



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:29 PM UTC

PDB ID : 1JLH / pdb_00001jlh
Title : Human Glucose-6-phosphate Isomerase
Authors : Cordeiro, A.T.
Deposited on : 2001-07-16
Resolution : 2.10 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

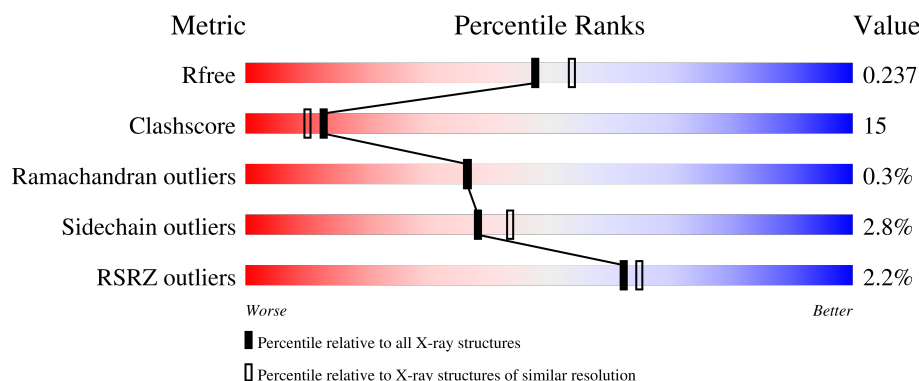
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	558	72% 25% .
1	B	558	69% 27% .
1	C	558	4% 67% 29% ..
1	D	558	3% 73% 23% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19037 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 phosphoglucose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4437	2826	781	812	18			
1	B	556	Total	C	N	O	S	0	0	0
			4437	2826	781	812	18			
1	C	556	Total	C	N	O	S	0	0	0
			4437	2826	781	812	18			
1	D	556	Total	C	N	O	S	0	0	0
			4437	2826	781	812	18			

There are 4 discrepancies between the modelled and reference sequences:

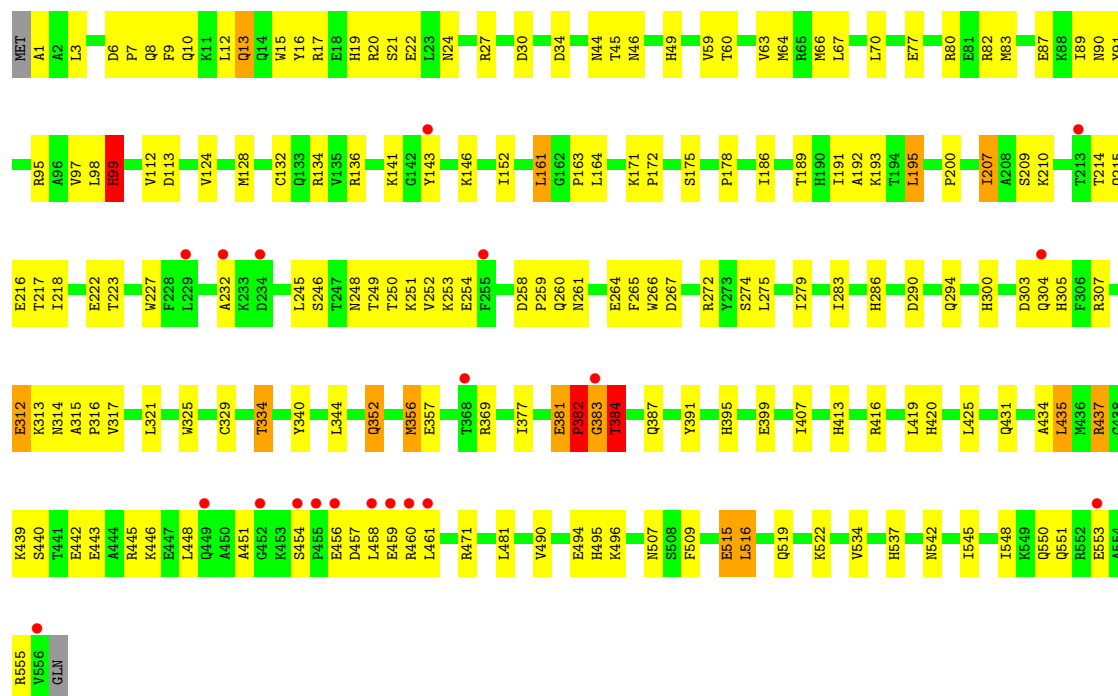
Chain	Residue	Modelled	Actual	Comment	Reference
A	399	GLU	LYS	see remark 999	UNP P06744
B	399	GLU	LYS	see remark 999	UNP P06744
C	399	GLU	LYS	see remark 999	UNP P06744
D	399	GLU	LYS	see remark 999	UNP P06744

- Molecule 2 is water.

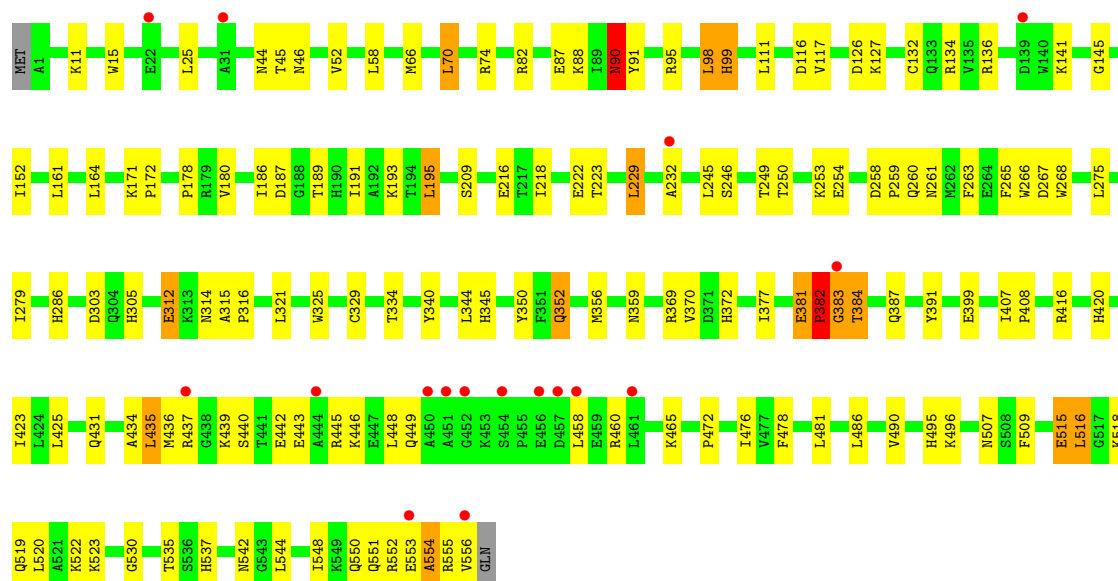
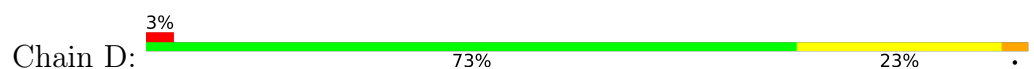
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	350	Total	O	0	0
			350	350		
2	B	352	Total	O	0	0
			352	352		
2	C	275	Total	O	0	0
			275	275		
2	D	312	Total	O	0	0
			312	312		



- Molecule 1: phosphoglucose isomerase



- Molecule 1: phosphoglucose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.75Å 108.02Å 271.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.21 – 2.10 22.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (22.21-2.10) 99.6 (22.21-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.09Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.237 0.197 , 0.237	Depositor DCC
R_{free} test set	6914 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19037	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3155e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.41	1/4545 (0.0%)	0.91	16/6155 (0.3%)
1	B	0.58	3/4545 (0.1%)	0.95	22/6155 (0.4%)
1	C	0.46	2/4545 (0.0%)	0.90	21/6155 (0.3%)
1	D	0.85	1/4545 (0.0%)	0.92	14/6155 (0.2%)
All	All	0.60	7/18180 (0.0%)	0.92	73/24620 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	382	PRO	C-O	50.99	1.79	1.23
1	B	382	PRO	CA-C	24.42	1.84	1.52
1	C	382	PRO	CA-C	13.64	1.70	1.52
1	B	382	PRO	C-O	11.21	1.36	1.23
1	C	382	PRO	C-O	10.95	1.35	1.23
1	A	384	THR	CA-CB	5.84	1.63	1.53
1	B	384	THR	CA-CB	5.57	1.62	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	PRO	O-C-N	14.04	140.33	123.06
1	C	383	GLY	CA-C-N	10.44	141.47	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	GLY	C-N-CA	10.44	141.47	121.54
1	B	383	GLY	CA-C-N	10.08	140.79	121.54
1	B	383	GLY	C-N-CA	10.08	140.79	121.54
1	A	383	GLY	CA-C-N	9.92	140.48	121.54
1	A	383	GLY	C-N-CA	9.92	140.48	121.54
1	D	383	GLY	CA-C-N	9.60	139.88	121.54
1	D	383	GLY	C-N-CA	9.60	139.88	121.54
1	D	91	TYR	N-CA-C	8.27	120.29	111.28
1	B	98	LEU	N-CA-C	8.20	121.38	110.88
1	C	384	THR	N-CA-CB	7.98	123.98	110.49
1	A	352	GLN	N-CA-C	-7.80	102.86	111.36
1	C	352	GLN	N-CA-C	-7.59	103.08	111.36
1	B	515	GLU	N-CA-C	7.57	119.61	111.36
1	D	384	THR	N-CA-CB	7.53	123.21	110.49
1	D	98	LEU	N-CA-C	7.42	119.34	110.44
1	A	384	THR	N-CA-CB	7.26	122.75	110.49
1	A	91	TYR	N-CA-C	7.25	120.05	111.71
1	D	515	GLU	N-CA-C	7.25	118.83	111.07
1	B	471	ARG	CA-C-N	7.20	126.96	119.76
1	B	471	ARG	C-N-CA	7.20	126.96	119.76
1	D	352	GLN	N-CA-C	-7.06	103.59	111.28
1	A	515	GLU	N-CA-C	6.99	118.90	111.28
1	A	98	LEU	N-CA-C	6.91	118.74	110.44
1	C	98	LEU	N-CA-C	6.88	118.70	110.44
1	C	382	PRO	CA-C-O	-6.82	113.13	121.31
1	B	91	TYR	N-CA-C	6.60	119.31	111.71
1	C	91	TYR	N-CA-C	6.60	118.47	111.28
1	C	356	MET	N-CA-C	6.59	118.46	111.28
1	B	352	GLN	N-CA-C	-6.58	104.14	111.71
1	C	471	ARG	CA-C-N	6.55	126.31	119.76
1	C	471	ARG	C-N-CA	6.55	126.31	119.76
1	B	384	THR	N-CA-CB	6.53	121.53	110.49
1	B	437	ARG	N-CA-C	6.49	118.15	111.14
1	B	356	MET	N-CA-C	6.41	118.26	111.28
1	A	471	ARG	CA-C-N	6.40	126.16	119.76
1	A	471	ARG	C-N-CA	6.40	126.16	119.76
1	A	274	SER	N-CA-C	6.35	121.19	113.38
1	A	509	PHE	N-CA-C	6.22	121.71	112.94
1	C	437	ARG	N-CA-C	6.17	118.09	111.36
1	D	496	LYS	N-CA-C	-6.04	104.61	111.07
1	C	381	GLU	CA-C-N	5.96	125.72	119.76
1	C	381	GLU	C-N-CA	5.96	125.72	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	LYS	N-CA-C	-5.90	104.76	111.07
1	A	359	ASN	N-CA-C	5.86	120.13	112.92
1	B	509	PHE	N-CA-C	5.84	121.12	113.30
1	B	383	GLY	O-C-N	5.83	130.28	122.70
1	C	509	PHE	N-CA-C	5.82	121.14	112.94
1	B	359	ASN	N-CA-C	5.73	119.97	112.92
1	B	264	GLU	N-CA-C	5.68	119.22	110.42
1	A	437	ARG	N-CA-C	5.57	117.16	111.14
1	C	161	LEU	N-CA-C	5.48	117.69	111.11
1	D	359	ASN	N-CA-C	5.47	119.94	112.88
1	C	266	TRP	N-CA-C	5.46	118.17	109.81
1	B	538	ASP	N-CA-C	-5.45	103.29	110.43
1	C	334	THR	N-CA-C	5.43	118.12	109.81
1	D	509	PHE	N-CA-C	5.40	120.55	112.94
1	A	161	LEU	N-CA-C	5.39	117.58	111.11
1	B	311	LEU	N-CA-C	5.37	117.83	111.33
1	D	381	GLU	CA-C-N	5.36	125.12	119.76
1	D	381	GLU	C-N-CA	5.36	125.12	119.76
1	B	90	ASN	N-CA-C	-5.34	99.27	108.56
1	A	99	HIS	N-CA-C	-5.30	106.07	112.54
1	D	90	ASN	N-CA-C	-5.27	99.39	108.56
1	C	515	GLU	N-CA-C	5.24	117.79	111.40
1	B	496	LYS	N-CA-C	-5.17	105.65	111.28
1	C	383	GLY	O-C-N	5.16	129.41	122.70
1	C	496	LYS	N-CA-C	-5.11	105.60	111.07
1	D	266	TRP	N-CA-C	5.08	117.59	109.81
1	C	99	HIS	N-CA-C	-5.02	106.42	112.54
1	B	462	LEU	N-CA-C	5.01	120.89	109.81
1	B	334	THR	N-CA-C	5.00	117.47	109.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	382	PRO	Mainchain
1	C	382	PRO	Mainchain
1	D	382	PRO	Mainchain

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	4437	0	4388	140	0
1	B	4437	0	4388	147	0
1	C	4437	0	4388	160	0
1	D	4437	0	4388	118	0
2	A	350	0	0	13	0
2	B	352	0	0	20	0
2	C	275	0	0	20	0
2	D	312	0	0	13	0
All	All	19037	0	17552	533	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 15.

All (533) 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:B:382:PRO:C	1:B:382:PRO:CA	1.84	1.48
1:D:382:PRO:O	1:D:382:PRO:C	1.79	1.24
1:C:304:GLN:HG3	2:C:558:HOH:O	1.45	1.14
1:B:304:GLN:HG3	2:B:558:HOH:O	1.53	1.05
1:A:550:GLN:HE21	1:A:551:GLN:HE21	1.04	0.97
1:C:134:ARG:HD2	2:C:803:HOH:O	1.67	0.94
1:B:382:PRO:CA	1:B:383:GLY:N	2.37	0.87
1:A:537:HIS:H	1:A:542:ASN:HD21	1.20	0.87
1:B:537:HIS:H	1:B:542:ASN:HD21	1.23	0.86
1:D:340:TYR:HA	1:D:383:GLY:HA3	1.58	0.85
1:C:305:HIS:HE1	1:C:315:ALA:H	1.25	0.85
1:C:442:GLU:HG2	1:C:446:LYS:HE2	1.60	0.84
1:B:340:TYR:HA	1:B:383:GLY:HA3	1.58	0.84
1:B:11:LYS:HE2	2:B:612:HOH:O	1.75	0.84
1:A:59:VAL:HG21	1:A:64:MET:SD	2.17	0.84
1:C:340:TYR:HA	1:C:383:GLY:HA3	1.59	0.83
1:D:253:LYS:HG2	1:D:259:PRO:HG3	1.61	0.83
1:C:439:LYS:NZ	1:D:519:GLN:HE22	1.78	0.81
1:D:209:SER:O	1:D:246:SER:HB3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:GLN:HE21	1:D:551:GLN:HE21	1.26	0.80
1:A:519:GLN:HE22	1:B:439:LYS:NZ	1.80	0.78
1:D:537:HIS:H	1:D:542:ASN:HD21	1.31	0.77
1:D:370:VAL:HG12	1:D:372:HIS:H	1.48	0.76
1:C:90:ASN:ND2	1:C:507:ASN:HD21	1.83	0.76
1:C:59:VAL:HG21	1:C:64:MET:SD	2.25	0.76
1:D:250:THR:O	1:D:254:GLU:HG3	1.86	0.76
1:A:439:LYS:NZ	1:B:519:GLN:HE22	1.84	0.75
1:C:132:CYS:O	1:C:136:ARG:HG3	1.86	0.75
1:C:321:LEU:HG	2:C:639:HOH:O	1.85	0.75
1:C:550:GLN:HE21	1:C:551:GLN:HE21	1.34	0.75
1:B:317:VAL:O	1:B:321:LEU:HD13	1.86	0.75
1:A:272:ARG:HH12	1:A:511:GLN:HE21	1.35	0.75
1:B:132:CYS:O	1:B:136:ARG:HG3	1.87	0.74
1:C:264:GLU:HG2	2:C:564:HOH:O	1.86	0.74
1:B:59:VAL:HG21	1:B:64:MET:SD	2.27	0.74
1:A:59:VAL:HG23	1:A:63:VAL:HB	1.71	0.72
1:A:305:HIS:HE1	1:A:315:ALA:H	1.38	0.71
1:A:90:ASN:ND2	1:A:507:ASN:HD21	1.88	0.71
1:C:209:SER:O	1:C:246:SER:HB3	1.91	0.70
1:C:59:VAL:HG23	1:C:63:VAL:HB	1.71	0.70
1:A:272:ARG:HH12	1:A:511:GLN:NE2	1.89	0.70
1:D:553:GLU:O	1:D:555:ARG:HD2	1.91	0.70
1:B:305:HIS:HE1	1:B:315:ALA:H	1.38	0.70
1:B:315:ALA:HB3	1:B:316:PRO:HD3	1.74	0.70
1:C:537:HIS:H	1:C:542:ASN:HD21	1.38	0.70
1:B:59:VAL:HG23	1:B:63:VAL:HB	1.74	0.69
1:B:550:GLN:HE21	1:B:551:GLN:HE21	1.40	0.69
1:C:317:VAL:O	1:C:321:LEU:HD13	1.92	0.69
1:A:387:GLN:HA	1:A:391:TYR:CD1	2.28	0.69
1:A:85:ASN:HB3	2:A:703:HOH:O	1.92	0.69
1:B:300:HIS:O	1:B:304:GLN:HG2	1.93	0.69
1:A:515:GLU:O	1:A:519:GLN:HG3	1.93	0.68
1:B:90:ASN:ND2	1:B:507:ASN:HD21	1.90	0.68
1:D:90:ASN:ND2	1:D:507:ASN:HD21	1.92	0.68
1:A:445:ARG:O	1:A:449:GLN:HG3	1.93	0.68
1:D:305:HIS:HE1	1:D:315:ALA:H	1.39	0.68
1:A:314:ASN:OD1	1:A:316:PRO:HD2	1.93	0.67
1:C:272:ARG:NH1	1:C:357:GLU:HG2	2.09	0.67
1:A:12:LEU:HD11	1:A:67:LEU:HD23	1.77	0.67
1:C:515:GLU:O	1:C:519:GLN:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:GLN:HA	1:C:391:TYR:CD1	2.30	0.66
1:A:25:LEU:HB3	1:A:436:MET:HG3	1.77	0.66
1:A:409:VAL:HG22	1:B:548:ILE:HD13	1.76	0.66
1:C:459:GLU:HB2	1:C:460:ARG:NH1	2.11	0.66
1:D:25:LEU:HB3	1:D:436:MET:HG3	1.77	0.66
1:D:387:GLN:HA	1:D:391:TYR:CD1	2.30	0.66
1:A:209:SER:O	1:A:246:SER:HB3	1.97	0.65
1:A:434:ALA:HB1	1:B:516:LEU:HD13	1.77	0.65
1:B:218:ILE:O	1:B:222:GLU:HG3	1.95	0.65
1:B:522:LYS:HE2	1:B:522:LYS:HA	1.79	0.64
1:D:186:ILE:HD13	1:D:216:GLU:HA	1.79	0.64
1:A:340:TYR:HA	1:A:383:GLY:HA3	1.80	0.64
1:A:522:LYS:HG2	2:A:640:HOH:O	1.96	0.64
1:C:186:ILE:HD13	1:C:216:GLU:HA	1.78	0.64
1:D:522:LYS:HE2	1:D:522:LYS:HA	1.77	0.64
1:A:191:ILE:HG13	1:A:195:LEU:HD22	1.79	0.63
1:C:548:ILE:HD13	1:D:425:LEU:HD22	1.80	0.63
1:A:132:CYS:O	1:A:136:ARG:HG3	1.99	0.63
1:C:352:GLN:O	1:C:356:MET:HB2	1.98	0.63
1:C:407:ILE:HD13	1:C:425:LEU:HD23	1.81	0.63
1:D:249:THR:HG22	1:D:253:LYS:HE3	1.79	0.63
1:B:522:LYS:HG2	2:B:903:HOH:O	1.96	0.63
1:C:439:LYS:HZ1	1:D:519:GLN:HE22	1.46	0.63
1:B:248:ASN:O	1:B:252:VAL:HG23	1.99	0.62
1:D:258:ASP:OD1	1:D:260:GLN:HG2	1.99	0.62
1:B:314:ASN:OD1	1:B:316:PRO:HD2	1.97	0.62
1:C:314:ASN:OD1	1:C:316:PRO:HD2	1.99	0.62
1:A:552:ARG:HB2	2:A:664:HOH:O	1.99	0.62
1:D:436:MET:HE3	1:D:437:ARG:HG3	1.81	0.62
1:A:15:TRP:CG	1:A:66:MET:HE1	2.34	0.62
1:A:218:ILE:O	1:A:222:GLU:HG3	1.99	0.62
1:A:439:LYS:HZ3	1:B:519:GLN:HE22	1.46	0.62
1:C:90:ASN:HD22	1:C:507:ASN:HD21	1.46	0.62
1:B:250:THR:O	1:B:254:GLU:HG3	2.00	0.62
1:C:519:GLN:HE22	1:D:439:LYS:NZ	1.96	0.62
1:D:15:TRP:CG	1:D:66:MET:HE1	2.33	0.62
1:B:387:GLN:HA	1:B:391:TYR:CD1	2.34	0.62
1:A:456:GLU:O	1:A:460:ARG:HG2	2.00	0.62
1:C:305:HIS:HD2	2:C:560:HOH:O	1.83	0.62
1:B:161:LEU:HD12	1:B:350:TYR:HA	1.82	0.61
1:C:19:HIS:O	1:C:22:GLU:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:HG12	1:C:128:MET:HE2	1.82	0.61
1:B:61:GLU:HG2	2:B:757:HOH:O	2.00	0.61
1:A:550:GLN:HE21	1:A:551:GLN:NE2	1.87	0.61
1:D:431:GLN:O	1:D:435:LEU:HD22	2.00	0.61
1:A:519:GLN:HE22	1:B:439:LYS:HZ1	1.48	0.60
1:C:45:THR:O	1:C:46:ASN:HB2	2.00	0.60
1:D:132:CYS:O	1:D:136:ARG:HG3	2.01	0.60
1:C:315:ALA:HB3	1:C:316:PRO:HD3	1.83	0.60
1:D:134:ARG:HD2	2:D:575:HOH:O	2.01	0.60
1:A:19:HIS:O	1:A:22:GLU:HB3	2.02	0.60
1:D:315:ALA:HB3	1:D:316:PRO:HD3	1.84	0.60
1:A:258:ASP:OD1	1:A:260:GLN:HG2	2.01	0.60
1:C:178:PRO:O	1:C:286:HIS:HD2	1.84	0.60
1:A:95:ARG:HD2	1:A:267:ASP:OD2	2.01	0.60
1:C:522:LYS:HA	1:C:522:LYS:HE2	1.82	0.60
1:C:249:THR:HG22	1:C:253:LYS:HE2	1.83	0.60
1:A:44:ASN:ND2	1:A:46:ASN:H	2.00	0.60
1:B:191:ILE:HG13	1:B:195:LEU:HD22	1.84	0.59
1:B:407:ILE:HD13	1:B:425:LEU:HD23	1.84	0.59
1:C:434:ALA:HB1	1:D:516:LEU:HD13	1.82	0.59
1:D:45:THR:O	1:D:46:ASN:HB2	2.00	0.59
1:B:352:GLN:O	1:B:356:MET:HB2	2.02	0.59
1:D:275:LEU:C	1:D:275:LEU:HD12	2.27	0.59
1:B:370:VAL:HG12	1:B:372:HIS:H	1.68	0.59
1:A:59:VAL:HG23	1:A:63:VAL:CG1	2.33	0.59
1:A:223:THR:OG1	1:B:420:HIS:HE1	1.86	0.59
1:D:556:VAL:HG12	1:D:556:VAL:O	2.02	0.59
1:B:109:PRO:HG2	2:B:614:HOH:O	2.03	0.59
1:B:544:LEU:O	1:B:548:ILE:HG12	2.02	0.59
1:C:59:VAL:HG23	1:C:63:VAL:CG1	2.33	0.59
1:D:191:ILE:HG13	1:D:195:LEU:HD22	1.85	0.59
1:D:522:LYS:HG2	2:D:637:HOH:O	2.03	0.58
1:A:442:GLU:HG3	2:A:907:HOH:O	2.02	0.58
1:D:258:ASP:CG	1:D:260:GLN:HG2	2.28	0.58
1:C:83:MET:HE2	1:C:97:VAL:CG1	2.33	0.58
1:C:12:LEU:HD11	1:C:67:LEU:HD23	1.86	0.58
1:B:59:VAL:HG23	1:B:63:VAL:CG1	2.34	0.58
1:C:253:LYS:HG2	1:C:259:PRO:HG3	1.85	0.58
1:A:230:GLN:O	1:A:233:LYS:HE3	2.03	0.58
1:A:519:GLN:HE22	1:B:439:LYS:HZ3	1.50	0.58
2:A:561:HOH:O	1:B:49:HIS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:HIS:HE1	1:B:223:THR:OG1	1.87	0.57
1:B:461:LEU:HG	1:B:465:LYS:HD2	1.85	0.57
1:C:16:TYR:O	1:C:20:ARG:HB2	2.04	0.57
1:A:164:LEU:C	1:A:164:LEU:HD23	2.29	0.57
1:B:442:GLU:HG2	1:B:446:LYS:HE2	1.87	0.57
1:D:265:PHE:CE2	1:D:279:ILE:HD11	2.40	0.57
1:C:305:HIS:CE1	1:C:315:ALA:H	2.15	0.57
1:D:440:SER:OG	1:D:443:GLU:HG3	2.05	0.57
1:A:45:THR:O	1:A:46:ASN:HB2	2.03	0.57
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.87	0.57
2:A:566:HOH:O	1:B:49:HIS:HE1	1.87	0.57
1:A:440:SER:OG	1:A:443:GLU:HG3	2.05	0.56
1:D:90:ASN:C	1:D:90:ASN:HD22	2.13	0.56
1:B:258:ASP:HB3	1:B:261:ASN:ND2	2.19	0.56
1:C:395:HIS:HD2	2:C:820:HOH:O	1.87	0.56
1:A:387:GLN:HA	1:A:391:TYR:CG	2.40	0.56
1:A:553:GLU:O	1:A:555:ARG:HD2	2.05	0.56
1:B:45:THR:O	1:B:46:ASN:HB2	2.05	0.56
1:C:439:LYS:HZ3	1:D:519:GLN:HE22	1.51	0.56
1:C:420:HIS:HE1	1:D:223:THR:OG1	1.87	0.56
1:D:442:GLU:HG2	1:D:446:LYS:HE2	1.87	0.56
1:A:456:GLU:HG3	1:A:460:ARG:NH2	2.20	0.56
1:C:59:VAL:HG23	1:C:63:VAL:CB	2.35	0.56
1:C:152:ILE:HD12	1:C:152:ILE:N	2.21	0.56
1:B:59:VAL:CG2	1:B:63:VAL:HB	2.35	0.56
1:B:264:GLU:HG2	2:B:833:HOH:O	2.05	0.56
1:B:251:LYS:HD3	1:B:254:GLU:OE1	2.06	0.56
1:D:442:GLU:O	1:D:446:LYS:HG3	2.06	0.56
1:C:193:LYS:HE2	2:D:739:HOH:O	2.06	0.55
1:B:210:LYS:O	1:B:246:SER:HB2	2.06	0.55
1:B:395:HIS:HD2	2:B:791:HOH:O	1.88	0.55
1:D:515:GLU:O	1:D:519:GLN:HG3	2.05	0.55
1:A:152:ILE:HD12	1:A:152:ILE:N	2.20	0.55
1:C:395:HIS:NE2	1:C:435:LEU:HD13	2.22	0.55
1:A:13:GLN:HG2	1:A:17:ARG:NH1	2.22	0.55
1:A:90:ASN:HD22	1:A:507:ASN:HD21	1.52	0.55
1:B:59:VAL:HG23	1:B:63:VAL:CB	2.36	0.55
1:B:258:ASP:CG	1:B:260:GLN:HG2	2.31	0.55
1:C:83:MET:HE2	1:C:97:VAL:HG12	1.89	0.55
1:B:518:LYS:HE2	2:B:764:HOH:O	2.07	0.55
1:C:13:GLN:HG2	1:C:17:ARG:HH12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HG2	1:A:369:ARG:HH11	1.72	0.55
1:B:164:LEU:C	1:B:164:LEU:HD13	2.32	0.55
1:B:258:ASP:HB3	1:B:261:ASN:HD22	1.72	0.55
1:C:248:ASN:O	1:C:252:VAL:HG23	2.07	0.55
1:A:538:ASP:CG	1:B:436:MET:HE1	2.32	0.55
1:C:440:SER:OG	1:C:443:GLU:HG3	2.07	0.55
1:B:209:SER:O	1:B:246:SER:CB	2.55	0.54
1:D:314:ASN:OD1	1:D:316:PRO:HD2	2.07	0.54
1:A:59:VAL:CG2	1:A:63:VAL:HB	2.36	0.54
1:B:83:MET:HE2	1:B:97:VAL:HG11	1.89	0.54
1:B:99:HIS:HD2	2:B:752:HOH:O	1.90	0.54
1:B:228:PHE:HD2	1:B:229:LEU:HD12	1.72	0.54
1:C:15:TRP:CG	1:C:66:MET:HE1	2.43	0.54
1:C:413:HIS:HD2	1:D:189:THR:HG22	1.73	0.54
1:C:124:VAL:HG12	1:C:128:MET:CE	2.37	0.54
1:C:210:LYS:HD3	1:C:265:PHE:CE1	2.43	0.54
1:C:442:GLU:O	1:C:446:LYS:HG3	2.08	0.54
1:A:59:VAL:HG23	1:A:63:VAL:CB	2.36	0.54
1:A:409:VAL:HG22	1:B:548:ILE:CD1	2.38	0.54
1:B:15:TRP:CG	1:B:66:MET:HE1	2.42	0.54
1:C:146:LYS:HB2	2:C:618:HOH:O	2.08	0.54
1:A:534:VAL:HG21	1:A:545:ILE:HG21	1.89	0.54
1:D:352:GLN:O	1:D:356:MET:HB2	2.08	0.54
1:A:458:LEU:C	1:A:458:LEU:HD23	2.33	0.54
1:A:525:GLU:O	1:B:422:LYS:HE3	2.06	0.54
1:B:90:ASN:HD22	1:B:507:ASN:HD21	1.56	0.54
1:C:44:ASN:ND2	1:C:46:ASN:H	2.05	0.54
1:D:535:THR:HG22	2:D:686:HOH:O	2.08	0.54
1:C:312:GLU:CD	1:C:312:GLU:H	2.16	0.54
1:A:516:LEU:HD13	1:B:434:ALA:HB1	1.90	0.54
1:B:275:LEU:HD12	1:B:275:LEU:C	2.32	0.54
1:D:189:THR:HG21	2:D:690:HOH:O	2.08	0.54
1:A:522:LYS:HA	1:A:522:LYS:HE2	1.89	0.53
1:B:225:LYS:O	1:B:229:LEU:HD13	2.08	0.53
1:C:191:ILE:HG13	1:C:195:LEU:HD22	1.89	0.53
1:B:14:GLN:O	1:B:18:GLU:HG3	2.07	0.53
1:C:59:VAL:CG2	1:C:63:VAL:HB	2.37	0.53
1:C:210:LYS:O	1:C:246:SER:HB2	2.07	0.53
1:A:91:TYR:CE2	1:A:365:LYS:HA	2.43	0.53
1:C:209:SER:O	1:C:246:SER:CB	2.56	0.53
1:A:90:ASN:HD22	1:A:90:ASN:C	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASP:OD1	1:A:495:HIS:HE1	1.92	0.53
1:B:175:SER:HB3	2:B:638:HOH:O	2.08	0.53
1:B:312:GLU:CD	1:B:312:GLU:H	2.15	0.53
1:D:265:PHE:CZ	1:D:279:ILE:HD11	2.44	0.53
1:A:253:LYS:NZ	1:A:259:PRO:HG2	2.24	0.53
1:C:258:ASP:HB3	1:C:261:ASN:HD22	1.74	0.53
1:C:381:GLU:HG3	1:C:382:PRO:HD2	1.90	0.53
1:A:13:GLN:HG2	1:A:17:ARG:HH12	1.72	0.53
1:B:44:ASN:ND2	1:B:46:ASN:H	2.06	0.53
1:C:49:HIS:HE1	2:D:574:HOH:O	1.91	0.53
1:D:44:ASN:ND2	1:D:46:ASN:H	2.07	0.53
1:A:209:SER:O	1:A:246:SER:CB	2.57	0.52
1:D:58:LEU:CD2	1:D:472:PRO:HB3	2.39	0.52
1:C:245:LEU:HD13	1:C:279:ILE:HA	1.91	0.52
1:C:200:PRO:HG3	1:C:227:TRP:CZ2	2.45	0.52
1:B:98:LEU:HB2	1:B:268:TRP:CE3	2.45	0.52
1:B:189:THR:HG21	2:B:571:HOH:O	2.09	0.52
1:A:210:LYS:HD3	1:A:265:PHE:CE1	2.45	0.52
1:A:537:HIS:N	1:A:542:ASN:HD21	2.00	0.52
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.75	0.52
1:A:550:GLN:NE2	1:A:551:GLN:HE21	1.88	0.52
1:A:264:GLU:HG2	2:A:620:HOH:O	2.10	0.51
1:A:352:GLN:O	1:A:356:MET:HB2	2.11	0.51
1:B:258:ASP:OD1	1:B:260:GLN:HG2	2.09	0.51
1:B:294:GLN:HG3	2:B:650:HOH:O	2.10	0.51
1:B:229:LEU:HD11	1:B:238:VAL:CG2	2.40	0.51
1:A:395:HIS:HE1	1:A:431:GLN:OE1	1.93	0.51
1:B:186:ILE:HD13	1:B:216:GLU:HA	1.93	0.51
1:C:77:GLU:HG3	2:C:731:HOH:O	2.10	0.51
1:C:143:TYR:CZ	1:C:232:ALA:HB2	2.46	0.51
1:C:294:GLN:HE21	1:C:294:GLN:HA	1.76	0.51
1:D:325:TRP:O	1:D:329:CYS:HB2	2.10	0.51
1:C:294:GLN:HA	1:C:294:GLN:NE2	2.25	0.51
1:D:381:GLU:HG3	1:D:382:PRO:HD2	1.91	0.51
1:A:449:GLN:HG2	1:A:458:LEU:HD11	1.92	0.51
1:D:164:LEU:C	1:D:164:LEU:HD23	2.36	0.51
1:A:25:LEU:CB	1:A:436:MET:HG3	2.40	0.51
1:B:141:LYS:HD3	1:B:145:GLY:O	2.11	0.51
1:D:218:ILE:O	1:D:222:GLU:HG3	2.11	0.51
1:B:134:ARG:NH2	2:B:809:HOH:O	2.44	0.50
1:B:395:HIS:HE1	1:B:431:GLN:OE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:THR:O	1:C:254:GLU:HG3	2.11	0.50
1:C:253:LYS:NZ	1:C:259:PRO:HG2	2.24	0.50
1:A:434:ALA:CB	1:B:516:LEU:HD13	2.41	0.50
1:C:325:TRP:O	1:C:329:CYS:HB2	2.10	0.50
1:D:229:LEU:HA	1:D:232:ALA:O	2.11	0.50
1:A:16:TYR:O	1:A:20:ARG:HB2	2.11	0.50
1:A:395:HIS:NE2	1:A:435:LEU:HD13	2.26	0.50
1:C:82:ARG:HG2	1:C:87:GLU:CD	2.37	0.50
1:C:6:ASP:O	1:C:10:GLN:HG3	2.12	0.50
1:D:258:ASP:HB3	1:D:261:ASN:HD22	1.76	0.50
1:D:58:LEU:HD22	1:D:472:PRO:HB3	1.93	0.50
1:B:83:MET:HE2	1:B:97:VAL:CG1	2.42	0.50
1:C:163:PRO:HA	1:C:283:ILE:HD11	1.93	0.50
1:C:334:THR:HG22	1:C:377:ILE:HB	1.94	0.50
1:D:518:LYS:HG3	2:D:637:HOH:O	2.09	0.50
1:A:439:LYS:HZ1	1:B:519:GLN:HE22	1.57	0.50
1:C:218:ILE:O	1:C:222:GLU:HG3	2.11	0.50
1:D:436:MET:CE	1:D:437:ARG:HG3	2.42	0.50
1:B:515:GLU:O	1:B:519:GLN:HG3	2.11	0.49
1:D:141:LYS:HD3	1:D:145:GLY:O	2.11	0.49
1:D:209:SER:O	1:D:246:SER:CB	2.57	0.49
1:A:58:LEU:CD2	1:A:472:PRO:HB3	2.42	0.49
1:C:258:ASP:HB3	1:C:261:ASN:ND2	2.27	0.49
1:B:209:SER:O	1:B:246:SER:HB2	2.12	0.49
1:B:230:GLN:HG3	2:B:674:HOH:O	2.12	0.49
1:C:191:ILE:HG23	1:C:192:ALA:N	2.27	0.49
1:A:58:LEU:HD22	1:A:472:PRO:HB3	1.95	0.49
1:B:19:HIS:O	1:B:22:GLU:HB3	2.11	0.49
1:B:25:LEU:CB	1:B:436:MET:HG3	2.42	0.49
1:C:164:LEU:C	1:C:164:LEU:HD23	2.37	0.49
1:D:387:GLN:HA	1:D:391:TYR:CG	2.48	0.49
1:B:395:HIS:CD2	1:B:435:LEU:HD13	2.47	0.49
1:A:20:ARG:C	1:A:22:GLU:H	2.20	0.49
1:A:325:TRP:O	1:A:329:CYS:HB2	2.12	0.49
1:B:384:THR:HA	1:B:387:GLN:HB3	1.94	0.49
1:C:416:ARG:NH2	1:D:222:GLU:HB2	2.28	0.49
1:D:303:ASP:OD1	1:D:495:HIS:HE1	1.96	0.49
1:B:440:SER:OG	1:B:443:GLU:HG3	2.12	0.49
1:D:88:LYS:HD2	1:D:88:LYS:N	2.27	0.49
1:A:29:PHE:CD1	1:A:436:MET:HE1	2.48	0.48
1:A:324:ILE:CD1	1:A:503:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASN:HB3	1:B:317:VAL:HB	1.93	0.48
1:C:490:VAL:O	1:C:494:GLU:HG3	2.12	0.48
1:A:275:LEU:C	1:A:275:LEU:HD12	2.37	0.48
1:A:324:ILE:HD13	1:A:503:ILE:HD12	1.95	0.48
1:B:23:LEU:HB3	1:B:58:LEU:HD12	1.94	0.48
1:D:312:GLU:H	1:D:312:GLU:CD	2.21	0.48
1:B:304:GLN:CG	2:B:558:HOH:O	2.34	0.48
1:C:82:ARG:NH2	2:C:788:HOH:O	2.47	0.48
1:B:25:LEU:HB3	1:B:436:MET:HG3	1.95	0.48
1:B:382:PRO:CA	1:B:383:GLY:H	2.21	0.48
1:C:13:GLN:HG2	1:C:17:ARG:NH1	2.28	0.48
1:A:141:LYS:HD3	1:A:145:GLY:O	2.12	0.48
1:B:370:VAL:CG1	1:B:372:HIS:H	2.26	0.48
1:D:445:ARG:O	1:D:449:GLN:HG3	2.14	0.48
1:D:458:LEU:C	1:D:458:LEU:HD23	2.38	0.48
1:B:209:SER:O	1:B:246:SER:HB3	2.13	0.48
1:C:20:ARG:C	1:C:22:GLU:H	2.20	0.48
1:A:132:CYS:O	1:A:136:ARG:CG	2.62	0.48
1:A:82:ARG:HG2	1:A:87:GLU:CD	2.39	0.48
1:A:384:THR:HA	1:A:387:GLN:HB3	1.96	0.48
1:C:214:THR:O	1:C:218:ILE:HG12	2.14	0.48
1:A:16:TYR:CZ	1:A:20:ARG:HG3	2.49	0.47
1:C:458:LEU:C	1:C:458:LEU:HD23	2.38	0.47
1:A:320:ALA:HB1	1:A:500:GLN:HG3	1.97	0.47
1:C:519:GLN:HE22	1:D:439:LYS:HZ2	1.62	0.47
1:D:189:THR:O	1:D:193:LYS:HG2	2.15	0.47
1:A:305:HIS:HD2	2:A:867:HOH:O	1.98	0.47
1:C:215:GLN:OE1	1:D:423:ILE:HD12	2.14	0.47
1:D:407:ILE:HD13	1:D:425:LEU:HD23	1.96	0.47
1:C:445:ARG:HD3	2:C:787:HOH:O	2.14	0.47
1:D:161:LEU:HD12	1:D:350:TYR:HA	1.95	0.47
1:A:530:GLY:O	1:A:552:ARG:NH2	2.48	0.47
1:C:313:LYS:HD3	2:C:778:HOH:O	2.15	0.47
1:D:334:THR:HG22	1:D:377:ILE:HB	1.96	0.47
1:B:132:CYS:O	1:B:136:ARG:CG	2.60	0.47
1:B:253:LYS:NZ	1:B:259:PRO:HG2	2.30	0.47
1:C:124:VAL:O	1:C:128:MET:HG3	2.14	0.47
1:A:59:VAL:HG22	1:A:60:THR:N	2.29	0.47
1:A:99:HIS:HE1	2:A:869:HOH:O	1.97	0.47
1:B:272:ARG:HH12	1:B:511:GLN:HE21	1.63	0.47
1:B:537:HIS:N	1:B:542:ASN:HD21	2.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:LEU:HD12	2:C:593:HOH:O	2.15	0.47
1:D:90:ASN:HD22	1:D:507:ASN:HD21	1.62	0.47
1:B:303:ASP:OD1	1:B:495:HIS:HE1	1.98	0.46
1:A:29:PHE:CD1	1:A:436:MET:CE	2.98	0.46
1:C:200:PRO:HG3	1:C:227:TRP:CH2	2.50	0.46
1:D:132:CYS:O	1:D:136:ARG:CG	2.62	0.46
1:C:300:HIS:O	1:C:304:GLN:HG2	2.15	0.46
1:A:481:LEU:HD12	2:A:812:HOH:O	2.15	0.46
1:B:305:HIS:CE1	1:B:315:ALA:H	2.26	0.46
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.51	0.46
1:C:99:HIS:HD2	2:C:683:HOH:O	1.99	0.46
1:C:249:THR:O	1:C:253:LYS:HG3	2.16	0.46
1:B:178:PRO:O	1:B:286:HIS:HD2	1.99	0.46
1:B:228:PHE:CD2	1:B:229:LEU:HD12	2.50	0.46
1:C:253:LYS:HZ3	1:C:259:PRO:HG2	1.80	0.46
1:D:95:ARG:HD2	1:D:267:ASP:HB2	1.98	0.46
1:A:258:ASP:HB3	1:A:261:ASN:HD22	1.80	0.46
1:C:303:ASP:OD1	1:C:495:HIS:HE1	1.99	0.46
1:A:189:THR:HG21	2:B:607:HOH:O	2.16	0.46
1:A:222:GLU:HB2	1:B:416:ARG:NH2	2.31	0.46
1:A:486:LEU:O	1:A:490:VAL:HG23	2.16	0.46
1:B:20:ARG:C	1:B:22:GLU:H	2.23	0.46
1:B:234:ASP:HA	1:B:235:PRO:HD2	1.87	0.46
1:D:111:LEU:HD23	1:D:116:ASP:HA	1.97	0.46
1:B:164:LEU:HD23	1:B:182:TYR:CD2	2.51	0.45
1:B:456:GLU:O	1:B:460:ARG:HG2	2.16	0.45
1:C:519:GLN:HE22	1:D:439:LYS:HZ1	1.63	0.45
1:D:370:VAL:HG13	1:D:372:HIS:CE1	2.51	0.45
1:A:439:LYS:N	1:A:467:PHE:HB2	2.31	0.45
1:B:305:HIS:HD2	2:B:667:HOH:O	1.99	0.45
1:A:245:LEU:HD13	1:A:279:ILE:HA	1.98	0.45
1:C:80:ARG:HD2	1:C:307:ARG:HA	1.97	0.45
1:C:395:HIS:HE1	1:C:431:GLN:OE1	1.99	0.45
1:D:70:LEU:HD22	1:D:74:ARG:HG2	1.98	0.45
1:D:126:ASP:HB3	2:D:759:HOH:O	2.16	0.45
1:A:247:THR:HG22	1:A:264:GLU:HB2	1.97	0.45
1:C:387:GLN:HA	1:C:391:TYR:CG	2.51	0.45
1:D:82:ARG:HG2	1:D:87:GLU:CD	2.41	0.45
1:B:187:ASP:OD2	1:B:189:THR:HG23	2.17	0.45
1:D:522:LYS:HA	1:D:522:LYS:CE	2.45	0.45
1:D:152:ILE:HD12	1:D:152:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ARG:HG2	1:C:460:ARG:HH11	1.82	0.45
1:A:395:HIS:HD2	2:A:897:HOH:O	2.00	0.45
1:B:495:HIS:O	1:B:499:VAL:HG23	2.17	0.45
1:C:275:LEU:C	1:C:275:LEU:HD12	2.41	0.45
1:D:99:HIS:HE1	2:D:683:HOH:O	1.99	0.45
1:C:6:ASP:OD2	1:C:8:GLN:HB2	2.16	0.45
1:C:522:LYS:HA	1:C:522:LYS:CE	2.46	0.44
1:D:11:LYS:HD3	2:D:860:HOH:O	2.16	0.44
1:D:369:ARG:HH11	1:D:369:ARG:HG2	1.82	0.44
1:A:258:ASP:HB3	1:A:261:ASN:ND2	2.32	0.44
1:B:171:LYS:N	1:B:172:PRO:CD	2.80	0.44
1:C:34:ASP:HA	2:C:694:HOH:O	2.16	0.44
1:D:460:ARG:HG2	1:D:460:ARG:HH11	1.81	0.44
1:B:229:LEU:HD11	1:B:238:VAL:HG22	1.98	0.44
1:C:95:ARG:HD2	1:C:267:ASP:HB2	1.99	0.44
1:C:305:HIS:HE1	1:C:315:ALA:N	2.05	0.44
1:A:186:ILE:O	1:B:420:HIS:HD2	2.00	0.44
1:A:214:THR:O	1:A:218:ILE:HG12	2.18	0.44
1:A:324:ILE:HD13	1:A:503:ILE:CD1	2.48	0.44
1:B:382:PRO:C	1:B:382:PRO:N	2.68	0.44
1:D:530:GLY:O	1:D:552:ARG:NH2	2.50	0.44
1:B:496:LYS:O	1:B:500:GLN:HG3	2.17	0.44
1:A:98:LEU:HB2	1:A:268:TRP:CE3	2.53	0.44
1:C:516:LEU:HD13	1:D:434:ALA:HB1	2.00	0.44
1:C:303:ASP:HA	1:C:495:HIS:HE1	1.82	0.44
1:D:523:LYS:HE3	2:D:558:HOH:O	2.17	0.44
1:A:320:ALA:O	1:A:324:ILE:HD12	2.17	0.44
1:C:251:LYS:HD3	1:C:254:GLU:OE1	2.18	0.44
1:D:553:GLU:O	1:D:554:ALA:C	2.61	0.44
1:C:3:LEU:HD13	1:C:3:LEU:C	2.43	0.43
1:C:6:ASP:HA	1:C:7:PRO:HD3	1.89	0.43
1:A:253:LYS:HG2	1:A:259:PRO:HG3	2.01	0.43
1:B:334:THR:HG22	1:B:377:ILE:HB	2.01	0.43
1:D:544:LEU:O	1:D:548:ILE:HG13	2.18	0.43
1:A:232:ALA:O	1:A:233:LYS:HB2	2.19	0.43
1:A:490:VAL:O	1:A:494:GLU:HG3	2.19	0.43
1:C:3:LEU:HD11	1:C:9:PHE:CE1	2.54	0.43
1:B:370:VAL:CG1	1:B:372:HIS:O	2.67	0.43
1:C:171:LYS:N	1:C:172:PRO:CD	2.81	0.43
1:C:207:ILE:HD12	1:C:207:ILE:N	2.33	0.43
1:C:456:GLU:O	1:C:460:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PRO:O	1:D:286:HIS:HD2	2.01	0.43
1:C:1:ALA:HB1	2:C:722:HOH:O	2.16	0.43
1:C:437:ARG:HB3	1:C:437:ARG:CZ	2.49	0.43
1:D:370:VAL:HG13	1:D:372:HIS:CD2	2.53	0.43
1:A:305:HIS:CE1	1:A:315:ALA:H	2.27	0.43
1:B:387:GLN:HA	1:B:391:TYR:CG	2.53	0.43
1:D:481:LEU:C	1:D:481:LEU:HD13	2.43	0.43
1:A:195:LEU:HG	1:A:227:TRP:CD2	2.54	0.43
1:A:356:MET:HA	2:A:633:HOH:O	2.19	0.43
1:C:207:ILE:N	1:C:207:ILE:CD1	2.81	0.43
1:A:155:GLY:O	1:A:184:SER:HA	2.19	0.43
1:B:448:LEU:O	1:B:453:LYS:HB2	2.19	0.43
1:A:530:GLY:HA3	2:A:701:HOH:O	2.18	0.42
1:B:351:PHE:CZ	1:B:493:TYR:HB2	2.54	0.42
1:B:382:PRO:HA	1:B:383:GLY:N	2.32	0.42
1:C:141:LYS:HE3	2:C:580:HOH:O	2.19	0.42
1:D:171:LYS:N	1:D:172:PRO:CD	2.82	0.42
1:D:381:GLU:CG	1:D:382:PRO:HD2	2.49	0.42
1:D:381:GLU:OE2	1:D:382:PRO:HD2	2.19	0.42
1:A:312:GLU:H	1:A:312:GLU:CD	2.27	0.42
1:B:12:LEU:HD11	1:B:67:LEU:HD23	2.01	0.42
1:C:454:SER:C	1:C:456:GLU:N	2.76	0.42
1:C:456:GLU:OE1	1:C:456:GLU:HA	2.19	0.42
1:D:486:LEU:O	1:D:490:VAL:HG23	2.19	0.42
1:A:189:THR:O	1:A:193:LYS:HG2	2.19	0.42
1:C:459:GLU:HB2	1:C:460:ARG:HH11	1.82	0.42
1:C:553:GLU:O	1:C:555:ARG:HD2	2.19	0.42
1:D:245:LEU:HD13	1:D:279:ILE:HA	2.02	0.42
1:B:22:GLU:O	1:B:22:GLU:HG2	2.18	0.42
1:C:112:VAL:O	1:C:113:ASP:HB2	2.20	0.42
1:A:49:HIS:HD2	2:B:587:HOH:O	2.03	0.42
1:A:191:ILE:HG23	1:A:192:ALA:N	2.34	0.42
1:C:132:CYS:O	1:C:136:ARG:CG	2.63	0.42
1:C:381:GLU:HG2	2:D:699:HOH:O	2.18	0.42
1:C:448:LEU:O	1:C:451:ALA:HB3	2.19	0.42
1:D:90:ASN:ND2	1:D:90:ASN:C	2.76	0.42
1:D:408:PRO:HA	1:D:478:PHE:O	2.19	0.42
1:A:481:LEU:C	1:A:481:LEU:HD13	2.45	0.42
1:B:6:ASP:HA	1:B:7:PRO:HD3	1.85	0.42
1:D:356:MET:HA	2:D:641:HOH:O	2.19	0.42
1:A:187:ASP:OD2	1:A:189:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LYS:HG2	1:D:263:PHE:CE2	2.55	0.42
1:A:230:GLN:HA	1:A:230:GLN:NE2	2.35	0.42
1:A:381:GLU:HG3	1:A:382:PRO:HD2	2.02	0.42
1:A:439:LYS:H	1:A:467:PHE:HB2	1.85	0.42
1:C:195:LEU:HG	1:C:227:TRP:CD2	2.55	0.42
1:C:321:LEU:CD1	2:C:639:HOH:O	2.68	0.42
1:D:111:LEU:HD23	1:D:116:ASP:CA	2.50	0.42
1:A:90:ASN:ND2	1:A:90:ASN:C	2.77	0.41
1:B:298:GLY:HA3	1:B:484:PHE:O	2.20	0.41
1:D:52:VAL:HG13	1:D:476:ILE:CD1	2.50	0.41
1:C:24:ASN:HB3	1:C:27:ARG:HE	1.85	0.41
1:C:134:ARG:NH2	2:C:681:HOH:O	2.51	0.41
1:C:223:THR:OG1	1:D:420:HIS:HE1	2.03	0.41
1:C:290:ASP:HB2	2:C:714:HOH:O	2.19	0.41
1:C:416:ARG:NH1	1:C:419:LEU:HD23	2.35	0.41
1:B:59:VAL:HG22	1:B:60:THR:N	2.34	0.41
1:B:408:PRO:HA	1:B:478:PHE:O	2.21	0.41
1:C:59:VAL:HG22	1:C:60:THR:N	2.36	0.41
1:C:274:SER:O	1:C:279:ILE:HB	2.20	0.41
1:C:384:THR:HA	1:C:387:GLN:HB3	2.02	0.41
1:C:550:GLN:NE2	1:C:551:GLN:HE21	2.10	0.41
1:D:98:LEU:HB2	1:D:268:TRP:CE3	2.54	0.41
1:B:216:GLU:H	1:B:216:GLU:CD	2.26	0.41
1:C:369:ARG:HG2	1:C:369:ARG:HH11	1.85	0.41
1:C:381:GLU:CG	1:C:382:PRO:HD2	2.51	0.41
1:C:457:ASP:O	1:C:461:LEU:HB2	2.21	0.41
1:D:387:GLN:HA	1:D:391:TYR:CE1	2.55	0.41
1:A:320:ALA:HB1	1:A:500:GLN:CG	2.50	0.41
1:B:90:ASN:HD22	1:B:90:ASN:C	2.28	0.41
1:B:352:GLN:HG3	1:B:378:VAL:O	2.19	0.41
1:B:382:PRO:HA	1:B:383:GLY:H	1.84	0.41
1:B:550:GLN:NE2	1:B:551:GLN:HE21	2.14	0.41
1:D:180:VAL:HG11	1:D:286:HIS:HB2	2.01	0.41
1:A:246:SER:O	1:A:262:MET:HE3	2.21	0.41
1:B:408:PRO:HB3	1:B:478:PHE:CE1	2.56	0.41
1:A:6:ASP:HA	1:A:7:PRO:HD3	1.87	0.41
1:A:407:ILE:HD13	1:A:425:LEU:HD23	2.02	0.41
1:B:370:VAL:HG13	1:B:372:HIS:CD2	2.55	0.41
1:C:175:SER:HB3	2:C:582:HOH:O	2.20	0.41
1:C:258:ASP:OD1	1:C:260:GLN:HG2	2.20	0.41
1:D:82:ARG:HG2	1:D:87:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:O	1:A:246:SER:HB2	2.21	0.41
1:A:253:LYS:HZ1	1:A:259:PRO:HG2	1.86	0.41
1:C:214:THR:HB	1:C:217:THR:HB	2.02	0.41
1:B:152:ILE:N	1:B:152:ILE:HD12	2.36	0.40
1:B:247:THR:HG22	1:B:264:GLU:HB2	2.03	0.40
1:B:534:VAL:HA	2:B:719:HOH:O	2.21	0.40
1:D:187:ASP:OD2	1:D:189:THR:HG23	2.21	0.40
1:C:303:ASP:OD1	1:C:495:HIS:CE1	2.74	0.40
1:C:434:ALA:HB2	1:D:520:LEU:HD12	2.03	0.40
1:C:534:VAL:HG21	1:C:545:ILE:HG21	2.03	0.40
1:A:178:PRO:O	1:A:286:HIS:HD2	2.04	0.40
1:C:83:MET:HB2	1:C:89:ILE:HD13	2.02	0.40
1:C:90:ASN:HD22	1:C:90:ASN:C	2.29	0.40
1:A:317:VAL:O	1:A:321:LEU:HD13	2.21	0.40
1:A:435:LEU:HD23	1:A:473:THR:HG21	2.03	0.40
1:B:458:LEU:HD23	1:B:458:LEU:C	2.46	0.40
1:B:516:LEU:HD22	1:B:520:LEU:HG	2.02	0.40
1:B:552:ARG:HD3	2:B:692:HOH:O	2.21	0.40
1:D:370:VAL:HG13	1:D:372:HIS:NE2	2.36	0.40
1:D:448:LEU:HD21	1:D:465:LYS:HD3	2.02	0.40
1:C:189:THR:O	1:C:193:LYS:HG2	2.21	0.40
1:D:345:HIS:HA	1:D:382:PRO:HG3	2.03	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	554/558 (99%)	533 (96%)	19 (3%)	2 (0%)	30	28
1	B	554/558 (99%)	532 (96%)	22 (4%)	0	100	100
1	C	554/558 (99%)	526 (95%)	26 (5%)	2 (0%)	30	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	554/558 (99%)	524 (95%)	28 (5%)	2 (0%)	30	28
All	All	2216/2232 (99%)	2115 (95%)	95 (4%)	6 (0%)	36	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	384	THR
1	A	21	SER
1	C	21	SER
1	D	384	THR
1	A	384	THR
1	D	554	ALA

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	475/477 (100%)	462 (97%)	13 (3%)	39	45
1	B	475/477 (100%)	459 (97%)	16 (3%)	32	35
1	C	475/477 (100%)	463 (98%)	12 (2%)	42	48
1	D	475/477 (100%)	462 (97%)	13 (3%)	39	45
All	All	1900/1908 (100%)	1846 (97%)	54 (3%)	38	43

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	90	ASN
1	A	99	HIS
1	A	117	VAL
1	A	161	LEU
1	A	195	LEU
1	A	229	LEU
1	A	324	ILE

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Mol	Chain	Res	Type
1	A	344	LEU
1	A	384	THR
1	A	435	LEU
1	A	511	GLN
1	A	516	LEU
1	B	70	LEU
1	B	90	ASN
1	B	117	VAL
1	B	161	LEU
1	B	189	THR
1	B	195	LEU
1	B	265	PHE
1	B	296	LEU
1	B	312	GLU
1	B	344	LEU
1	B	399	GLU
1	B	416	ARG
1	B	435	LEU
1	B	511	GLN
1	B	516	LEU
1	B	553	GLU
1	C	13	GLN
1	C	30	ASP
1	C	70	LEU
1	C	99	HIS
1	C	161	LEU
1	C	195	LEU
1	C	207	ILE
1	C	312	GLU
1	C	344	LEU
1	C	399	GLU
1	C	435	LEU
1	C	516	LEU
1	D	70	LEU
1	D	90	ASN
1	D	99	HIS
1	D	117	VAL
1	D	195	LEU
1	D	229	LEU
1	D	312	GLU
1	D	321	LEU
1	D	344	LEU

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Mol	Chain	Res	Type
1	D	399	GLU
1	D	416	ARG
1	D	435	LEU
1	D	516	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	10	GLN
1	A	44	ASN
1	A	49	HIS
1	A	90	ASN
1	A	99	HIS
1	A	153	ASN
1	A	215	GLN
1	A	230	GLN
1	A	261	ASN
1	A	286	HIS
1	A	294	GLN
1	A	305	HIS
1	A	335	HIS
1	A	352	GLN
1	A	395	HIS
1	A	410	GLN
1	A	420	HIS
1	A	495	HIS
1	A	511	GLN
1	A	519	GLN
1	A	533	GLN
1	A	542	ASN
1	A	551	GLN
1	B	10	GLN
1	B	14	GLN
1	B	44	ASN
1	B	49	HIS
1	B	57	ASN
1	B	90	ASN
1	B	99	HIS
1	B	107	ASN
1	B	122	ASN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	215	GLN
1	B	230	GLN
1	B	286	HIS
1	B	294	GLN
1	B	305	HIS
1	B	352	GLN
1	B	353	GLN
1	B	373	GLN
1	B	395	HIS
1	B	420	HIS
1	B	474	ASN
1	B	495	HIS
1	B	511	GLN
1	B	519	GLN
1	B	542	ASN
1	B	550	GLN
1	C	8	GLN
1	C	10	GLN
1	C	44	ASN
1	C	49	HIS
1	C	90	ASN
1	C	99	HIS
1	C	153	ASN
1	C	197	GLN
1	C	286	HIS
1	C	294	GLN
1	C	305	HIS
1	C	352	GLN
1	C	353	GLN
1	C	395	HIS
1	C	410	GLN
1	C	420	HIS
1	C	495	HIS
1	C	519	GLN
1	C	542	ASN
1	C	550	GLN
1	D	8	GLN
1	D	10	GLN
1	D	13	GLN
1	D	44	ASN
1	D	49	HIS
1	D	57	ASN

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Mol	Chain	Res	Type
1	D	90	ASN
1	D	99	HIS
1	D	153	ASN
1	D	215	GLN
1	D	261	ASN
1	D	286	HIS
1	D	294	GLN
1	D	305	HIS
1	D	395	HIS
1	D	410	GLN
1	D	420	HIS
1	D	495	HIS
1	D	519	GLN
1	D	533	GLN
1	D	542	ASN
1	D	551	GLN

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 ⓘ

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	556/558 (99%)	-0.23	7 (1%) 75 77	14, 22, 39, 53	0
1	B	556/558 (99%)	-0.20	6 (1%) 78 80	14, 22, 41, 53	0
1	C	556/558 (99%)	0.20	20 (3%) 46 48	15, 28, 52, 74	0
1	D	556/558 (99%)	-0.00	17 (3%) 51 54	16, 25, 46, 72	0
All	All	2224/2232 (99%)	-0.06	50 (2%) 62 65	14, 24, 44, 74	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	GLY	5.0
1	D	232	ALA	4.9
1	C	232	ALA	4.8
1	B	383	GLY	4.3
1	A	383	GLY	4.2
1	D	383	GLY	4.1
1	C	458	LEU	4.0
1	C	556	VAL	3.9
1	C	455	PRO	3.6
1	B	556	VAL	3.5
1	D	454	SER	3.4
1	C	460	ARG	3.4
1	C	461	LEU	3.3
1	D	451	ALA	3.1
1	A	553	GLU	3.1
1	A	556	VAL	3.1
1	B	304	GLN	2.9
1	C	454	SER	2.9
1	C	304	GLN	2.8
1	C	456	GLU	2.8
1	C	368	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	458	LEU	2.7
1	D	556	VAL	2.7
1	D	139	ASP	2.7
1	C	459	GLU	2.6
1	D	452	GLY	2.6
1	C	452	GLY	2.5
1	D	450	ALA	2.4
1	A	460	ARG	2.4
1	D	437	ARG	2.4
1	C	213	THR	2.4
1	D	31	ALA	2.3
1	A	384	THR	2.3
1	B	18	GLU	2.2
1	B	460	ARG	2.2
1	D	456	GLU	2.2
1	D	553	GLU	2.2
1	C	229	LEU	2.2
1	C	143	TYR	2.2
1	C	553	GLU	2.1
1	B	31	ALA	2.1
1	D	444	ALA	2.1
1	A	454	SER	2.1
1	D	461	LEU	2.1
1	D	22	GLU	2.1
1	C	255	PHE	2.1
1	A	436	MET	2.1
1	C	234	ASP	2.1
1	D	457	ASP	2.1
1	C	449	GLN	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.