:HB2	1.57	0.84
1:D:513:ALA:O	1:D:517:GLN:HG3	1.79	0.83
1:A:226:SER:HB2	1:A:229:GLN:H	1.41	0.83
1:D:226:SER:HB2	1:D:228:GLN:HE21	1.38	0.83
1:B:411:LEU:HD12	1:B:412:TRP:N	1.93	0.83
1:C:233:MSE:HE1	1:C:262:ILE:HD11	1.59	0.82
1:A:386:VAL:HG11	1:A:394:GLY:HA2	1.59	0.82
1:B:441:THR:HB	1:B:485:THR:HG21	1.62	0.82
1:C:386:VAL:HG11	1:C:394:GLY:HA2	1.61	0.81
1:D:569:GLN:HA	1:D:572:MSE:HE3	1.60	0.81
1:A:713:PHE:H	1:B:48:ASN:HD21	1.28	0.80
1:A:80:LEU:HB2	1:A:88:PRO:HG3	1.64	0.80
1:D:502:HIS:HE1	2:D:1432:HOH:O	1.64	0.80
1:A:223:MSE:HE3	1:A:487:MSE:SE	2.32	0.79
1:A:531:GLY:HA2	2:A:1331:HOH:O	1.81	0.79
1:C:313:ALA:CB	1:C:568:PRO:HG3	2.13	0.79
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.48	0.79
1:C:353:VAL:HG13	1:C:407:MSE:HE1	1.63	0.79
1:A:48:ASN:ND2	1:B:713:PHE:H	1.80	0.79
1:A:681:ARG:HD3	1:A:710:ALA:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:SER:HB2	1:B:538:MSE:HE3	1.64	0.78
1:D:55:ARG:H	1:D:69:GLN:HE22	1.31	0.78
1:A:233:MSE:HE1	1:A:262:ILE:CD1	2.10	0.78
1:A:308:LEU:HG	1:A:312:MSE:HE2	1.64	0.78
1:D:484:ALA:HB3	1:D:487:MSE:HE2	1.67	0.77
1:A:412:TRP:HD1	1:A:477:LYS:HD3	1.47	0.77
1:D:655:GLN:HE22	1:D:685:LYS:H	1.32	0.77
1:A:694:GLN:HG3	1:A:737:ILE:HD11	1.65	0.77
1:C:345:ASN:HA	1:C:390:LYS:HB3	1.67	0.77
1:B:212:ARG:H	1:B:216:GLN:HE22	1.33	0.77
1:B:226:SER:HB2	1:B:228:GLN:HE21	1.50	0.75
1:D:233:MSE:CE	1:D:262:ILE:HD11	2.16	0.75
1:B:216:GLN:HB2	1:C:212:ARG:HH21	1.52	0.75
1:C:579:VAL:HG21	1:C:588:THR:H	1.50	0.75
1:D:599:PHE:CD1	1:D:654:TRP:CZ3	2.76	0.74
1:A:415:PRO:HB3	1:A:464:MSE:HE1	1.70	0.74
1:C:550:ASP:O	1:C:556:ARG:HD3	1.87	0.74
1:D:26:MSE:HE1	1:D:73:ILE:HG21	1.69	0.74
1:A:243:GLU:OE1	1:A:685:LYS:HE3	1.88	0.74
1:B:655:GLN:HE22	1:B:685:LYS:H	1.33	0.74
1:D:14:LEU:HB3	1:D:153:ILE:HD11	1.67	0.74
1:D:330:ARG:HD3	1:D:544:GLN:OE1	1.88	0.74
1:D:371:PHE:CZ	1:D:374:ARG:HG3	2.23	0.74
1:C:223:MSE:HE1	1:C:500:LEU:HD13	1.69	0.73
1:C:243:GLU:CD	1:C:685:LYS:HE3	2.12	0.73
1:C:3:ILE:H	1:C:132:GLN:HE22	1.35	0.73
1:B:538:MSE:HE2	2:B:908:HOH:O	1.87	0.73
1:C:484:ALA:HB3	1:C:487:MSE:HE2	1.68	0.73
1:A:493:THR:HG22	1:A:495:ASP:N	2.04	0.73
1:A:48:ASN:HD21	1:B:713:PHE:N	1.80	0.72
1:B:226:SER:HB2	1:B:228:GLN:NE2	2.04	0.72
1:D:3:ILE:N	2:D:944:HOH:O	2.21	0.72
1:B:254:TYR:OH	1:B:502:HIS:HD2	1.72	0.72
1:C:55:ARG:H	1:C:69:GLN:HE22	1.35	0.72
1:D:313:ALA:HB1	1:D:568:PRO:HG3	1.72	0.72
1:B:82:LYS:HD2	1:B:102:GLU:HG2	1.71	0.72
1:C:82:LYS:HD2	1:C:102:GLU:HG2	1.71	0.72
1:C:412:TRP:CZ2	1:C:414:GLU:HG3	2.24	0.72
1:B:6:ASN:ND2	1:B:9:ASN:HD22	1.87	0.72
1:A:226:SER:HB3	1:A:228:GLN:H	1.55	0.71
1:D:581:ASN:HD21	1:D:583:GLN:NE2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:MSE:HE1	1:D:262:ILE:CD1	2.18	0.71
1:C:6:ASN:HD21	1:C:9:ASN:HD22	1.40	0.70
1:C:243:GLU:OE1	1:C:685:LYS:HE3	1.91	0.70
1:A:233:MSE:CE	1:A:262:ILE:HD11	2.13	0.70
1:A:654:TRP:CH2	1:A:669:TYR:OH	2.44	0.70
1:B:74:LYS:HE2	2:B:1377:HOH:O	1.91	0.70
1:B:87:GLN:CG	1:B:215:MSE:HE1	2.21	0.70
1:A:3:ILE:H	1:A:132:GLN:HE22	1.39	0.69
1:C:334:ILE:HG13	1:C:335:ASN:H	1.55	0.69
1:A:425:TYR:O	1:A:429:PRO:HG3	1.92	0.69
1:A:569:GLN:HA	1:A:572:MSE:HE3	1.75	0.69
1:D:599:PHE:CE1	1:D:654:TRP:HZ3	2.10	0.69
1:D:465:SER:HB2	1:D:519:TYR:OH	1.92	0.69
1:C:6:ASN:ND2	1:C:9:ASN:HD22	1.91	0.69
1:C:396:GLU:CD	1:C:396:GLU:H	2.01	0.69
1:B:650:ASN:HD21	1:B:672:LEU:H	1.40	0.68
1:D:235:LEU:HD21	1:D:262:ILE:HD12	1.76	0.68
1:C:668:ARG:HD3	1:C:730:GLN:HE22	1.57	0.68
1:A:226:SER:CB	1:A:229:GLN:H	2.06	0.68
1:C:2:SER:HB2	1:C:132:GLN:HE22	1.57	0.68
1:C:611:MSE:HE2	1:C:615:GLU:HB3	1.76	0.68
1:C:485:THR:HG22	1:C:486:GLU:CD	2.19	0.68
1:A:329:GLU:HB3	1:A:630:ARG:HD3	1.76	0.68
1:A:212:ARG:H	1:A:216:GLN:HE22	1.39	0.67
1:B:362:GLU:OE1	1:B:630:ARG:NH2	2.26	0.67
1:C:332:VAL:HG23	1:C:630:ARG:HH21	1.58	0.67
1:D:262:ILE:HD13	1:D:272:ILE:HG13	1.76	0.67
1:C:48:ASN:HD21	1:D:713:PHE:H	1.41	0.67
1:C:371:PHE:CZ	1:C:374:ARG:HD2	2.29	0.67
1:D:254:TYR:OH	1:D:502:HIS:HD2	1.76	0.67
1:A:306:ASN:O	1:A:310:GLN:HG3	1.94	0.67
1:C:383:ASP:OD1	1:C:423:ASP:HB3	1.95	0.67
1:B:526:SER:HB2	1:B:538:MSE:CE	2.24	0.67
1:C:584:MSE:HE1	1:C:586:ARG:CB	2.22	0.66
1:D:313:ALA:CB	1:D:568:PRO:HG3	2.24	0.66
1:B:24:GLN:HB2	1:B:34:ILE:HD11	1.78	0.66
1:B:716:THR:HG23	2:B:1077:HOH:O	1.94	0.66
1:C:230:ASN:HD22	1:C:232:PHE:H	1.40	0.66
1:B:386:VAL:HG22	1:B:395:ILE:HG12	1.78	0.66
1:C:223:MSE:HE2	1:C:501:PRO:HA	1.76	0.66
1:A:468:ILE:HG12	1:A:473:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ILE:HD12	1:D:448:VAL:HG22	1.78	0.65
1:C:243:GLU:HG2	2:C:1365:HOH:O	1.94	0.65
1:C:223:MSE:HE1	1:C:500:LEU:CD1	2.25	0.65
1:A:212:ARG:NH2	1:A:215:MSE:O	2.29	0.65
1:A:590:LEU:HD23	1:A:618:GLN:CD	2.22	0.65
1:D:550:ASP:O	1:D:556:ARG:HD3	1.96	0.65
1:C:233:MSE:CE	1:C:262:ILE:HD11	2.27	0.65
1:C:443:GLY:O	1:C:446:GLN:HG3	1.97	0.65
1:C:550:ASP:HA	1:C:583:GLN:NE2	2.11	0.65
1:D:230:ASN:ND2	1:D:232:PHE:H	1.91	0.65
1:C:349:LEU:HD21	1:C:364:PHE:CZ	2.31	0.64
1:A:550:ASP:OD2	1:C:675:PRO:HG3	1.97	0.64
1:C:325:PHE:O	1:C:330:ARG:NH2	2.30	0.64
1:A:654:TRP:NE1	2:A:1399:HOH:O	2.28	0.64
1:A:675:PRO:HD3	1:C:584:MSE:HG2	1.80	0.64
1:C:557:LEU:HD21	1:C:669:TYR:CB	2.28	0.63
1:A:482:ARG:NH2	1:A:485:THR:HB	2.12	0.63
1:B:3:ILE:H	1:B:132:GLN:HE22	1.44	0.63
1:B:216:GLN:CB	1:C:212:ARG:HH21	2.12	0.63
1:B:371:PHE:CZ	1:B:374:ARG:HD2	2.32	0.63
1:B:353:VAL:HG13	1:B:407:MSE:CE	2.27	0.63
1:A:668:ARG:HH11	1:A:730:GLN:HE22	1.46	0.63
1:D:24:GLN:HB2	1:D:34:ILE:HD11	1.81	0.63
1:C:167:THR:O	1:C:169:PRO:HD3	1.98	0.63
1:C:226:SER:HB2	1:C:228:GLN:HE21	1.60	0.62
1:C:227:HIS:CD2	1:C:483:TYR:OH	2.52	0.62
1:C:334:ILE:HG13	1:C:335:ASN:N	2.14	0.62
1:A:399:SER:HB2	1:A:409:PHE:CD2	2.34	0.62
1:A:644:PRO:HG3	1:A:652:THR:OG1	1.99	0.62
1:C:226:SER:HB2	1:C:228:GLN:HE22	1.65	0.62
1:C:227:HIS:HD2	1:C:483:TYR:OH	1.82	0.62
1:C:655:GLN:HE22	1:C:685:LYS:H	1.47	0.62
1:C:654:TRP:CH2	1:C:669:TYR:OH	2.49	0.62
1:D:579:VAL:HG22	1:D:587:ILE:HA	1.80	0.62
1:B:99:ARG:HG3	1:B:99:ARG:NH1	2.15	0.61
1:D:26:MSE:SE	1:D:50:MSE:HE1	2.49	0.61
1:A:3:ILE:H	1:A:132:GLN:NE2	1.97	0.61
1:C:228:GLN:NE2	1:C:228:GLN:H	1.99	0.61
1:D:538:MSE:HE2	2:D:939:HOH:O	2.00	0.61
1:C:87:GLN:HG3	1:C:215:MSE:HE1	1.82	0.61
1:C:353:VAL:HG13	1:C:407:MSE:CE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:THR:O	1:C:380:SER:HB2	2.00	0.61
1:A:599:PHE:CE1	1:A:654:TRP:HZ3	2.19	0.61
1:B:6:ASN:ND2	1:B:9:ASN:H	1.99	0.61
1:B:212:ARG:HB3	1:C:209:HIS:CE1	2.36	0.61
1:C:414:GLU:OE2	1:C:417:MSE:HG3	2.01	0.61
1:D:482:ARG:NH2	1:D:485:THR:HB	2.15	0.61
1:A:547:THR:OG1	1:A:572:MSE:HB3	2.01	0.61
1:B:277:ASN:HD22	1:B:278:PRO:HD2	1.66	0.61
1:B:526:SER:CB	1:B:538:MSE:HE3	2.31	0.61
1:C:668:ARG:HD3	1:C:730:GLN:NE2	2.16	0.61
1:A:382:GLY:HA3	1:A:424:LEU:HD12	1.81	0.61
1:D:329:GLU:OE1	1:D:630:ARG:HD2	2.01	0.61
1:D:353:VAL:HG13	1:D:407:MSE:HE1	1.83	0.61
1:A:568:PRO:HD2	1:A:571:MSE:SE	2.52	0.60
1:B:167:THR:HG23	1:B:290:THR:HG22	1.82	0.60
1:B:299:SER:HB3	1:B:312:MSE:CE	2.06	0.60
1:C:612:ALA:HB1	1:C:613:PRO:HD2	1.84	0.60
1:B:684:PHE:O	1:B:708:MSE:HG2	2.00	0.60
1:A:556:ARG:O	1:A:560:GLN:HG3	2.02	0.60
1:B:2:SER:HB2	1:B:132:GLN:HE22	1.67	0.60
1:B:369:GLY:O	1:B:390:LYS:HE2	2.02	0.60
1:B:6:ASN:HD21	1:B:9:ASN:HD22	1.49	0.60
1:B:52:GLN:HE22	1:B:68:PHE:HA	1.67	0.60
1:A:226:SER:HB3	1:A:228:GLN:N	2.16	0.59
1:B:249:GLY:HA3	1:B:312:MSE:HE1	1.83	0.59
1:C:413:PHE:CD1	1:C:464:MSE:HE2	2.37	0.59
1:A:550:ASP:O	1:A:556:ARG:HD3	2.02	0.59
1:B:386:VAL:HG11	1:B:394:GLY:HA2	1.83	0.59
1:B:588:THR:HG21	1:B:593:ARG:HG2	1.82	0.59
1:A:411:LEU:HD12	1:A:412:TRP:N	2.17	0.59
1:A:599:PHE:CE1	1:A:654:TRP:CZ3	2.90	0.59
1:D:272:ILE:N	1:D:272:ILE:HD12	2.17	0.59
1:D:599:PHE:CG	1:D:654:TRP:CZ3	2.91	0.59
1:A:412:TRP:CD1	1:A:477:LYS:HD3	2.35	0.58
1:A:655:GLN:HE22	1:A:685:LYS:H	1.51	0.58
1:C:336:ASN:HB2	1:C:340:THR:OG1	2.03	0.58
1:B:266:GLN:HB2	1:C:199:THR:HB	1.84	0.58
1:D:599:PHE:CD1	1:D:654:TRP:HZ3	2.18	0.58
1:C:478:TRP:CD1	1:C:478:TRP:C	2.81	0.58
1:C:569:GLN:O	1:C:600:GLY:HA2	2.03	0.58
1:D:485:THR:HG22	2:D:1153:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:GLU:HB3	1:D:630:ARG:CD	2.32	0.58
1:B:411:LEU:HD12	1:B:411:LEU:C	2.28	0.58
1:B:487:MSE:HG3	2:B:1034:HOH:O	2.04	0.58
1:A:493:THR:CG2	1:A:494:SER:N	2.67	0.58
1:B:277:ASN:HD22	1:B:278:PRO:CD	2.17	0.58
1:B:6:ASN:HD22	1:B:9:ASN:H	1.52	0.58
1:C:212:ARG:NH1	1:C:213:PRO:O	2.37	0.57
1:A:595:ALA:HA	1:A:598:PHE:CD2	2.38	0.57
1:D:329:GLU:HB3	1:D:630:ARG:HD3	1.86	0.57
1:B:212:ARG:NH2	1:B:215:MSE:O	2.37	0.57
1:B:308:LEU:HG	1:B:312:MSE:HE3	1.87	0.57
1:C:444:ARG:O	1:C:446:GLN:HG2	2.04	0.57
1:D:235:LEU:HD21	1:D:262:ILE:CD1	2.34	0.57
1:B:368:ASP:OD1	1:B:374:ARG:HD3	2.04	0.57
1:B:695:ILE:HG22	1:B:695:ILE:O	2.05	0.57
1:C:223:MSE:SE	1:C:487:MSE:HE2	2.55	0.57
1:D:650:ASN:HD21	1:D:672:LEU:HB2	1.70	0.57
1:D:226:SER:CB	1:D:228:GLN:HE21	2.14	0.57
1:A:660:ASP:O	1:A:661:GLN:HB2	2.04	0.56
1:B:445:HIS:HD2	1:C:63:GLU:OE1	1.88	0.56
1:C:349:LEU:HD22	1:C:398:PHE:CE1	2.40	0.56
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.70	0.56
1:A:654:TRP:CZ2	2:A:1399:HOH:O	2.53	0.56
1:D:23:PHE:HA	1:D:34:ILE:HG13	1.87	0.56
1:A:478:TRP:CD1	1:A:478:TRP:C	2.83	0.56
1:A:230:ASN:ND2	1:A:232:PHE:H	2.03	0.56
1:B:191:TYR:HB2	1:B:211:LEU:HD22	1.86	0.56
1:D:6:ASN:HD22	1:D:9:ASN:H	1.53	0.56
1:D:16:THR:HG22	1:D:155:PRO:HA	1.87	0.56
1:D:462:LYS:O	1:D:466:GLN:HG3	2.06	0.56
1:A:500:LEU:HB3	1:A:501:PRO:HD3	1.88	0.56
1:B:588:THR:HG22	1:B:593:ARG:HH11	1.71	0.56
1:B:502:HIS:HE1	2:B:1015:HOH:O	1.88	0.56
1:D:485:THR:HG23	1:D:486:GLU:CD	2.31	0.56
1:A:330:ARG:HD2	1:A:330:ARG:N	2.21	0.56
1:B:539:MSE:HA	1:B:542:ALA:O	2.05	0.56
1:C:332:VAL:O	1:C:361:ILE:HG23	2.06	0.56
1:C:413:PHE:HB3	1:C:415:PRO:HD3	1.88	0.56
1:D:485:THR:CG2	1:D:486:GLU:OE1	2.54	0.56
1:D:681:ARG:HD3	1:D:710:ALA:O	2.06	0.56
1:A:154:PHE:CG	1:A:315:PHE:HE1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TRP:CE3	1:A:456:VAL:HG22	2.41	0.55
1:A:655:GLN:NE2	1:A:685:LYS:H	2.03	0.55
1:D:655:GLN:NE2	1:D:685:LYS:H	2.03	0.55
1:A:226:SER:HB2	1:A:229:GLN:N	2.17	0.55
1:C:223:MSE:CE	1:C:500:LEU:HD13	2.34	0.55
1:B:6:ASN:HD21	1:B:8:ALA:HB3	1.72	0.55
1:B:460:LEU:HB3	1:B:464:MSE:CE	2.36	0.55
1:B:692:ARG:HB2	1:B:692:ARG:HH11	1.71	0.55
1:A:599:PHE:CD1	1:A:654:TRP:CZ3	2.94	0.55
1:C:650:ASN:HD21	1:C:672:LEU:H	1.53	0.55
1:D:500:LEU:HB3	1:D:501:PRO:HD3	1.88	0.55
1:D:539:MSE:HA	1:D:542:ALA:O	2.06	0.55
1:A:277:ASN:HD22	1:A:278:PRO:HD2	1.71	0.55
1:A:436:PRO:HG2	1:D:96:ASN:ND2	2.21	0.55
1:B:206:LEU:C	1:B:206:LEU:HD23	2.31	0.55
1:D:228:GLN:NE2	1:D:228:GLN:H	2.03	0.55
1:D:283:TRP:CE3	1:D:499:GLU:HG2	2.42	0.55
1:D:485:THR:HG23	1:D:486:GLU:OE1	2.06	0.55
1:D:266:GLN:HG3	1:D:267:TYR:CD2	2.42	0.55
1:B:362:GLU:CD	1:B:630:ARG:HH22	2.14	0.55
1:A:579:VAL:HG11	1:A:587:ILE:HG23	1.88	0.55
1:A:676:ASN:O	1:C:202:ARG:NH1	2.39	0.55
1:B:15:GLN:O	1:B:153:ILE:HD11	2.06	0.55
1:C:2:SER:HB2	1:C:132:GLN:NE2	2.22	0.55
1:A:443:GLY:O	1:A:446:GLN:HG2	2.07	0.54
1:B:308:LEU:HD11	1:B:312:MSE:CE	2.37	0.54
1:B:344:PHE:O	1:B:390:LYS:HD3	2.07	0.54
1:B:538:MSE:HE1	2:B:1032:HOH:O	2.06	0.54
1:C:454:PRO:HD2	1:C:491:ARG:NH1	2.21	0.54
1:A:533:ARG:HE	1:A:538:MSE:HE2	1.71	0.54
1:B:87:GLN:HG3	1:B:215:MSE:CE	2.30	0.54
1:C:371:PHE:CZ	1:C:384:TRP:CZ3	2.95	0.54
1:C:415:PRO:HG3	1:C:464:MSE:HE1	1.88	0.54
1:D:411:LEU:HD11	1:D:413:PHE:CE2	2.42	0.54
1:D:450:ASP:HB3	1:D:453:ARG:HD2	1.89	0.54
1:A:55:ARG:H	1:A:69:GLN:HE22	1.53	0.54
1:B:568:PRO:HD2	1:B:571:MSE:SE	2.58	0.54
1:C:579:VAL:HA	1:C:580:PRO:C	2.32	0.54
1:B:48:ASN:HB3	2:B:1111:HOH:O	2.07	0.54
1:B:376:ASP:HB3	1:B:378:THR:H	1.73	0.54
1:C:479:ASP:HA	1:C:527:CYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:O	1:B:464:MSE:HE3	2.08	0.54
1:A:153:ILE:HG22	1:A:155:PRO:HD3	1.89	0.53
1:B:199:THR:HB	1:C:266:GLN:HB2	1.90	0.53
1:B:308:LEU:CD1	1:B:312:MSE:HE3	2.38	0.53
1:D:415:PRO:HB3	1:D:464:MSE:HE1	1.90	0.53
1:A:650:ASN:HD21	1:A:672:LEU:N	1.93	0.53
1:C:415:PRO:CG	1:C:464:MSE:HE1	2.38	0.53
1:A:581:ASN:HD21	1:A:583:GLN:NE2	2.05	0.53
1:B:500:LEU:HB3	1:B:501:PRO:HD3	1.91	0.53
1:C:412:TRP:HD1	1:C:477:LYS:HD3	1.73	0.53
1:C:425:TYR:CE1	1:C:429:PRO:HB3	2.43	0.53
1:B:411:LEU:HB2	2:B:1017:HOH:O	2.07	0.53
1:A:623:VAL:O	1:A:627:LYS:HG3	2.09	0.53
1:D:54:TRP:HB2	1:D:67:ASN:ND2	2.23	0.53
1:A:453:ARG:HG2	1:A:491:ARG:HD2	1.91	0.53
1:A:662:LYS:HD3	1:A:738:LEU:HD11	1.89	0.53
1:B:590:LEU:HD23	1:B:618:GLN:CD	2.32	0.53
1:C:557:LEU:HD13	1:C:596:VAL:HG22	1.89	0.53
1:D:443:GLY:O	1:D:446:GLN:HG2	2.07	0.53
1:A:227:HIS:ND1	1:A:483:TYR:OH	2.34	0.53
1:B:491:ARG:HH11	1:B:491:ARG:CG	2.22	0.53
1:A:146:ALA:HB3	1:A:167:THR:HB	1.91	0.53
1:C:13:HIS:HD2	2:C:1273:HOH:O	1.91	0.53
1:C:599:PHE:CE1	1:C:654:TRP:CZ3	2.97	0.53
1:A:313:ALA:CB	1:A:568:PRO:HG3	2.39	0.52
1:A:654:TRP:HH2	1:A:669:TYR:OH	1.88	0.52
1:B:414:GLU:OE2	1:B:417:MSE:HG3	2.09	0.52
1:B:329:GLU:CB	1:B:630:ARG:HD3	2.35	0.52
1:B:491:ARG:HG2	1:B:491:ARG:NH1	2.22	0.52
1:C:492:LEU:HB3	1:C:496:GLN:HB2	1.91	0.52
1:B:588:THR:CG2	1:B:593:ARG:CG	2.88	0.52
1:D:333:LEU:C	1:D:333:LEU:HD12	2.34	0.52
1:D:386:VAL:HG11	1:D:394:GLY:HA2	1.92	0.52
1:A:599:PHE:CZ	1:A:654:TRP:HZ3	2.27	0.52
1:B:369:GLY:HA2	1:B:374:ARG:HG2	1.90	0.52
1:D:255:SER:HA	1:D:535:ASP:OD2	2.10	0.52
1:A:6:ASN:HD22	1:A:9:ASN:H	1.57	0.52
1:A:26:MSE:HE1	1:A:73:ILE:HG21	1.90	0.52
1:B:477:LYS:NZ	2:B:1219:HOH:O	2.42	0.52
1:B:641:ILE:HB	1:B:653:SER:OG	2.09	0.52
1:B:644:PRO:HA	1:B:649:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ILE:O	1:C:695:ILE:HG22	2.09	0.52
1:B:478:TRP:HH2	1:B:511:LEU:HB3	1.74	0.52
1:D:478:TRP:C	1:D:478:TRP:CD1	2.88	0.52
1:B:396:GLU:CD	1:B:396:GLU:H	2.18	0.52
1:C:90:PHE:HA	1:C:178:ARG:O	2.10	0.52
1:C:168:ASN:HB2	1:C:285:LEU:HD23	1.92	0.52
1:B:655:GLN:NE2	1:B:685:LYS:H	2.05	0.51
1:C:191:TYR:HB2	1:C:211:LEU:HD22	1.92	0.51
1:A:482:ARG:HH22	1:A:485:THR:HB	1.75	0.51
1:B:353:VAL:HG13	1:B:407:MSE:HE3	1.91	0.51
1:D:441:THR:HB	1:D:485:THR:HG21	1.91	0.51
1:C:223:MSE:CE	1:C:501:PRO:HA	2.39	0.51
1:D:223:MSE:HE2	1:D:501:PRO:HA	1.91	0.51
1:D:325:PHE:O	1:D:330:ARG:NH2	2.44	0.51
1:A:222:ARG:HB3	1:A:483:TYR:CD1	2.45	0.51
1:A:410:GLY:HA3	1:A:475:TYR:HB3	1.92	0.51
1:B:33:GLN:HE22	1:B:35:TYR:C	2.18	0.51
1:B:225:SER:O	1:B:532:GLY:O	2.27	0.51
1:C:599:PHE:CD1	1:C:654:TRP:CZ3	2.99	0.51
1:D:300:TYR:CD1	1:D:301:THR:N	2.78	0.51
1:A:328:GLU:O	1:A:330:ARG:HD2	2.10	0.51
1:B:353:VAL:HG13	1:B:407:MSE:HE1	1.91	0.51
1:A:485:THR:HG23	1:A:486:GLU:CD	2.36	0.51
1:B:142:ILE:HG23	1:C:437:LYS:HB2	1.93	0.51
1:C:413:PHE:CG	1:C:464:MSE:HE2	2.45	0.51
1:C:599:PHE:CE1	1:C:654:TRP:HZ3	2.28	0.51
1:B:277:ASN:HD22	1:B:278:PRO:N	2.07	0.51
1:C:588:THR:HG22	1:C:589:SER:O	2.11	0.51
1:D:322:ASN:OD1	1:D:324:ARG:HB3	2.10	0.51
1:C:371:PHE:CE1	1:C:374:ARG:HD2	2.46	0.51
1:C:489:SER:HB3	1:C:492:LEU:HD12	1.92	0.51
1:B:193:LEU:HD13	1:B:262:ILE:CD1	2.41	0.51
1:C:641:ILE:HG22	1:C:642:ASP:N	2.25	0.51
1:A:254:TYR:OH	1:A:502:HIS:HD2	1.94	0.50
1:A:475:TYR:HA	1:A:523:LEU:O	2.11	0.50
1:A:611:MSE:HB2	1:A:616:LEU:HD13	1.92	0.50
1:C:99:ARG:HG3	1:C:99:ARG:HH11	1.75	0.50
1:D:551:THR:H	1:D:583:GLN:NE2	2.09	0.50
1:C:441:THR:HB	1:C:485:THR:HG21	1.92	0.50
1:A:87:GLN:HG3	1:A:215:MSE:CE	2.32	0.50
1:C:546:TRP:HA	1:C:546:TRP:CE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:PHE:CE1	1:D:654:TRP:CZ3	2.97	0.50
1:A:300:TYR:CG	1:A:301:THR:N	2.80	0.50
1:B:209:HIS:CE1	1:C:212:ARG:HB3	2.46	0.50
1:B:491:ARG:O	1:B:491:ARG:HG3	2.12	0.50
1:B:585:GLY:O	1:D:724:SER:HA	2.12	0.50
1:A:414:GLU:N	1:A:415:PRO:HD3	2.27	0.50
1:A:460:LEU:HB3	1:A:464:MSE:HE3	1.92	0.50
1:C:87:GLN:HG3	1:C:215:MSE:CE	2.41	0.50
1:D:433:ILE:HD12	1:D:448:VAL:CG2	2.41	0.50
1:A:355:GLN:NE2	1:A:616:LEU:HD21	2.27	0.50
1:A:370:TRP:NE1	1:A:411:LEU:HD13	2.27	0.50
1:A:676:ASN:OD1	1:B:55:ARG:HD2	2.12	0.50
1:B:590:LEU:HD23	1:B:618:GLN:NE2	2.27	0.50
1:A:313:ALA:HB1	1:A:568:PRO:HG3	1.93	0.49
1:A:425:TYR:CE1	1:A:429:PRO:HB3	2.47	0.49
1:A:552:ASP:OD1	1:A:586:ARG:HB3	2.12	0.49
1:B:370:TRP:CZ2	1:B:411:LEU:HD11	2.47	0.49
1:B:569:GLN:HA	1:B:572:MSE:HE3	1.94	0.49
1:C:3:ILE:H	1:C:132:GLN:NE2	2.08	0.49
1:D:233:MSE:HE1	1:D:262:ILE:CG1	2.41	0.49
1:A:303:ALA:HB3	1:A:307:GLN:HG2	1.94	0.49
1:C:252:LEU:HD13	1:C:254:TYR:HB3	1.94	0.49
1:C:420:VAL:O	1:C:425:TYR:HD2	1.96	0.49
1:D:225:SER:O	1:D:532:GLY:O	2.30	0.49
1:A:193:LEU:HD13	1:A:262:ILE:HD12	1.94	0.49
1:B:216:GLN:HB2	1:C:212:ARG:NH2	2.25	0.49
1:C:277:ASN:C	1:C:277:ASN:HD22	2.20	0.49
1:C:349:LEU:HD22	1:C:398:PHE:CZ	2.47	0.49
1:C:557:LEU:HD21	1:C:669:TYR:CG	2.48	0.49
1:D:584:MSE:HE1	1:D:586:ARG:CZ	2.42	0.49
1:C:440:PRO:HB2	1:C:447:PHE:HE2	1.77	0.49
1:C:500:LEU:HB3	1:C:501:PRO:HD3	1.94	0.49
1:A:225:SER:O	1:A:532:GLY:O	2.29	0.49
1:C:96:ASN:OD1	1:C:98:SER:HB3	2.11	0.49
1:C:329:GLU:OE1	1:C:630:ARG:HD2	2.12	0.49
1:A:212:ARG:HB3	1:D:209:HIS:CE1	2.47	0.49
1:D:224:ALA:HA	1:D:255:SER:O	2.13	0.49
1:B:233:MSE:CE	1:B:262:ILE:HD11	2.35	0.49
1:C:277:ASN:HD22	1:C:278:PRO:N	2.11	0.49
1:C:332:VAL:HG23	1:C:630:ARG:NH2	2.26	0.49
1:C:349:LEU:HD23	1:C:349:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:THR:HB	2:D:1317:HOH:O	2.13	0.49
1:A:684:PHE:O	1:A:708:MSE:HG2	2.13	0.49
1:A:717:ILE:HG12	1:A:728:TYR:CE2	2.48	0.49
1:B:588:THR:HG21	1:B:593:ARG:CG	2.42	0.49
1:A:13:HIS:HE1	1:A:20:SER:OG	1.96	0.49
1:A:231:PRO:O	1:A:260:ASP:OD2	2.31	0.49
1:A:259:LEU:O	1:A:274:THR:HA	2.13	0.49
1:A:579:VAL:HG21	1:A:588:THR:H	1.78	0.49
1:D:479:ASP:HA	1:D:527:CYS:HB3	1.93	0.49
1:B:354:ASN:HD22	1:B:405:GLN:HE21	1.60	0.48
1:B:579:VAL:HA	1:B:580:PRO:C	2.38	0.48
1:C:6:ASN:HD22	1:C:9:ASN:H	1.61	0.48
1:C:420:VAL:HA	1:C:425:TYR:CD2	2.48	0.48
1:D:212:ARG:NH1	1:D:213:PRO:O	2.46	0.48
1:D:579:VAL:HG21	1:D:588:THR:H	1.78	0.48
1:D:349:LEU:CD1	1:D:366:LEU:HD13	2.43	0.48
1:A:599:PHE:CZ	1:A:654:TRP:CZ3	3.01	0.48
1:D:127:THR:O	1:D:128:ASP:C	2.56	0.48
1:D:136:VAL:HG12	1:D:138:PHE:CE1	2.48	0.48
1:D:226:SER:HB2	1:D:228:GLN:H	1.77	0.48
1:D:411:LEU:C	1:D:411:LEU:HD12	2.38	0.48
1:A:16:THR:OG1	1:A:158:ASP:OD1	2.24	0.48
1:A:632:LEU:HD13	1:A:658:SER:HB3	1.95	0.48
1:B:92:VAL:HG22	1:B:176:LEU:HD23	1.94	0.48
1:C:228:GLN:HE21	1:C:228:GLN:H	1.59	0.48
1:C:370:TRP:CE2	1:C:411:LEU:HD13	2.49	0.48
1:D:76:GLU:CG	1:D:151:TYR:OH	2.62	0.48
1:A:223:MSE:HE3	1:A:487:MSE:CG	2.44	0.48
1:A:145:LEU:HD13	1:A:174:LEU:HD13	1.96	0.48
1:A:411:LEU:HD12	1:A:411:LEU:C	2.38	0.48
1:A:581:ASN:HD21	1:A:583:GLN:HE22	1.60	0.48
1:C:206:LEU:HD23	1:C:207:TYR:N	2.29	0.48
1:C:354:ASN:HD22	1:C:405:GLN:HE21	1.60	0.48
1:D:681:ARG:CD	1:D:710:ALA:O	2.62	0.48
1:A:191:TYR:HB2	1:A:211:LEU:HD22	1.95	0.48
1:A:322:ASN:HA	1:A:323:PRO:HD3	1.75	0.48
1:B:308:LEU:CG	1:B:312:MSE:HE3	2.43	0.48
1:D:415:PRO:HB3	1:D:464:MSE:CE	2.44	0.48
1:A:725:LYS:HD2	1:A:725:LYS:HA	1.52	0.48
1:D:277:ASN:C	1:D:277:ASN:HD22	2.22	0.48
1:A:277:ASN:HD22	1:A:278:PRO:CD	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:O	1:A:593:ARG:NH1	2.47	0.47
1:C:415:PRO:HG2	1:C:478:TRP:CE2	2.49	0.47
1:D:14:LEU:CB	1:D:153:ILE:HD11	2.38	0.47
1:A:411:LEU:HD11	1:A:413:PHE:CE2	2.49	0.47
1:B:332:VAL:O	1:B:361:ILE:HG23	2.14	0.47
1:C:329:GLU:HB3	1:C:630:ARG:HD3	1.95	0.47
1:C:584:MSE:HE2	1:C:584:MSE:C	2.39	0.47
1:D:412:TRP:CH2	1:D:414:GLU:HB2	2.50	0.47
1:D:655:GLN:HE22	1:D:685:LYS:N	2.07	0.47
1:B:2:SER:N	2:B:1316:HOH:O	2.47	0.47
1:B:724:SER:HA	1:D:585:GLY:O	2.15	0.47
1:D:353:VAL:HG13	1:D:407:MSE:CE	2.44	0.47
1:B:243:GLU:HG2	1:B:685:LYS:HE3	1.97	0.47
1:B:26:MSE:HE1	1:B:73:ILE:HG21	1.97	0.47
1:C:129:ASP:O	1:C:130:ASP:HB2	2.14	0.47
1:C:478:TRP:C	1:C:478:TRP:HD1	2.21	0.47
1:C:552:ASP:OD1	1:C:586:ARG:HB3	2.14	0.47
1:D:505:ILE:HD13	1:D:505:ILE:HA	1.61	0.47
1:D:588:THR:HG22	1:D:589:SER:O	2.15	0.47
1:A:6:ASN:ND2	1:A:9:ASN:HD22	2.11	0.47
1:A:344:PHE:O	1:A:390:LYS:HE2	2.15	0.47
1:A:413:PHE:C	1:A:415:PRO:HD3	2.39	0.47
1:A:599:PHE:CD1	1:A:654:TRP:CH2	3.03	0.47
1:B:60:SER:O	1:C:441:THR:HG23	2.15	0.47
1:C:344:PHE:O	1:C:390:LYS:HD2	2.15	0.47
1:C:703:TYR:CD2	1:D:41:HIS:ND1	2.83	0.47
1:D:6:ASN:ND2	1:D:9:ASN:HD22	2.13	0.47
1:D:76:GLU:CG	1:D:151:TYR:HH	2.28	0.47
1:D:378:THR:HG22	1:D:445:HIS:CG	2.50	0.47
1:D:504:TYR:CD1	1:D:504:TYR:C	2.92	0.47
1:B:180:LEU:HD23	1:B:273:LEU:HD22	1.97	0.47
1:B:387:ASP:OD1	1:B:387:ASP:C	2.57	0.47
1:C:349:LEU:HD11	1:C:366:LEU:HD13	1.97	0.47
1:C:550:ASP:HA	1:C:583:GLN:HE21	1.80	0.47
1:A:493:THR:HG22	1:A:494:SER:N	2.29	0.47
1:B:38:PRO:HD3	1:B:300:TYR:CZ	2.50	0.47
1:B:198:GLY:O	1:B:228:GLN:HA	2.15	0.47
1:B:252:LEU:HD13	1:B:254:TYR:HB3	1.97	0.47
1:D:584:MSE:HE2	1:D:584:MSE:HB2	1.90	0.47
1:B:235:LEU:HD21	1:B:262:ILE:HD13	1.98	0.46
1:C:364:PHE:CD1	1:C:364:PHE:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:HB2	1:C:456:VAL:HG23	1.97	0.46
1:C:504:TYR:CD1	1:C:504:TYR:C	2.93	0.46
1:C:568:PRO:HD2	1:C:571:MSE:SE	2.65	0.46
1:A:63:GLU:OE1	1:D:445:HIS:HD2	1.98	0.46
1:A:333:LEU:C	1:A:333:LEU:HD12	2.40	0.46
1:A:716:THR:OG1	1:B:53:GLU:OE1	2.34	0.46
1:A:239:GLN:HB2	2:A:942:HOH:O	2.15	0.46
1:A:650:ASN:ND2	1:A:671:LEU:HB2	2.31	0.46
1:B:378:THR:OG1	1:B:379:THR:HG23	2.14	0.46
1:D:324:ARG:HG2	1:D:520:PRO:O	2.15	0.46
1:D:355:GLN:OE1	1:D:616:LEU:HD21	2.15	0.46
1:C:151:TYR:CE2	1:C:162:LYS:HE3	2.51	0.46
1:C:209:HIS:HD2	2:C:1202:HOH:O	1.98	0.46
1:C:368:ASP:OD1	1:C:374:ARG:NH1	2.48	0.46
1:C:579:VAL:HG22	1:C:587:ILE:HA	1.97	0.46
1:D:277:ASN:ND2	1:D:279:ASP:H	2.14	0.46
1:A:300:TYR:CD1	1:A:300:TYR:C	2.93	0.46
1:B:52:GLN:NE2	1:B:68:PHE:HA	2.29	0.46
1:B:491:ARG:CG	1:B:491:ARG:NH1	2.77	0.46
1:D:450:ASP:OD1	1:D:452:ALA:HB3	2.15	0.46
1:A:378:THR:OG1	1:A:379:THR:HG23	2.16	0.46
1:A:533:ARG:HH21	1:A:538:MSE:HE1	1.80	0.46
1:B:254:TYR:CD1	1:B:294:PRO:HG3	2.51	0.46
1:B:713:PHE:CD1	1:B:713:PHE:C	2.94	0.46
1:C:167:THR:HG23	1:C:290:THR:CG2	2.32	0.46
1:C:200:TRP:O	1:C:201:ALA:HB3	2.15	0.46
1:C:692:ARG:HD3	1:C:703:TYR:CZ	2.50	0.46
1:C:412:TRP:CH2	1:C:414:GLU:HG3	2.50	0.46
1:D:371:PHE:CD2	1:D:371:PHE:N	2.84	0.46
1:D:411:LEU:HD11	1:D:413:PHE:CZ	2.51	0.46
1:A:363:MSE:HE2	1:A:408:LYS:HB3	1.98	0.46
1:A:638:PHE:HZ	1:A:654:TRP:CD1	2.33	0.46
1:B:15:GLN:C	1:B:153:ILE:HD11	2.41	0.46
1:B:450:ASP:HB3	1:B:453:ARG:HD2	1.98	0.46
1:C:265:ASP:OD1	1:C:265:ASP:C	2.58	0.46
1:D:694:GLN:HE21	1:D:701:THR:HG22	1.81	0.46
1:A:223:MSE:HG3	1:A:487:MSE:CE	2.46	0.46
1:A:223:MSE:CE	1:A:487:MSE:SE	3.10	0.46
1:A:262:ILE:HG23	1:A:272:ILE:HG13	1.98	0.46
1:B:166:PHE:O	1:B:290:THR:HA	2.15	0.46
1:C:730:GLN:HE21	1:C:730:GLN:HB2	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:SER:HB3	1:A:228:GLN:HB2	1.97	0.45
1:A:552:ASP:HA	2:A:1195:HOH:O	2.16	0.45
1:B:455:GLU:OE1	1:B:491:ARG:NH2	2.46	0.45
1:B:479:ASP:CG	1:B:480:MSE:H	2.25	0.45
1:C:694:GLN:HG3	1:C:737:ILE:HD11	1.98	0.45
1:A:96:ASN:ND2	1:D:436:PRO:HG2	2.31	0.45
1:A:300:TYR:CD1	1:A:301:THR:N	2.84	0.45
1:B:478:TRP:CD1	1:B:478:TRP:C	2.94	0.45
1:C:330:ARG:HA	1:C:331:PRO:HD3	1.81	0.45
1:C:384:TRP:HB2	1:C:463:LEU:HD13	1.99	0.45
1:C:569:GLN:HA	1:C:572:MSE:HE3	1.98	0.45
1:D:526:SER:HB2	1:D:538:MSE:HE3	1.98	0.45
1:A:24:GLN:HB2	1:A:34:ILE:HD11	1.97	0.45
1:A:287:PRO:O	1:A:288:GLN:HB2	2.17	0.45
1:D:90:PHE:HA	1:D:178:ARG:O	2.16	0.45
1:B:199:THR:OG1	1:B:200:TRP:N	2.49	0.45
1:C:114:LYS:HD3	1:C:152:SER:OG	2.16	0.45
1:C:420:VAL:HG13	1:C:425:TYR:HE2	1.81	0.45
1:C:515:LEU:HD13	1:C:524:PHE:HZ	1.82	0.45
1:D:264:VAL:HA	1:D:269:THR:O	2.16	0.45
1:A:694:GLN:HG3	1:A:737:ILE:CD1	2.42	0.45
1:B:681:ARG:HD3	1:B:710:ALA:O	2.16	0.45
1:C:713:PHE:H	1:D:48:ASN:HD21	1.63	0.45
1:D:556:ARG:O	1:D:557:LEU:C	2.57	0.45
1:A:63:GLU:OE1	1:A:63:GLU:HA	2.16	0.45
1:A:556:ARG:HA	1:A:556:ARG:HD2	1.73	0.45
1:A:632:LEU:HD21	1:A:664:ALA:HA	1.97	0.45
1:B:227:HIS:ND1	1:B:483:TYR:OH	2.46	0.45
1:B:349:LEU:O	1:B:353:VAL:HG23	2.17	0.45
1:B:695:ILE:O	1:B:696:ASN:HB2	2.17	0.45
1:C:349:LEU:HD23	1:C:349:LEU:C	2.41	0.45
1:C:378:THR:OG1	1:C:379:THR:HG23	2.15	0.45
1:B:202:ARG:HD2	1:D:675:PRO:O	2.17	0.45
1:B:353:VAL:O	1:B:407:MSE:HE1	2.17	0.45
1:B:478:TRP:CH2	1:B:511:LEU:HD13	2.50	0.45
1:B:484:ALA:HB3	1:B:487:MSE:HE2	1.98	0.45
1:B:588:THR:CG2	1:B:593:ARG:HH11	2.29	0.45
1:D:3:ILE:HG13	1:D:132:GLN:NE2	2.31	0.45
1:D:108:TYR:CD2	1:D:108:TYR:C	2.95	0.45
1:D:252:LEU:HG	2:D:1317:HOH:O	2.17	0.45
1:A:26:MSE:SE	1:A:50:MSE:HE1	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ARG:NH2	1:B:573:GLY:O	2.44	0.45
1:D:262:ILE:CD1	1:D:272:ILE:HG13	2.44	0.45
1:A:330:ARG:HG2	1:A:330:ARG:HH11	1.80	0.45
1:A:662:LYS:HE3	2:A:1123:HOH:O	2.16	0.45
1:C:485:THR:HG22	1:C:486:GLU:OE1	2.16	0.45
1:C:48:ASN:ND2	1:D:713:PHE:H	2.13	0.45
1:A:145:LEU:HG	1:A:146:ALA:N	2.31	0.44
1:C:34:ILE:HG12	1:C:50:MSE:HE2	1.99	0.44
1:C:147:LEU:HD13	1:C:166:PHE:CE2	2.51	0.44
1:C:226:SER:CB	1:C:228:GLN:HE21	2.28	0.44
1:D:725:LYS:HD2	1:D:725:LYS:HA	1.66	0.44
1:A:53:GLU:OE1	1:B:716:THR:OG1	2.32	0.44
1:B:74:LYS:HE3	2:B:1140:HOH:O	2.17	0.44
1:A:221:LEU:HD11	1:D:87:GLN:HE22	1.81	0.44
1:A:227:HIS:CE1	1:A:529:SER:HB2	2.53	0.44
1:A:370:TRP:CE2	1:A:411:LEU:HD13	2.52	0.44
1:C:54:TRP:HB2	1:C:67:ASN:ND2	2.32	0.44
1:A:153:ILE:CG2	1:A:155:PRO:HD3	2.47	0.44
1:A:286:ALA:O	1:A:289:ALA:HB3	2.17	0.44
1:B:13:HIS:HE1	1:B:20:SER:OG	2.01	0.44
1:B:22:ILE:HG22	1:B:34:ILE:HD12	1.99	0.44
1:B:350:MSE:HE1	1:B:398:PHE:HD1	1.83	0.44
1:B:612:ALA:HB1	1:B:613:PRO:HD2	2.00	0.44
1:D:575:HIS:HA	1:D:603:GLY:O	2.17	0.44
1:A:82:LYS:HE3	1:D:486:GLU:OE2	2.16	0.44
1:A:154:PHE:CD1	1:A:315:PHE:HE1	2.34	0.44
1:A:382:GLY:CA	1:A:424:LEU:HD12	2.47	0.44
1:A:391:PHE:HE1	1:A:398:PHE:CD2	2.35	0.44
1:C:198:GLY:O	1:C:228:GLN:HA	2.18	0.44
1:C:519:TYR:HB3	1:C:522:VAL:HG23	2.00	0.44
1:A:329:GLU:OE1	1:A:630:ARG:HD2	2.17	0.44
1:A:411:LEU:HD11	1:A:413:PHE:CZ	2.53	0.44
1:B:127:THR:O	1:B:128:ASP:HB3	2.18	0.44
1:B:681:ARG:CD	1:B:710:ALA:O	2.66	0.44
1:A:199:THR:OG1	1:A:200:TRP:N	2.47	0.44
1:C:425:TYR:HE1	1:C:429:PRO:HB3	1.81	0.44
1:D:418:VAL:HG11	1:D:432:LEU:HD12	2.00	0.44
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.84	0.44
1:B:538:MSE:CE	2:B:1032:HOH:O	2.64	0.44
1:C:346:GLU:N	1:C:390:LYS:O	2.51	0.44
1:C:386:VAL:HG12	1:C:387:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:PRO:O	1:C:676:ASN:C	2.61	0.44
1:A:579:VAL:CG1	1:A:587:ILE:HG23	2.48	0.43
1:A:724:SER:HB2	1:C:587:ILE:HG13	1.99	0.43
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.83	0.43
1:D:370:TRP:CE2	1:D:411:LEU:HD13	2.53	0.43
1:D:606:LEU:HD11	1:D:611:MSE:HE3	1.99	0.43
1:A:350:MSE:HE1	1:A:398:PHE:HD1	1.83	0.43
1:B:485:THR:CG2	1:B:486:GLU:OE1	2.58	0.43
1:C:650:ASN:ND2	1:C:672:LEU:H	2.17	0.43
1:D:92:VAL:HB	2:D:994:HOH:O	2.18	0.43
1:A:233:MSE:SE	1:A:260:ASP:HB3	2.69	0.43
1:A:654:TRP:CE2	2:A:1399:HOH:O	2.65	0.43
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.64	0.43
1:C:370:TRP:HE3	1:C:370:TRP:O	2.02	0.43
1:D:146:ALA:HB3	1:D:167:THR:HB	2.00	0.43
1:B:415:PRO:HB3	1:B:464:MSE:CE	2.49	0.43
1:A:595:ALA:CB	1:A:729:THR:HG21	2.48	0.43
1:B:505:ILE:HD13	1:B:505:ILE:HA	1.79	0.43
1:C:277:ASN:HD22	1:C:278:PRO:CD	2.31	0.43
1:C:551:THR:H	1:C:583:GLN:HE22	1.66	0.43
1:A:228:GLN:H	1:A:228:GLN:NE2	2.16	0.43
1:A:345:ASN:OD1	1:A:347:ALA:HB3	2.19	0.43
1:C:154:PHE:CG	1:C:315:PHE:HE1	2.37	0.43
1:C:425:TYR:O	1:C:429:PRO:HG3	2.18	0.43
1:D:741:HIS:O	1:D:743:HIS:CD2	2.72	0.43
1:A:230:ASN:HD22	1:A:232:PHE:H	1.65	0.43
1:B:617:ASP:O	1:B:621:LYS:HG2	2.19	0.43
1:B:688:ARG:HA	1:B:689:PRO:HD3	1.84	0.43
1:D:300:TYR:CG	1:D:301:THR:N	2.86	0.43
1:B:120:LEU:O	1:B:121:PRO:C	2.60	0.43
1:B:479:ASP:OD1	1:B:480:MSE:N	2.47	0.43
1:B:500:LEU:HD23	1:B:500:LEU:HA	1.79	0.43
1:C:254:TYR:OH	1:C:502:HIS:HD2	2.02	0.43
1:C:415:PRO:HG2	1:C:478:TRP:NE1	2.34	0.43
1:C:433:ILE:HD12	1:C:448:VAL:HG22	2.00	0.43
1:D:74:LYS:HB2	1:D:74:LYS:HE3	1.81	0.43
1:D:381:LEU:HD12	1:D:381:LEU:HA	1.82	0.43
1:A:714:VAL:HA	1:A:715:PRO:HD3	1.91	0.43
1:C:373:HIS:CD2	1:C:373:HIS:O	2.71	0.43
1:C:436:PRO:HD3	1:C:488:PHE:CD1	2.54	0.43
1:C:737:ILE:HD12	1:C:737:ILE:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:SER:HA	1:D:567:TYR:O	2.16	0.43
1:A:371:PHE:CZ	1:A:374:ARG:CD	2.93	0.43
1:A:654:TRP:HZ2	2:A:1399:HOH:O	1.94	0.43
1:D:69:GLN:HB2	2:D:1283:HOH:O	2.19	0.43
1:D:353:VAL:O	1:D:407:MSE:HE1	2.19	0.43
1:D:502:HIS:CE1	2:D:1432:HOH:O	2.51	0.43
1:D:567:TYR:HA	1:D:568:PRO:HD3	1.76	0.43
1:D:713:PHE:CD1	1:D:713:PHE:C	2.96	0.43
1:A:277:ASN:HD22	1:A:277:ASN:C	2.27	0.42
1:A:478:TRP:C	1:A:478:TRP:HD1	2.23	0.42
1:A:741:HIS:HB3	1:A:743:HIS:CE1	2.54	0.42
1:B:350:MSE:HE1	1:B:398:PHE:CD1	2.54	0.42
1:C:34:ILE:CG1	1:C:50:MSE:HE2	2.49	0.42
1:D:230:ASN:CG	1:D:231:PRO:HD2	2.44	0.42
1:A:264:VAL:HA	1:A:269:THR:O	2.19	0.42
1:A:277:ASN:HD22	1:A:278:PRO:N	2.18	0.42
1:B:524:PHE:O	1:B:542:ALA:HB1	2.19	0.42
1:D:374:ARG:HG2	1:D:380:SER:HB2	2.01	0.42
1:D:684:PHE:O	1:D:708:MSE:HG2	2.19	0.42
1:A:386:VAL:HG22	1:A:395:ILE:HG12	2.01	0.42
1:A:496:GLN:O	1:A:499:GLU:HB2	2.18	0.42
1:B:346:GLU:HB2	1:B:391:PHE:CD1	2.54	0.42
1:B:692:ARG:HB2	1:B:692:ARG:NH1	2.34	0.42
1:C:612:ALA:HB3	1:C:615:GLU:OE2	2.19	0.42
1:A:54:TRP:HB2	1:A:67:ASN:ND2	2.34	0.42
1:B:606:LEU:HD11	1:B:611:MSE:HE3	2.00	0.42
1:C:718:LEU:O	1:C:725:LYS:HE2	2.19	0.42
1:D:539:MSE:HG3	1:D:571:MSE:SE	2.69	0.42
1:A:14:LEU:HD12	1:A:14:LEU:N	2.34	0.42
1:A:450:ASP:C	1:A:450:ASP:OD1	2.62	0.42
1:C:632:LEU:HG	1:C:656:VAL:HG23	2.01	0.42
1:A:99:ARG:HG3	1:A:99:ARG:NH1	2.33	0.42
1:D:464:MSE:CE	1:D:511:LEU:HD11	2.50	0.42
1:B:153:ILE:HG23	1:B:153:ILE:O	2.19	0.42
1:B:676:ASN:O	1:D:202:ARG:NH1	2.52	0.42
1:C:6:ASN:ND2	1:C:9:ASN:H	2.18	0.42
1:D:218:ILE:HG12	1:D:260:ASP:HB2	2.02	0.42
1:D:300:TYR:CD1	1:D:300:TYR:C	2.97	0.42
1:A:266:GLN:HB2	1:D:199:THR:HB	2.01	0.42
1:B:5:VAL:HG11	1:B:108:TYR:CZ	2.55	0.42
1:B:567:TYR:HA	1:B:568:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:HG3	1:C:99:ARG:NH1	2.35	0.42
1:C:546:TRP:HA	1:C:546:TRP:HE3	1.82	0.42
1:C:611:MSE:HB2	1:C:616:LEU:CD2	2.50	0.42
1:D:378:THR:C	1:D:379:THR:HG22	2.44	0.42
1:D:556:ARG:NH2	1:D:573:GLY:O	2.53	0.42
1:A:193:LEU:HD13	1:A:262:ILE:CD1	2.50	0.42
1:A:206:LEU:C	1:A:206:LEU:HD23	2.44	0.42
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.73	0.42
1:B:196:PHE:CZ	1:B:565:TYR:HB2	2.55	0.42
1:C:195:GLN:HG2	1:C:207:TYR:HB2	2.01	0.42
1:D:132:GLN:O	1:D:152:SER:HA	2.19	0.42
1:D:159:VAL:HG21	1:D:315:PHE:CG	2.55	0.42
1:D:254:TYR:OH	1:D:502:HIS:CD2	2.65	0.42
1:A:2:SER:HB2	1:A:132:GLN:HE22	1.85	0.42
1:C:324:ARG:HG2	1:C:520:PRO:O	2.20	0.42
1:C:611:MSE:HB2	1:C:616:LEU:HD22	2.02	0.42
1:B:55:ARG:H	1:B:69:GLN:HE22	1.67	0.41
1:B:303:ALA:HB3	1:B:307:GLN:HG2	2.01	0.41
1:C:371:PHE:CZ	1:C:374:ARG:CD	3.02	0.41
1:D:76:GLU:HG2	1:D:151:TYR:OH	2.19	0.41
1:D:209:HIS:HA	1:D:210:PRO:HD3	1.95	0.41
1:A:223:MSE:HE3	1:A:487:MSE:HG2	2.02	0.41
1:A:675:PRO:O	1:A:676:ASN:C	2.62	0.41
1:C:205:HIS:CE1	1:C:558:LEU:HD23	2.55	0.41
1:A:92:VAL:O	1:A:99:ARG:HA	2.21	0.41
1:A:226:SER:HB2	1:A:229:GLN:O	2.20	0.41
1:A:359:LEU:HD21	1:A:616:LEU:HG	2.02	0.41
1:A:431:TRP:CD2	1:A:456:VAL:HG22	2.55	0.41
1:A:599:PHE:CG	1:A:654:TRP:CZ3	3.09	0.41
1:C:228:GLN:NE2	1:C:228:GLN:N	2.68	0.41
1:C:262:ILE:HA	1:C:271:ARG:O	2.19	0.41
1:C:599:PHE:CD1	1:C:654:TRP:CH2	3.09	0.41
1:C:698:ASP:HA	1:C:699:PRO:HD2	1.89	0.41
1:A:183:GLN:HB2	1:A:273:LEU:HD23	2.01	0.41
1:A:710:ALA:HA	1:B:35:TYR:CE1	2.55	0.41
1:B:114:LYS:HD3	1:B:152:SER:OG	2.20	0.41
1:B:224:ALA:O	1:B:225:SER:C	2.63	0.41
1:C:370:TRP:CZ2	1:C:411:LEU:HD13	2.55	0.41
1:C:569:GLN:HG3	1:C:633:PHE:O	2.21	0.41
1:C:606:LEU:HD23	1:C:606:LEU:H	1.86	0.41
1:C:651:VAL:HG22	1:C:670:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:PHE:CE1	1:D:374:ARG:HG3	2.54	0.41
1:D:688:ARG:HA	1:D:689:PRO:HD3	1.95	0.41
1:A:383:ASP:OD1	1:A:423:ASP:OD2	2.39	0.41
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.77	0.41
1:A:703:TYR:O	1:A:706:GLU:HB2	2.21	0.41
1:B:212:ARG:H	1:B:216:GLN:NE2	2.09	0.41
1:B:313:ALA:CB	1:B:568:PRO:HG3	2.50	0.41
1:C:328:GLU:O	1:C:329:GLU:C	2.63	0.41
1:D:272:ILE:N	1:D:272:ILE:CD1	2.84	0.41
1:D:371:PHE:CE2	1:D:374:ARG:HG3	2.54	0.41
1:D:464:MSE:HE1	1:D:511:LEU:HD11	2.03	0.41
1:A:199:THR:HB	1:D:266:GLN:HB2	2.02	0.41
1:A:551:THR:H	1:A:583:GLN:HE22	1.68	0.41
1:A:698:ASP:HA	1:A:699:PRO:HD2	1.87	0.41
1:B:186:LEU:O	1:B:269:THR:HB	2.21	0.41
1:C:330:ARG:HD3	1:C:544:GLN:OE1	2.21	0.41
1:C:359:LEU:HD21	1:C:616:LEU:HD12	2.03	0.41
1:C:371:PHE:O	1:C:371:PHE:CG	2.74	0.41
1:D:58:THR:HA	1:D:59:PRO:HD3	1.87	0.41
1:D:65:ASN:ND2	1:D:65:ASN:N	2.69	0.41
1:D:277:ASN:HD22	1:D:278:PRO:N	2.18	0.41
1:A:383:ASP:OD1	1:A:422:SER:HB2	2.20	0.41
1:A:441:THR:HG23	1:D:60:SER:O	2.21	0.41
1:A:584:MSE:HE3	1:C:673:ASN:O	2.20	0.41
1:C:428:HIS:N	1:C:429:PRO:HD3	2.36	0.41
1:C:450:ASP:HB3	1:C:453:ARG:HD2	2.03	0.41
1:C:539:MSE:HG3	1:C:571:MSE:SE	2.70	0.41
1:C:588:THR:O	1:C:593:ARG:NH1	2.51	0.41
1:D:153:ILE:CG2	1:D:155:PRO:HD3	2.40	0.41
1:D:475:TYR:HA	1:D:523:LEU:O	2.20	0.41
1:D:644:PRO:HA	1:D:649:GLY:HA2	2.03	0.41
1:A:31:ALA:HB3	1:A:76:GLU:HB3	2.03	0.41
1:A:209:HIS:CE1	1:D:212:ARG:HB3	2.56	0.41
1:A:557:LEU:HD12	1:A:557:LEU:HA	1.94	0.41
1:A:724:SER:HA	1:C:585:GLY:O	2.21	0.41
1:B:325:PHE:CD2	1:B:523:LEU:HD13	2.54	0.41
1:C:13:HIS:CD2	2:C:1273:HOH:O	2.71	0.41
1:C:254:TYR:CE2	1:C:256:GLY:HA3	2.56	0.41
1:C:602:LEU:HB3	1:C:626:TYR:CE2	2.56	0.41
1:D:374:ARG:HD3	1:D:379:THR:O	2.20	0.41
1:D:374:ARG:NH1	1:D:381:LEU:HD13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:THR:C	1:D:379:THR:CG2	2.94	0.41
1:A:211:LEU:HA	1:A:216:GLN:NE2	2.36	0.40
1:B:55:ARG:HD3	1:B:55:ARG:HA	1.89	0.40
1:B:211:LEU:HD12	1:B:211:LEU:HA	1.94	0.40
1:C:12:PHE:CD1	1:C:134:LEU:HD21	2.56	0.40
1:C:588:THR:HB	1:C:593:ARG:NH1	2.35	0.40
1:D:482:ARG:HH21	1:D:485:THR:HB	1.85	0.40
1:A:202:ARG:NH1	1:C:676:ASN:O	2.51	0.40
1:B:9:ASN:ND2	1:B:9:ASN:N	2.69	0.40
1:B:588:THR:O	1:B:593:ARG:NH1	2.54	0.40
1:C:712:TYR:HA	1:D:48:ASN:HD21	1.87	0.40
1:D:381:LEU:O	1:D:418:VAL:HA	2.20	0.40
1:A:86:ARG:NH1	2:A:1408:HOH:O	2.54	0.40
1:A:246:ALA:HA	1:A:301:THR:O	2.21	0.40
1:A:391:PHE:CE1	1:A:398:PHE:CD2	3.10	0.40
1:C:604:TYR:CE1	1:C:619:VAL:HG13	2.56	0.40
1:D:478:TRP:C	1:D:478:TRP:HD1	2.27	0.40
1:D:673:ASN:HB2	1:D:725:LYS:O	2.22	0.40
1:A:703:TYR:CE2	1:B:41:HIS:CD2	3.10	0.40
1:B:461:PHE:CD2	1:B:461:PHE:C	3.00	0.40
1:C:376:ASP:HB3	1:C:378:THR:HG23	2.04	0.40
1:C:420:VAL:HG13	1:C:425:TYR:CE2	2.56	0.40
1:C:561:PHE:CE1	1:C:640:ARG:HD2	2.56	0.40
1:C:626:TYR:O	1:C:630:ARG:N	2.55	0.40
1:D:500:LEU:O	1:D:501:PRO:C	2.64	0.40
1:A:62:ASN:HA	1:D:442:PRO:HG3	2.04	0.40
1:A:721:GLY:O	1:C:580:PRO:HG2	2.21	0.40
1:B:208:ARG:C	1:B:209:HIS:CD2	3.00	0.40
1:C:26:MSE:HE1	1:C:73:ILE:HG21	2.03	0.40
1:C:223:MSE:SE	1:C:487:MSE:CE	3.19	0.40
1:C:515:LEU:HD13	1:C:524:PHE:CZ	2.56	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	740/745 (99%)	698 (94%)	38 (5%)	4 (0%)	24	48
1	B	734/745 (98%)	697 (95%)	36 (5%)	1 (0%)	48	73
1	C	735/745 (99%)	677 (92%)	55 (8%)	3 (0%)	30	54
1	D	741/745 (100%)	691 (93%)	48 (6%)	2 (0%)	36	60
All	All	2950/2980 (99%)	2763 (94%)	177 (6%)	10 (0%)	36	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	386	VAL
1	D	374	ARG
1	A	77	TYR
1	A	480	MSE
1	C	337	TRP
1	C	373	HIS
1	D	337	TRP
1	A	436	PRO
1	B	641	ILE
1	A	641	ILE

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	645/624 (103%)	604 (94%)	41 (6%)	16	38
1	B	638/624 (102%)	595 (93%)	43 (7%)	15	36
1	C	638/624 (102%)	586 (92%)	52 (8%)	10	27
1	D	645/624 (103%)	598 (93%)	47 (7%)	13	32
All	All	2566/2496 (103%)	2383 (93%)	183 (7%)	13	33

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	45	THR
1	A	61	LEU
1	A	82	LYS
1	A	110	LEU
1	A	153	ILE
1	A	180	LEU
1	A	182	SER
1	A	202	ARG
1	A	211	LEU
1	A	212	ARG
1	A	216	GLN
1	A	218	ILE
1	A	252	LEU
1	A	268	SER
1	A	376	ASP
1	A	390	LYS
1	A	396	GLU
1	A	399	SER
1	A	411	LEU
1	A	419	SER
1	A	432	LEU
1	A	448	VAL
1	A	485	THR
1	A	493	THR
1	A	494	SER
1	A	511	LEU
1	A	517	GLN
1	A	526	SER
1	A	557	LEU
1	A	579	VAL
1	A	588	THR
1	A	606	LEU
1	A	616	LEU
1	A	654	TRP
1	A	672	LEU
1	A	700	SER
1	A	716	THR
1	A	725	LYS
1	A	735	THR
1	A	739	GLU
1	B	9	ASN
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	104	THR
1	B	110	LEU
1	B	145	LEU
1	B	167	THR
1	B	173	LYS
1	B	180	LEU
1	B	211	LEU
1	B	212	ARG
1	B	216	GLN
1	B	218	ILE
1	B	222	ARG
1	B	223	MSE
1	B	228	GLN
1	B	243	GLU
1	B	252	LEU
1	B	268	SER
1	B	328	GLU
1	B	376	ASP
1	B	386	VAL
1	B	396	GLU
1	B	404	GLN
1	B	411	LEU
1	B	420	VAL
1	B	424	LEU
1	B	439	THR
1	B	446	GLN
1	B	448	VAL
1	B	485	THR
1	B	491	ARG
1	B	500	LEU
1	B	505	ILE
1	B	511	LEU
1	B	557	LEU
1	B	579	VAL
1	B	588	THR
1	B	606	LEU
1	B	616	LEU
1	B	621	LYS
1	B	692	ARG
1	B	716	THR
1	B	737	ILE
1	C	19	THR

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Mol	Chain	Res	Type
1	C	47	GLN
1	C	61	LEU
1	C	82	LYS
1	C	110	LEU
1	C	145	LEU
1	C	153	ILE
1	C	167	THR
1	C	180	LEU
1	C	194	ILE
1	C	197	SER
1	C	202	ARG
1	C	211	LEU
1	C	216	GLN
1	C	223	MSE
1	C	228	GLN
1	C	252	LEU
1	C	255	SER
1	C	268	SER
1	C	285	LEU
1	C	328	GLU
1	C	330	ARG
1	C	334	ILE
1	C	353	VAL
1	C	396	GLU
1	C	418	VAL
1	C	424	LEU
1	C	427	GLN
1	C	428	HIS
1	C	430	ASP
1	C	432	LEU
1	C	441	THR
1	C	448	VAL
1	C	463	LEU
1	C	500	LEU
1	C	505	ILE
1	C	511	LEU
1	C	529	SER
1	C	557	LEU
1	C	579	VAL
1	C	582	ASP
1	C	584	MSE
1	C	614	THR

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Mol	Chain	Res	Type
1	C	616	LEU
1	C	618	GLN
1	C	650	ASN
1	C	654	TRP
1	C	663	GLN
1	C	672	LEU
1	C	700	SER
1	C	731	LEU
1	C	737	ILE
1	D	61	LEU
1	D	64	GLU
1	D	65	ASN
1	D	110	LEU
1	D	112	THR
1	D	145	LEU
1	D	153	ILE
1	D	180	LEU
1	D	202	ARG
1	D	211	LEU
1	D	212	ARG
1	D	216	GLN
1	D	218	ILE
1	D	252	LEU
1	D	262	ILE
1	D	268	SER
1	D	272	ILE
1	D	314	SER
1	D	330	ARG
1	D	354	ASN
1	D	376	ASP
1	D	379	THR
1	D	381	LEU
1	D	386	VAL
1	D	390	LYS
1	D	396	GLU
1	D	424	LEU
1	D	432	LEU
1	D	441	THR
1	D	448	VAL
1	D	485	THR
1	D	500	LEU
1	D	505	ILE

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Mol	Chain	Res	Type
1	D	511	LEU
1	D	526	SER
1	D	557	LEU
1	D	579	VAL
1	D	588	THR
1	D	606	LEU
1	D	616	LEU
1	D	630	ARG
1	D	654	TRP
1	D	672	LEU
1	D	685	LYS
1	D	701	THR
1	D	725	LYS
1	D	737	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	13	HIS
1	A	41	HIS
1	A	48	ASN
1	A	52	GLN
1	A	67	ASN
1	A	69	GLN
1	A	132	GLN
1	A	139	ASN
1	A	216	GLN
1	A	228	GLN
1	A	230	ASN
1	A	244	GLN
1	A	277	ASN
1	A	307	GLN
1	A	310	GLN
1	A	354	ASN
1	A	355	GLN
1	A	400	GLN
1	A	403	HIS
1	A	445	HIS
1	A	502	HIS
1	A	517	GLN
1	A	583	GLN

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Mol	Chain	Res	Type
1	A	618	GLN
1	A	650	ASN
1	A	655	GLN
1	A	663	GLN
1	A	670	GLN
1	A	730	GLN
1	A	741	HIS
1	B	6	ASN
1	B	9	ASN
1	B	13	HIS
1	B	15	GLN
1	B	33	GLN
1	B	48	ASN
1	B	52	GLN
1	B	62	ASN
1	B	65	ASN
1	B	67	ASN
1	B	69	GLN
1	B	87	GLN
1	B	119	ASN
1	B	132	GLN
1	B	150	ASN
1	B	209	HIS
1	B	216	GLN
1	B	228	GLN
1	B	230	ASN
1	B	239	GLN
1	B	244	GLN
1	B	277	ASN
1	B	288	GLN
1	B	307	GLN
1	B	310	GLN
1	B	327	HIS
1	B	354	ASN
1	B	400	GLN
1	B	404	GLN
1	B	427	GLN
1	B	445	HIS
1	B	502	HIS
1	B	583	GLN
1	B	618	GLN
1	B	650	ASN

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Mol	Chain	Res	Type
1	B	655	GLN
1	C	6	ASN
1	C	13	HIS
1	C	24	GLN
1	C	48	ASN
1	C	67	ASN
1	C	69	GLN
1	C	132	GLN
1	C	177	ASN
1	C	209	HIS
1	C	216	GLN
1	C	227	HIS
1	C	228	GLN
1	C	230	ASN
1	C	239	GLN
1	C	244	GLN
1	C	277	ASN
1	C	307	GLN
1	C	310	GLN
1	C	318	GLN
1	C	354	ASN
1	C	373	HIS
1	C	400	GLN
1	C	403	HIS
1	C	405	GLN
1	C	445	HIS
1	C	446	GLN
1	C	481	ASN
1	C	502	HIS
1	C	521	ASN
1	C	583	GLN
1	C	618	GLN
1	C	650	ASN
1	C	655	GLN
1	C	663	GLN
1	C	730	GLN
1	D	6	ASN
1	D	13	HIS
1	D	15	GLN
1	D	24	GLN
1	D	48	ASN
1	D	52	GLN

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Mol	Chain	Res	Type
1	D	67	ASN
1	D	69	GLN
1	D	87	GLN
1	D	91	GLN
1	D	132	GLN
1	D	150	ASN
1	D	190	ASN
1	D	209	HIS
1	D	216	GLN
1	D	228	GLN
1	D	230	ASN
1	D	239	GLN
1	D	277	ASN
1	D	288	GLN
1	D	310	GLN
1	D	318	GLN
1	D	354	ASN
1	D	400	GLN
1	D	403	HIS
1	D	404	GLN
1	D	445	HIS
1	D	446	GLN
1	D	481	ASN
1	D	502	HIS
1	D	583	GLN
1	D	618	GLN
1	D	650	ASN
1	D	655	GLN
1	D	670	GLN
1	D	694	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	718/745 (96%)	-0.48	0 100 100	24, 38, 84, 103	0
1	B	712/745 (95%)	-0.67	0 100 100	23, 35, 49, 80	0
1	C	713/745 (95%)	-0.26	8 (1%) 78 76	25, 44, 97, 104	0
1	D	719/745 (96%)	-0.50	3 (0%) 88 87	25, 39, 67, 94	0
All	All	2862/2980 (96%)	-0.48	11 (0%) 88 87	23, 38, 81, 104	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	VAL	3.5
1	C	738	LEU	2.7
1	C	384	TRP	2.5
1	D	423	ASP	2.5
1	C	382	GLY	2.4
1	C	385	PHE	2.4
1	C	342	PHE	2.3
1	C	347	ALA	2.2
1	D	349	LEU	2.1
1	C	377	ASP	2.1
1	D	376	ASP	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.