



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2017 – 03:25 AM EDT

PDB ID : 1E78
Title : Crystal structure of human serum albumin
Authors : Bhattacharya, A.A.; Curry, S.; Franks, N.P.
Deposited on : unknown
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

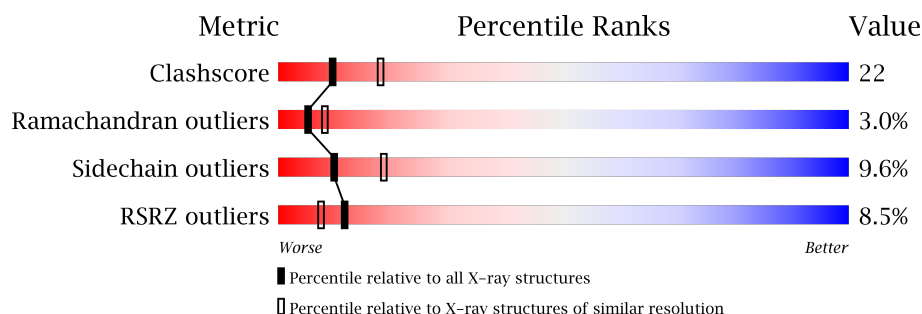
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	585	<div> <div>7%</div> <div>60%</div> <div>34%</div> <div>5% .</div> </div>
1	B	585	<div> <div>10%</div> <div>61%</div> <div>33%</div> <div>5% ..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8664 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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4339	2743	725	830	41			
1	B	578	Total	C	N	O	S	0	0	0
			4265	2692	718	815	40			

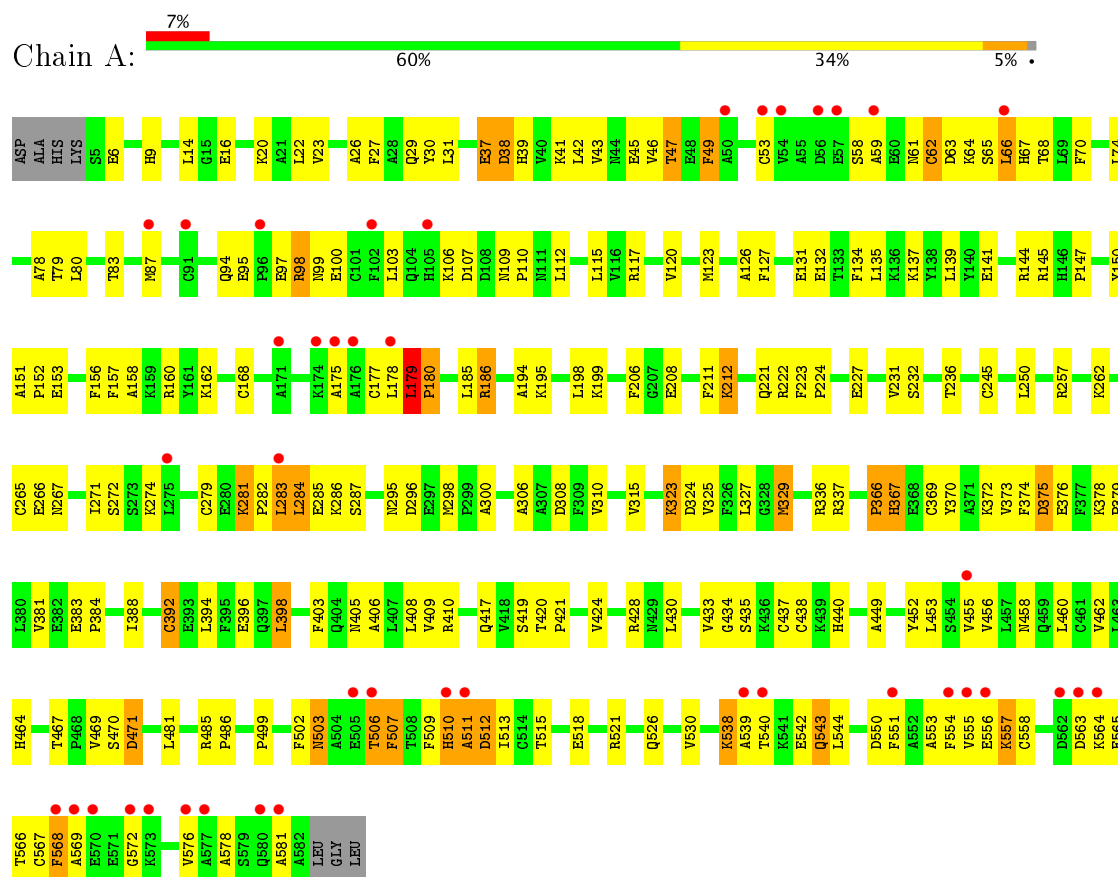
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	29	Total	O	0	0
			29	29		

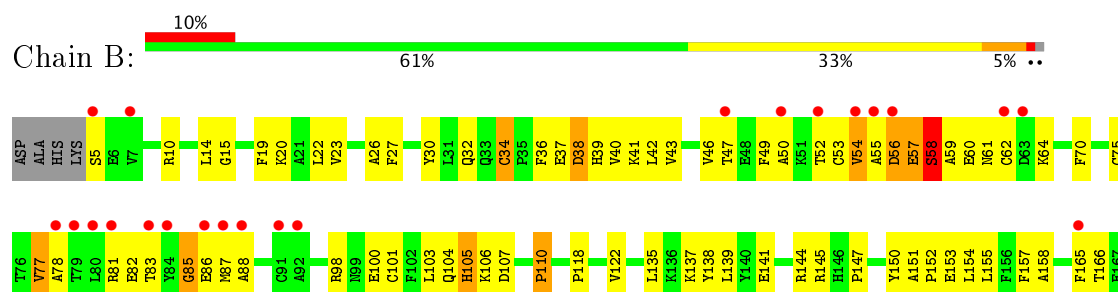
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: SERUM ALBUMIN



• Molecule 1: SERUM ALBUMIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.84Å 55.62Å 120.27Å 81.22° 91.08° 64.28°	Depositor
Resolution (Å)	40.00 – 2.60 36.16 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.60) 90.4 (36.16-2.58)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.247 , 0.277 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8664	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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	0.33	0/4425	0.55	0/6018
1	B	0.34	0/4347	0.54	3/5916 (0.1%)
All	All	0.33	0/8772	0.55	3/11934 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	540	THR	N-CA-C	8.09	132.84	111.00
1	B	541	LYS	N-CA-C	6.79	129.34	111.00
1	B	58	SER	CA-C-N	-5.05	106.10	117.20

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	4339	0	4009	196	0
1	B	4265	0	3898	163	0
2	A	31	0	0	4	0
2	B	29	0	0	5	0
All	All	8664	0	7907	359	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 22.

All (359) 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:557:LYS:NZ	1:B:571:GLU:HG3	1.58	1.18
1:A:503:ASN:HB2	1:A:506:THR:OG1	1.56	1.04
1:B:557:LYS:HZ1	1:B:571:GLU:HG3	1.05	1.01
1:A:94:GLN:O	1:A:98:ARG:HB3	1.60	1.00
1:A:503:ASN:HB3	1:A:506:THR:H	1.31	0.96
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.50	0.93
1:A:557:LYS:HG2	1:A:558:CYS:N	1.86	0.89
1:A:67:HIS:HB3	1:A:98:ARG:HH21	1.35	0.89
1:A:410:ARG:HD3	2:A:2020:HOH:O	1.76	0.84
1:A:392:CYS:O	1:A:396:GLU:HG3	1.79	0.83
1:A:98:ARG:NH2	1:A:99:ASN:HB2	1.94	0.83
1:A:503:ASN:HB2	1:A:506:THR:CB	2.09	0.82
1:A:186:ARG:HD3	2:A:2007:HOH:O	1.76	0.82
1:A:557:LYS:HG2	1:A:558:CYS:H	1.44	0.82
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.43	0.81
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.46	0.80
1:A:376:GLU:O	1:A:379:PRO:HD2	1.82	0.80
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.63	0.80
1:A:507:PHE:CZ	1:A:509:PHE:HZ	2.01	0.79
1:A:503:ASN:HB3	1:A:506:THR:N	1.98	0.77
1:B:39:HIS:O	1:B:43:VAL:HG23	1.85	0.77
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.67	0.75
1:A:507:PHE:O	1:A:507:PHE:CD1	2.39	0.75
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.52	0.75
1:A:23:VAL:O	1:A:27:PHE:HD1	1.67	0.75
1:A:98:ARG:CZ	1:A:99:ASN:HB2	2.16	0.75
1:B:557:LYS:HZ1	1:B:571:GLU:CG	1.95	0.74
1:A:503:ASN:HB2	1:A:506:THR:HG1	1.53	0.73
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.71	0.73
1:A:61:ASN:HB3	1:A:64:LYS:HD2	1.70	0.73
1:A:564:LYS:O	1:A:566:THR:N	2.17	0.73
1:A:424:VAL:O	1:A:428:ARG:HG3	1.89	0.73
1:A:540:THR:HG23	1:A:544:LEU:CD1	2.17	0.72
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.70	0.72
1:A:503:ASN:CB	1:A:506:THR:CB	2.68	0.71
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.05	0.71
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.06	0.71
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.71	0.71
1:A:557:LYS:CG	1:A:558:CYS:N	2.54	0.70
1:B:480:SER:HB2	2:B:2024:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.57	0.69
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.72	0.69
1:A:540:THR:HG23	1:A:544:LEU:HD11	1.74	0.69
1:B:507:PHE:CD1	1:B:507:PHE:O	2.46	0.69
1:A:323:LYS:HG3	1:A:324:ASP:N	2.07	0.68
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.73	0.68
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.77	0.67
1:B:511:ALA:HA	1:B:568:PHE:CZ	2.28	0.67
1:A:540:THR:CG2	1:A:544:LEU:HD11	2.23	0.67
1:A:117:ARG:HB2	1:A:123:MET:CE	2.25	0.67
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.25	0.66
1:B:378:LYS:HB2	1:B:379:PRO:CD	2.25	0.66
1:B:394:LEU:HD11	1:B:398:LEU:HD11	1.78	0.66
1:B:310:VAL:HG21	1:B:374:PHE:CE1	2.31	0.65
1:B:212:LYS:O	1:B:216:VAL:HG23	1.94	0.65
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.76	0.65
1:A:538:LYS:O	1:A:540:THR:N	2.30	0.65
1:A:39:HIS:O	1:A:43:VAL:HG23	1.96	0.65
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.79	0.65
1:B:373:VAL:HG13	1:B:374:PHE:N	2.12	0.65
1:A:503:ASN:CB	1:A:506:THR:HB	2.27	0.64
1:A:464:HIS:CE1	1:A:469:VAL:H	2.15	0.64
1:B:394:LEU:O	1:B:397:GLN:HG2	1.97	0.64
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.13	0.63
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.80	0.63
1:B:52:THR:HA	1:B:56:ASP:OD2	1.98	0.63
1:B:199:LYS:HG3	2:B:2010:HOH:O	1.99	0.63
1:B:36:PHE:O	1:B:40:VAL:HG23	1.99	0.63
1:B:557:LYS:HZ2	1:B:571:GLU:HG3	1.59	0.63
1:A:543:GLN:O	1:A:544:LEU:C	2.37	0.63
1:B:50:ALA:O	1:B:54:VAL:HG23	1.99	0.63
1:A:66:LEU:HD23	2:A:2015:HOH:O	1.97	0.62
1:B:276:LYS:HE3	1:B:280:GLU:OE2	1.99	0.62
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.81	0.62
1:B:342:SER:OG	1:B:344:VAL:HG23	1.99	0.62
1:A:502:PHE:CE1	1:A:507:PHE:CZ	2.86	0.62
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.82	0.62
1:A:117:ARG:HB2	1:A:123:MET:HE3	1.82	0.62
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.81	0.62
1:A:394:LEU:HG	1:A:398:LEU:HD11	1.82	0.62
1:B:81:ARG:HE	1:B:88:ALA:CB	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.82	0.61
1:A:283:LEU:HG	1:A:284:LEU:N	2.15	0.61
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.00	0.61
1:A:464:HIS:HE1	1:A:470:SER:H	1.48	0.61
1:A:434:GLY:O	1:A:438:CYS:HB2	2.00	0.61
1:B:531:GLU:O	1:B:535:HIS:HD2	1.83	0.61
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.83	0.60
1:A:564:LYS:C	1:A:566:THR:H	2.02	0.60
1:A:366:PRO:O	1:A:369:CYS:N	2.35	0.60
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.83	0.60
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.33	0.60
1:B:107:ASP:O	1:B:110:PRO:HD3	2.01	0.60
1:B:375:ASP:O	1:B:378:LYS:HG3	2.02	0.60
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.83	0.59
1:A:507:PHE:CE2	1:A:509:PHE:HZ	2.19	0.59
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.85	0.59
1:A:366:PRO:O	1:A:367:HIS:C	2.41	0.59
1:A:511:ALA:O	1:A:513:ILE:N	2.35	0.59
1:B:420:THR:HB	1:B:421:PRO:HD3	1.85	0.59
1:A:325:VAL:HG12	1:A:329:MET:CE	2.32	0.59
1:A:507:PHE:O	1:A:509:PHE:CE1	2.56	0.59
1:B:42:LEU:O	1:B:46:VAL:HG23	2.03	0.59
1:A:67:HIS:CB	1:A:98:ARG:HH21	2.12	0.59
1:B:293:VAL:HG22	1:B:294:GLU:N	2.17	0.59
1:B:323:LYS:HG3	1:B:324:ASP:N	2.17	0.59
1:B:186:ARG:O	1:B:190:LYS:HG3	2.02	0.58
1:A:153:GLU:O	1:A:157:PHE:HD1	1.86	0.58
1:B:475:LYS:O	1:B:479:GLU:HB2	2.03	0.58
1:A:199:LYS:HG2	1:A:211:PHE:HE2	1.68	0.58
1:A:553:ALA:O	1:A:556:GLU:HG2	2.03	0.57
1:A:42:LEU:O	1:A:46:VAL:HG23	2.04	0.57
1:A:430:LEU:O	1:A:433:VAL:HG12	2.02	0.57
1:B:23:VAL:O	1:B:27:PHE:HD1	1.87	0.57
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.86	0.57
1:A:511:ALA:C	1:A:513:ILE:H	2.07	0.57
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.57
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.35	0.56
1:B:507:PHE:HD1	1:B:507:PHE:O	1.88	0.56
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.05	0.56
1:B:426:VAL:HG21	1:B:460:LEU:HB2	1.87	0.56
1:A:502:PHE:HE1	1:A:507:PHE:CZ	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:GLU:HA	1:B:574:LYS:HB2	1.86	0.56
1:B:507:PHE:CE2	1:B:509:PHE:HZ	2.24	0.56
1:B:563:ASP:OD2	1:B:565:GLU:O	2.24	0.56
1:B:430:LEU:O	1:B:433:VAL:HG12	2.05	0.55
1:A:208:GLU:O	1:A:212:LYS:HB2	2.05	0.55
1:A:98:ARG:NH1	1:A:99:ASN:H	2.04	0.55
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.89	0.55
1:B:428:ARG:HD3	2:B:2020:HOH:O	2.06	0.55
1:B:540:THR:O	1:B:544:LEU:CG	2.55	0.55
1:A:554:PHE:HE1	1:A:568:PHE:CE1	2.25	0.54
1:A:567:CYS:SG	1:A:568:PHE:N	2.80	0.54
1:A:66:LEU:H	1:A:66:LEU:HD13	1.71	0.54
1:B:194:ALA:HB1	1:B:455:VAL:HG13	1.89	0.54
1:A:262:LYS:O	1:A:266:GLU:HG3	2.07	0.54
1:A:126:ALA:HB2	2:A:2004:HOH:O	2.07	0.54
1:B:459:GLN:O	1:B:462:VAL:HG22	2.09	0.53
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.91	0.53
1:B:464:HIS:CE1	1:B:469:VAL:H	2.26	0.53
1:B:153:GLU:O	1:B:157:PHE:HD1	1.91	0.53
1:B:424:VAL:O	1:B:428:ARG:HG3	2.08	0.53
1:B:398:LEU:O	1:B:402:LYS:HB2	2.08	0.53
1:B:541:LYS:HA	1:B:544:LEU:HD12	1.91	0.53
1:B:571:GLU:OE1	1:B:574:LYS:HD2	2.09	0.53
1:A:49:PHE:HE1	1:A:62:CYS:SG	2.32	0.53
1:B:384:PRO:O	1:B:388:ILE:HG12	2.10	0.52
1:A:100:GLU:OE1	1:A:103:LEU:HD12	2.09	0.52
1:A:23:VAL:HG13	1:A:70:PHE:HE1	1.73	0.52
1:B:394:LEU:CD1	1:B:398:LEU:HD11	2.38	0.52
1:B:516:LEU:HD22	1:B:520:GLU:CB	2.39	0.52
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.91	0.52
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.74	0.52
1:B:367:HIS:O	1:B:371:ALA:HB2	2.09	0.52
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.74	0.52
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.91	0.52
1:B:100:GLU:O	1:B:104:GLN:HG3	2.10	0.52
1:B:531:GLU:O	1:B:535:HIS:CD2	2.62	0.52
1:A:405:ASN:O	1:A:409:VAL:HG23	2.09	0.52
1:A:131:GLU:O	1:A:134:PHE:N	2.39	0.52
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.10	0.52
1:A:117:ARG:HB2	1:A:123:MET:HE1	1.92	0.51
1:A:518:GLU:HA	1:A:521:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ALA:C	1:A:513:ILE:N	2.63	0.51
1:B:405:ASN:O	1:B:409:VAL:HG23	2.11	0.51
1:B:511:ALA:C	1:B:513:ILE:H	2.13	0.51
1:B:283:LEU:HG	1:B:284:LEU:N	2.25	0.51
1:B:15:GLY:O	1:B:19:PHE:HB3	2.11	0.51
1:A:372:LYS:O	1:A:375:ASP:HB2	2.11	0.51
1:B:23:VAL:O	1:B:27:PHE:CD1	2.64	0.51
1:A:61:ASN:C	1:A:63:ASP:H	2.15	0.50
1:B:372:LYS:O	1:B:375:ASP:HB2	2.12	0.50
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.27	0.50
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.94	0.50
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.27	0.50
1:B:310:VAL:CG2	1:B:374:PHE:CE1	2.94	0.50
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.93	0.50
1:B:399:GLY:O	1:B:403:PHE:HB2	2.12	0.50
1:A:31:LEU:HG	1:A:74:LEU:HD22	1.93	0.49
1:A:464:HIS:HE1	1:A:469:VAL:H	1.60	0.49
1:A:512:ASP:O	1:A:515:THR:HG22	2.13	0.49
1:A:381:VAL:O	1:A:384:PRO:HD2	2.12	0.49
1:B:54:VAL:HG12	1:B:55:ALA:N	2.26	0.49
1:B:333:GLU:O	1:B:337:ARG:HG3	2.11	0.49
1:B:166:THR:CG2	2:B:2007:HOH:O	2.61	0.49
1:B:373:VAL:CG1	1:B:374:PHE:N	2.76	0.49
1:B:540:THR:O	1:B:544:LEU:HG	2.12	0.49
1:A:471:ASP:N	1:A:471:ASP:OD1	2.41	0.48
1:A:540:THR:HG23	1:A:544:LEU:CG	2.43	0.48
1:A:66:LEU:HD13	1:A:66:LEU:N	2.28	0.48
1:A:135:LEU:HD11	1:A:162:LYS:HD3	1.95	0.48
1:A:43:VAL:O	1:A:47:THR:OG1	2.30	0.48
1:A:373:VAL:HG13	1:A:374:PHE:N	2.29	0.48
1:A:543:GLN:HG2	1:A:544:LEU:H	1.78	0.48
1:A:420:THR:O	1:A:424:VAL:HG23	2.13	0.48
1:B:198:LEU:HA	1:B:458:ASN:ND2	2.28	0.48
1:B:571:GLU:HA	1:B:571:GLU:OE1	2.13	0.48
1:A:376:GLU:C	1:A:379:PRO:HD2	2.34	0.48
1:B:57:GLU:O	1:B:58:SER:C	2.51	0.48
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.95	0.48
1:B:290:ILE:O	1:B:293:VAL:HG12	2.13	0.48
1:A:38:ASP:O	1:A:42:LEU:HG	2.13	0.48
1:A:449:ALA:O	1:A:453:LEU:HG	2.14	0.48
1:B:293:VAL:CG2	1:B:294:GLU:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:O	1:A:141:GLU:HG2	2.14	0.47
1:B:542:GLU:C	1:B:544:LEU:N	2.67	0.47
1:B:141:GLU:O	1:B:145:ARG:HG3	2.13	0.47
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.80	0.47
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.14	0.47
1:B:310:VAL:HG21	1:B:374:PHE:CD1	2.49	0.47
1:A:222:ARG:C	1:A:224:PRO:HD3	2.35	0.47
1:A:227:GLU:O	1:A:231:VAL:HG23	2.13	0.47
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.43	0.47
1:B:19:PHE:CD1	1:B:19:PHE:C	2.88	0.47
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.49	0.47
1:B:516:LEU:O	1:B:521:ARG:NH2	2.46	0.47
1:A:310:VAL:O	1:A:370:TYR:HE1	1.98	0.46
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.45	0.46
1:A:578:ALA:O	1:A:581:ALA:HB3	2.15	0.46
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.96	0.46
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.51	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.96	0.46
1:A:221:GLN:O	1:A:224:PRO:HD3	2.16	0.46
1:A:49:PHE:CE1	1:A:53:CYS:SG	3.09	0.46
1:A:178:LEU:O	1:A:179:LEU:C	2.54	0.46
1:A:370:TYR:CD1	1:A:370:TYR:C	2.89	0.46
1:A:38:ASP:OD1	1:A:38:ASP:N	2.46	0.46
1:A:117:ARG:HG3	1:A:117:ARG:O	2.16	0.46
1:A:127:PHE:HB2	1:A:134:PHE:CE2	2.51	0.46
1:A:567:CYS:O	1:A:569:ALA:N	2.48	0.46
1:B:137:LYS:O	1:B:141:GLU:HG2	2.16	0.46
1:A:152:PRO:HB2	1:A:257:ARG:NH1	2.24	0.46
1:A:419:SER:HB2	1:A:421:PRO:HD2	1.98	0.46
1:B:22:LEU:HD21	1:B:155:LEU:HD11	1.97	0.46
1:B:34:CYS:HB3	1:B:39:HIS:CD2	2.50	0.46
1:B:34:CYS:HB3	1:B:39:HIS:HE2	1.79	0.46
1:A:542:GLU:O	1:A:543:GLN:C	2.52	0.45
1:A:384:PRO:O	1:A:388:ILE:HG12	2.15	0.45
1:A:572:GLY:O	1:A:576:VAL:HG23	2.16	0.45
1:B:249:ASP:HB3	1:B:252:GLU:OE1	2.17	0.45
1:B:374:PHE:O	1:B:375:ASP:C	2.54	0.45
1:B:507:PHE:HD1	1:B:507:PHE:H	1.64	0.45
1:A:518:GLU:OE1	1:A:521:ARG:HD2	2.15	0.45
1:B:483:ASN:C	1:B:486:PRO:HD2	2.36	0.45
1:B:70:PHE:N	1:B:70:PHE:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.16	0.45
1:A:152:PRO:CB	1:A:257:ARG:HH11	2.26	0.45
1:A:279:CYS:HA	1:A:286:LYS:CD	2.44	0.45
1:A:41:LYS:O	1:A:45:GLU:HG3	2.16	0.45
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.45	0.45
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.17	0.45
1:B:458:ASN:HB2	2:B:2022:HOH:O	2.16	0.45
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.52	0.45
1:A:6:GLU:O	1:A:9:HIS:HB3	2.16	0.45
1:A:95:GLU:O	1:A:98:ARG:NH1	2.50	0.44
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.99	0.44
1:B:563:ASP:OD2	1:B:565:GLU:C	2.55	0.44
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.98	0.44
1:A:540:THR:HG23	1:A:544:LEU:HG	1.99	0.44
1:A:66:LEU:HB3	1:A:70:PHE:CE2	2.53	0.44
1:B:540:THR:O	1:B:544:LEU:CB	2.66	0.44
1:A:141:GLU:O	1:A:145:ARG:HG3	2.17	0.44
1:A:507:PHE:CE2	1:A:509:PHE:CZ	3.02	0.44
1:B:38:ASP:O	1:B:41:LYS:HB3	2.17	0.44
1:B:563:ASP:O	1:B:564:LYS:O	2.35	0.44
1:B:276:LYS:HG3	1:B:277:GLU:N	2.30	0.44
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.48	0.44
1:A:540:THR:HG21	1:A:544:LEU:HD11	1.98	0.44
1:B:314:ASP:O	1:B:318:ASN:ND2	2.51	0.44
1:A:78:ALA:C	1:A:80:LEU:H	2.21	0.44
1:A:417:GLN:HB2	1:A:470:SER:HB2	2.00	0.44
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.89	0.44
1:B:38:ASP:N	1:B:38:ASP:OD1	2.48	0.44
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.58	0.44
1:A:509:PHE:O	1:A:510:HIS:C	2.57	0.44
1:A:16:GLU:O	1:A:20:LYS:HB2	2.18	0.43
1:B:434:GLY:O	1:B:438:CYS:HB2	2.18	0.43
1:A:115:LEU:HD22	1:A:145:ARG:HH12	1.83	0.43
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.48	0.43
1:A:97:GLU:C	1:A:99:ASN:N	2.71	0.43
1:B:529:LEU:HD13	1:B:548:MET:HG2	2.00	0.43
1:A:168:CYS:SG	1:A:177:CYS:C	2.97	0.43
1:A:23:VAL:HG13	1:A:27:PHE:HE1	1.83	0.43
1:A:509:PHE:N	1:A:509:PHE:CD1	2.85	0.43
1:A:61:ASN:C	1:A:63:ASP:N	2.72	0.43
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:O	1:A:49:PHE:HD1	2.01	0.43
1:A:464:HIS:CE1	1:A:470:SER:H	2.32	0.43
1:A:564:LYS:C	1:A:566:THR:N	2.63	0.43
1:B:139:LEU:HD21	1:B:158:ALA:HB2	2.00	0.43
1:A:298:MET:SD	1:A:337:ARG:HA	2.59	0.43
1:B:539:ALA:O	1:B:540:THR:HG23	2.19	0.43
1:B:511:ALA:C	1:B:513:ILE:N	2.72	0.43
1:B:49:PHE:O	1:B:53:CYS:SG	2.77	0.43
1:B:56:ASP:OD1	1:B:56:ASP:N	2.52	0.43
1:B:10:ARG:HA	1:B:10:ARG:HD3	1.79	0.43
1:B:118:PRO:HB2	1:B:122:VAL:HB	2.01	0.43
1:B:507:PHE:N	1:B:507:PHE:CD1	2.86	0.43
1:B:70:PHE:HD1	1:B:70:PHE:N	2.16	0.43
1:A:437:CYS:O	1:A:440:HIS:HB2	2.19	0.42
1:A:551:PHE:O	1:A:555:VAL:HG23	2.19	0.42
1:B:373:VAL:HG13	1:B:374:PHE:H	1.84	0.42
1:A:107:ASP:O	1:A:147:PRO:HG3	2.18	0.42
1:B:139:LEU:HD22	1:B:154:LEU:HG	2.00	0.42
1:A:366:PRO:O	1:A:369:CYS:HB3	2.18	0.42
1:A:78:ALA:C	1:A:80:LEU:N	2.72	0.42
1:B:366:PRO:O	1:B:369:CYS:N	2.52	0.42
1:A:131:GLU:O	1:A:132:GLU:C	2.56	0.42
1:A:141:GLU:OE1	1:A:144:ARG:HD3	2.20	0.42
1:A:452:TYR:O	1:A:456:VAL:HG23	2.19	0.42
1:A:458:ASN:O	1:A:462:VAL:HG13	2.19	0.42
1:A:554:PHE:CE1	1:A:568:PHE:CE1	3.07	0.42
1:A:61:ASN:O	1:A:63:ASP:N	2.53	0.42
1:B:364:ALA:O	1:B:366:PRO:HD3	2.19	0.42
1:A:563:ASP:C	1:A:564:LYS:O	2.55	0.42
1:A:394:LEU:O	1:A:398:LEU:HG	2.19	0.42
1:B:103:LEU:C	1:B:105:HIS:H	2.23	0.42
1:A:223:PHE:N	1:A:224:PRO:HD3	2.34	0.42
1:A:65:SER:O	1:A:66:LEU:C	2.58	0.42
1:B:165:PHE:O	1:B:169:CYS:HB2	2.20	0.42
1:B:333:GLU:OE1	1:B:336:ARG:HD3	2.19	0.42
1:A:553:ALA:O	1:A:557:LYS:HB3	2.20	0.42
1:B:38:ASP:O	1:B:42:LEU:HG	2.19	0.42
1:A:67:HIS:O	1:A:68:THR:C	2.57	0.42
1:B:563:ASP:O	1:B:564:LYS:C	2.56	0.42
1:A:49:PHE:CD1	1:A:49:PHE:C	2.93	0.41
1:B:135:LEU:O	1:B:138:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:O	1:A:271:ILE:HD12	2.20	0.41
1:A:403:PHE:O	1:A:406:ALA:HB3	2.21	0.41
1:B:168:CYS:SG	1:B:177:CYS:C	2.99	0.41
1:B:464:HIS:CE1	1:B:470:SER:H	2.38	0.41
1:B:540:THR:HG22	1:B:544:LEU:HG	2.02	0.41
1:A:460:LEU:O	1:A:460:LEU:HD12	2.20	0.41
1:B:23:VAL:HG13	1:B:27:PHE:CE1	2.56	0.41
1:B:384:PRO:O	1:B:385:GLN:C	2.58	0.41
1:B:464:HIS:HE1	1:B:470:SER:H	1.67	0.41
1:B:85:GLY:C	1:B:87:MET:H	2.24	0.41
1:A:160:ARG:HD3	1:A:185:LEU:HD21	2.01	0.41
1:B:5:SER:HA	1:B:62:CYS:O	2.21	0.41
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.60	0.41
1:A:274:LYS:HE3	1:A:296:ASP:HA	2.02	0.41
1:A:394:LEU:CG	1:A:398:LEU:HD11	2.48	0.41
1:B:345:LEU:O	1:B:349:LEU:HG	2.21	0.41
1:B:507:PHE:CZ	1:B:509:PHE:HZ	2.39	0.41
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.56	0.40
1:B:37:GLU:CD	1:B:37:GLU:H	2.24	0.40
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.96	0.40
1:B:75:CYS:HA	1:B:78:ALA:HB3	2.03	0.40
1:B:178:LEU:O	1:B:179:LEU:C	2.59	0.40
1:B:231:VAL:O	1:B:235:VAL:HG23	2.22	0.40
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.43	0.40
1:B:340:ASP:O	1:B:447:PRO:HD3	2.21	0.40
1:A:327:LEU:HA	1:A:327:LEU:HD23	1.96	0.40
1:A:367:HIS:HA	1:A:370:TYR:CZ	2.56	0.40
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.55	0.40
1:B:98:ARG:O	1:B:101:CYS:HB3	2.21	0.40
1:B:272:SER:HB3	1:B:275:LEU:HG	2.04	0.40
1:B:221:GLN:O	1:B:295:ASN:HB3	2.22	0.40
1:B:411:TYR:HA	1:B:414:LYS:HD3	2.04	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	576/585 (98%)	496 (86%)	60 (10%)	20 (4%)	4	6
1	B	576/585 (98%)	503 (87%)	59 (10%)	14 (2%)	7	12
All	All	1152/1170 (98%)	999 (87%)	119 (10%)	34 (3%)	5	8

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	A	511	ALA
1	A	538	LYS
1	A	539	ALA
1	B	54	VAL
1	B	60	GLU
1	B	300	ALA
1	B	538	LYS
1	B	566	THR
1	A	512	ASP
1	A	565	GLU
1	A	568	PHE
1	B	58	SER
1	B	85	GLY
1	B	539	ALA
1	A	58	SER
1	A	150	TYR
1	A	510	HIS
1	A	557	LYS
1	A	37	GLU
1	A	62	CYS
1	A	179	LEU
1	A	499	PRO
1	B	86	GLU
1	B	540	THR
1	A	180	PRO
1	A	315	VAL
1	A	367	HIS
1	B	564	LYS
1	A	366	PRO

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Mol	Chain	Res	Type
1	B	77	VAL
1	B	110	PRO
1	B	179	LEU

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	437/511 (86%)	399 (91%)	38 (9%)	12	23
1	B	418/511 (82%)	374 (90%)	44 (10%)	8	15
All	All	855/1022 (84%)	773 (90%)	82 (10%)	10	18

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	37	GLU
1	A	38	ASP
1	A	47	THR
1	A	49	PHE
1	A	66	LEU
1	A	79	THR
1	A	83	THR
1	A	87	MET
1	A	98	ARG
1	A	109	ASN
1	A	179	LEU
1	A	186	ARG
1	A	195	LYS
1	A	212	LYS
1	A	232	SER
1	A	236	THR
1	A	245	CYS
1	A	281	LYS
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	287	SER
1	A	295	ASN
1	A	308	ASP
1	A	323	LYS
1	A	329	MET
1	A	336	ARG
1	A	375	ASP
1	A	392	CYS
1	A	398	LEU
1	A	435	SER
1	A	467	THR
1	A	471	ASP
1	A	503	ASN
1	A	506	THR
1	A	507	PHE
1	A	543	GLN
1	A	550	ASP
1	B	20	LYS
1	B	34	CYS
1	B	38	ASP
1	B	47	THR
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	77	VAL
1	B	82	GLU
1	B	83	THR
1	B	105	HIS
1	B	150	TYR
1	B	179	LEU
1	B	212	LYS
1	B	232	SER
1	B	245	CYS
1	B	281	LYS
1	B	283	LEU
1	B	284	LEU
1	B	287	SER
1	B	323	LYS
1	B	324	ASP
1	B	336	ARG
1	B	337	ARG

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Mol	Chain	Res	Type
1	B	344	VAL
1	B	375	ASP
1	B	392	CYS
1	B	398	LEU
1	B	410	ARG
1	B	435	SER
1	B	467	THR
1	B	480	SER
1	B	489	SER
1	B	500	LYS
1	B	507	PHE
1	B	540	THR
1	B	544	LEU
1	B	545	LYS
1	B	548	MET
1	B	555	VAL
1	B	557	LYS
1	B	566	THR
1	B	567	CYS
1	B	568	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	A	503	ASN
1	B	111	ASN
1	B	196	GLN
1	B	318	ASN
1	B	385	GLN
1	B	464	HIS
1	B	483	ASN
1	B	535	HIS
1	B	543	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	578/585 (98%)	0.28	42 (7%) 16 11	28, 66, 136, 150	0
1	B	578/585 (98%)	0.39	56 (9%) 8 5	30, 72, 139, 150	0
All	All	1156/1170 (98%)	0.34	98 (8%) 11 7	28, 69, 138, 150	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	ALA	9.9
1	B	562	ASP	8.5
1	B	573	LYS	8.4
1	B	576	VAL	8.0
1	B	569	ALA	7.9
1	A	539	ALA	7.4
1	A	570	GLU	7.3
1	A	572	GLY	7.3
1	B	572	GLY	7.2
1	B	563	ASP	6.7
1	B	578	ALA	6.6
1	B	570	GLU	6.3
1	B	558	CYS	5.5
1	A	510	HIS	5.5
1	B	91	CYS	5.1
1	A	577	ALA	5.0
1	B	566	THR	4.8
1	A	554	PHE	4.7
1	A	506	THR	4.7
1	B	54	VAL	4.7
1	A	568	PHE	4.4
1	B	87	MET	4.3
1	B	504	ALA	4.3
1	B	568	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	559	CYS	4.2
1	A	569	ALA	4.1
1	A	576	VAL	4.0
1	A	580	GLN	4.0
1	A	555	VAL	3.9
1	B	560	LYS	3.9
1	B	513	ILE	3.9
1	B	92	ALA	3.8
1	B	62	CYS	3.8
1	A	505	GLU	3.7
1	B	580	GLN	3.7
1	A	178	LEU	3.7
1	B	539	ALA	3.7
1	B	79	THR	3.7
1	B	7	VAL	3.6
1	B	78	ALA	3.6
1	B	83	THR	3.5
1	B	175	ALA	3.5
1	B	508	THR	3.4
1	A	562	ASP	3.4
1	A	175	ALA	3.3
1	B	581	ALA	3.2
1	B	505	GLU	3.2
1	B	503	ASN	3.2
1	A	573	LYS	3.1
1	A	176	ALA	3.1
1	B	52	THR	3.1
1	B	275	LEU	2.9
1	A	275	LEU	2.9
1	A	54	VAL	2.8
1	B	55	ALA	2.8
1	B	84	TYR	2.8
1	B	174	LYS	2.8
1	A	283	LEU	2.8
1	A	551	PHE	2.8
1	B	81	ARG	2.7
1	B	515	THR	2.7
1	A	105	HIS	2.7
1	B	516	LEU	2.6
1	A	91	CYS	2.6
1	B	502	PHE	2.6
1	A	171	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	563	ASP	2.6
1	A	50	ALA	2.6
1	A	174	LYS	2.5
1	A	540	THR	2.5
1	B	47	THR	2.5
1	B	50	ALA	2.5
1	A	87	MET	2.5
1	A	564	LYS	2.5
1	B	86	GLU	2.5
1	B	278	CYS	2.5
1	B	555	VAL	2.5
1	B	5	SER	2.5
1	B	63	ASP	2.4
1	A	56	ASP	2.3
1	A	511	ALA	2.3
1	B	88	ALA	2.3
1	A	455	VAL	2.3
1	B	165	PHE	2.3
1	A	53	CYS	2.3
1	A	57	GLU	2.2
1	A	66	LEU	2.2
1	B	365	ASP	2.2
1	A	96	PRO	2.2
1	A	59	ALA	2.2
1	B	567	CYS	2.1
1	A	556	GLU	2.1
1	B	80	LEU	2.1
1	A	581	ALA	2.1
1	B	540	THR	2.1
1	B	56	ASP	2.1
1	B	575	LEU	2.1
1	A	102	PHE	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 carbohydrates 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.