



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:08 PM UTC

PDB ID : 7DJN / pdb_00007djn
Title : Human Serum Albumin
Authors : Xiang, W.; Yue, Z.; Su, J.
Deposited on : 2020-11-20
Resolution : 2.04 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

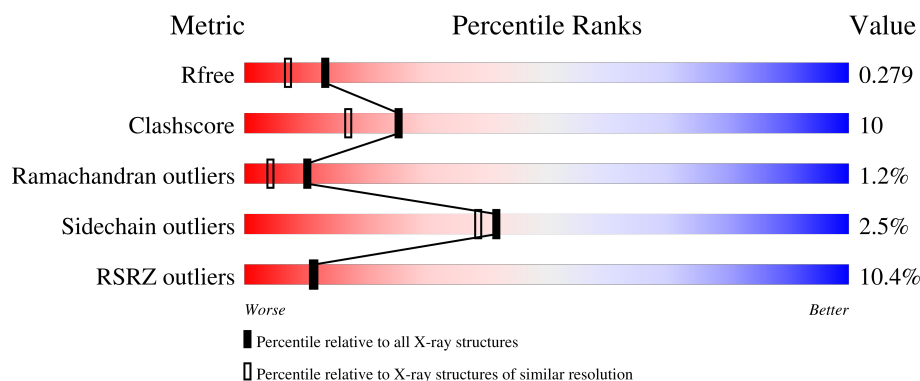
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	585	9% 78% 16% • •
1	B	585	11% 74% 21% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9164 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	561	Total	C	N	O	S	0	0	0
			4475	2827	754	853	41			
1	B	565	Total	C	N	O	S	0	0	0
			4502	2842	761	859	40			

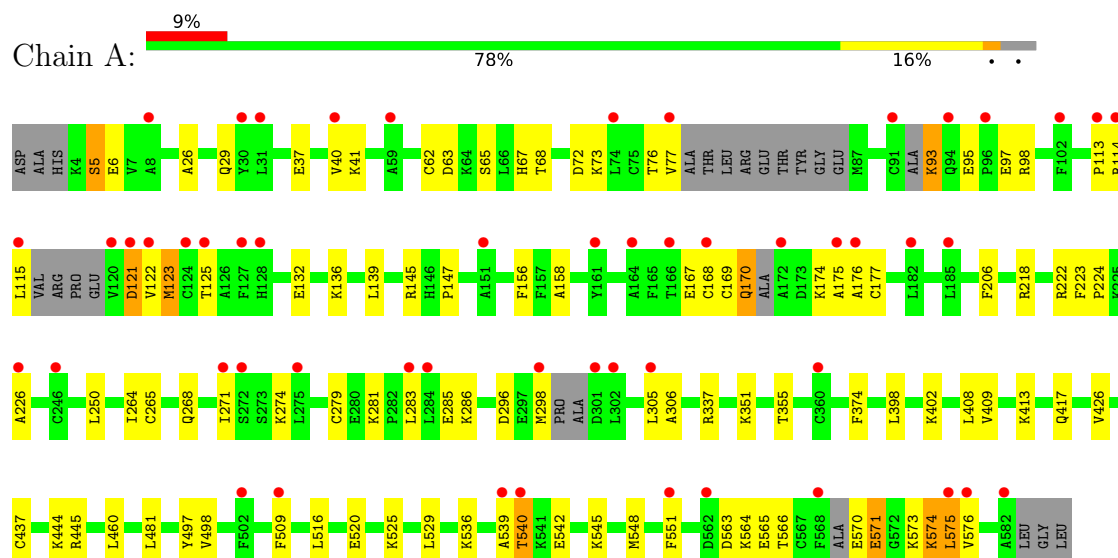
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	92	Total	O	0	0
			92	92		

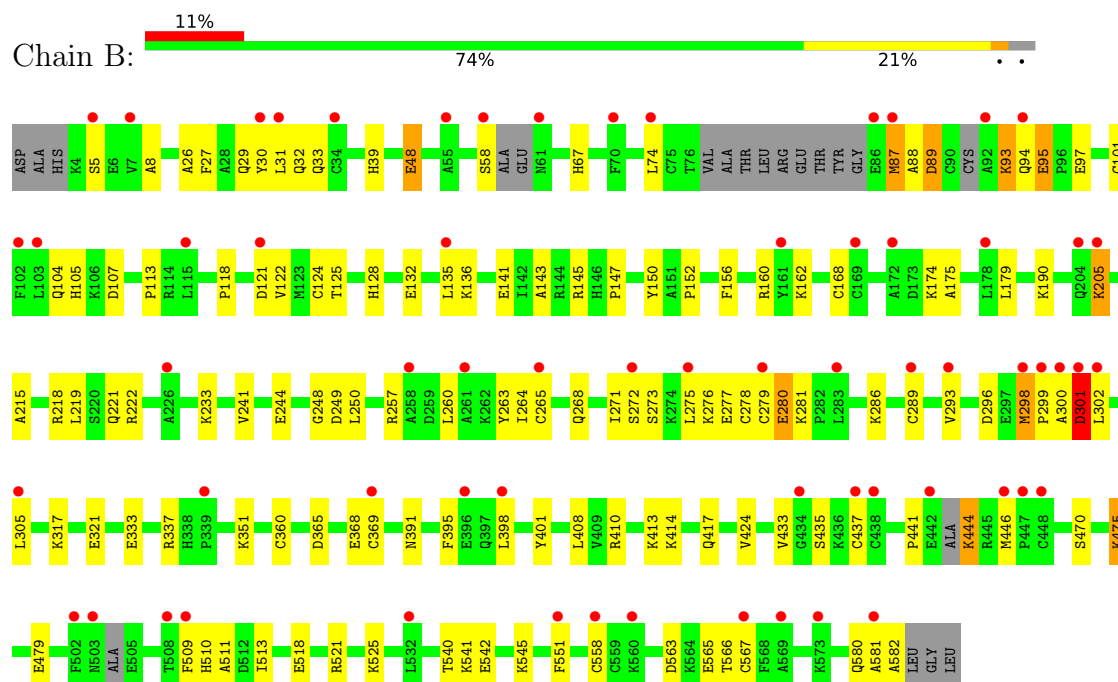
3 Residue-property plots

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: 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	52.09Å 53.03Å 117.42Å 99.17° 93.45° 117.64°	Depositor
Resolution (Å)	19.34 – 2.04 19.34 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.3 (19.34-2.04) 94.1 (19.34-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.04Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.242 , 0.276 0.246 , 0.279	Depositor DCC
R_{free} test set	1972 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9164	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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	0.23	0/4555	0.48	3/6130 (0.0%)
1	B	0.30	0/4584	0.52	3/6173 (0.0%)
All	All	0.27	0/9139	0.50	6/12303 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	MET	N-CA-C	-10.88	100.12	113.50
1	B	89	ASP	N-CA-C	-8.42	102.79	113.23
1	A	121	ASP	N-CA-C	-6.28	105.68	113.15
1	B	48	GLU	N-CA-C	-5.19	105.70	111.36
1	B	88	ALA	N-CA-C	-5.19	105.63	112.94
1	A	122	VAL	N-CA-C	-5.07	106.50	111.77

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	4475	0	4396	72	0
1	B	4502	0	4425	98	0
2	A	95	0	0	4	0
2	B	92	0	0	7	0
All	All	9164	0	8821	170	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 10.

All (170) 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:233:LYS:HE3	1:B:263:TYR:CZ	1.59	1.36
1:B:233:LYS:HE3	1:B:263:TYR:OH	1.51	1.11
1:A:509:PHE:CE1	1:A:551:PHE:CZ	2.50	1.00
1:A:509:PHE:CE1	1:A:551:PHE:CE1	2.65	0.85
1:B:233:LYS:CE	1:B:263:TYR:CZ	2.55	0.82
1:A:73:LYS:HA	1:A:76:THR:HG23	1.65	0.78
1:A:509:PHE:CE1	1:A:551:PHE:HZ	1.98	0.78
1:A:516:LEU:HB3	1:A:520:GLU:HG3	1.66	0.77
1:B:475:LYS:HD3	1:B:479:GLU:OE2	1.84	0.77
1:B:233:LYS:CE	1:B:263:TYR:OH	2.32	0.74
1:A:268:GLN:NE2	2:A:601:HOH:O	2.21	0.72
1:A:536:LYS:HD3	1:A:539:ALA:HB2	1.71	0.71
1:B:233:LYS:HE3	1:B:263:TYR:CE2	2.22	0.71
1:A:5:SER:HB2	1:A:62:CYS:HB3	1.73	0.70
1:A:509:PHE:HE1	1:A:551:PHE:CZ	2.05	0.70
1:B:33:GLN:NE2	2:B:602:HOH:O	2.25	0.69
1:B:475:LYS:NZ	1:B:479:GLU:OE2	2.23	0.68
1:B:222:ARG:HD3	1:B:293:VAL:HG13	1.77	0.67
1:B:141:GLU:HB3	1:B:145:ARG:HH21	1.61	0.66
1:A:408:LEU:HD23	1:A:529:LEU:HD23	1.79	0.65
1:B:27:PHE:HB3	1:B:39:HIS:HD2	1.62	0.64
1:B:32:GLN:HE22	1:B:107:ASP:HB3	1.63	0.64
1:B:268:GLN:HE22	1:B:276:LYS:HB3	1.62	0.64
1:A:121:ASP:OD2	1:A:175:ALA:CA	2.46	0.64
1:A:509:PHE:CZ	1:A:551:PHE:CE1	2.85	0.64
1:A:413:LYS:HZ2	1:A:540:THR:CG2	2.11	0.63
1:A:121:ASP:OD2	1:A:175:ALA:HB2	1.99	0.62
1:B:141:GLU:OE2	1:B:145:ARG:NH2	2.33	0.62
1:B:67:HIS:NE2	1:B:249:ASP:OD1	2.28	0.61
1:B:101:CYS:O	1:B:105:HIS:ND1	2.28	0.61
1:B:542:GLU:HA	1:B:545:LYS:HE3	1.83	0.61
1:B:525:LYS:HG2	1:B:551:PHE:HE1	1.66	0.61
1:B:95:GLU:HB3	1:B:97:GLU:H	1.66	0.60
1:B:281:LYS:O	1:B:286:LYS:HE3	2.03	0.59
1:A:121:ASP:OD2	1:A:175:ALA:N	2.36	0.59
1:A:571:GLU:HA	1:A:574:LYS:HB2	1.82	0.59
1:A:115:LEU:HD22	1:A:145:ARG:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:CG1	1:A:413:LYS:HZ3	2.16	0.58
1:B:475:LYS:CD	1:B:479:GLU:OE2	2.52	0.58
1:A:281:LYS:CG	1:A:285:GLU:HB3	2.34	0.57
1:B:265:CYS:HB3	1:B:275:LEU:HD21	1.86	0.57
1:A:283:LEU:HA	1:A:286:LYS:HE3	1.86	0.56
1:A:121:ASP:CG	1:A:175:ALA:HB2	2.29	0.56
1:A:226:ALA:HB2	1:A:271:ILE:HA	1.88	0.56
1:B:135:LEU:HD11	1:B:162:LYS:HB2	1.87	0.55
1:B:401:TYR:N	2:B:610:HOH:O	2.39	0.55
1:B:277:GLU:HA	1:B:280:GLU:HG3	1.89	0.55
1:B:433:VAL:O	1:B:437:CYS:HB2	2.07	0.55
1:A:279:CYS:SG	2:A:601:HOH:O	2.59	0.54
1:A:409:VAL:HG12	1:A:413:LYS:HZ3	1.71	0.54
1:A:156:PHE:CE1	1:A:285:GLU:HG3	2.43	0.54
1:B:152:PRO:HG2	1:B:257:ARG:HD3	1.88	0.54
1:A:218:ARG:HH21	1:A:222:ARG:HH22	1.54	0.54
1:A:37:GLU:O	1:A:41:LYS:HG2	2.08	0.54
1:A:218:ARG:HH21	1:A:222:ARG:NH2	2.06	0.54
1:A:351:LYS:NZ	1:A:355:THR:OG1	2.39	0.53
1:A:498:VAL:HG12	2:A:654:HOH:O	2.08	0.53
1:B:97:GLU:OE1	1:B:97:GLU:N	2.42	0.53
1:B:391:ASN:O	1:B:395:PHE:N	2.42	0.53
1:B:268:GLN:NE2	1:B:276:LYS:HB3	2.23	0.53
1:B:113:PRO:O	1:B:145:ARG:NH1	2.42	0.53
1:A:174:LYS:O	1:A:176:ALA:N	2.37	0.52
1:B:168:CYS:O	1:B:174:LYS:HG2	2.10	0.52
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.92	0.52
1:B:513:ILE:HG12	1:B:521:ARG:HG3	1.90	0.52
1:B:121:ASP:O	1:B:125:THR:HG23	2.10	0.52
1:B:264:ILE:HG23	1:B:271:ILE:HD13	1.91	0.51
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.75	0.51
1:A:281:LYS:HD2	1:A:285:GLU:CD	2.35	0.51
1:A:525:LYS:HB3	1:A:548:MET:HE1	1.92	0.50
1:B:27:PHE:HD1	1:B:74:LEU:HD13	1.76	0.50
1:B:244:GLU:HB3	1:B:249:ASP:HB2	1.93	0.50
1:A:65:SER:HG	1:A:68:THR:HG1	1.58	0.50
1:A:509:PHE:CZ	1:A:551:PHE:HE1	2.28	0.50
1:B:29:GLN:HG3	1:B:143:ALA:HB1	1.94	0.50
1:A:63:ASP:OD1	1:A:63:ASP:N	2.46	0.49
1:B:408:LEU:HD21	1:B:424:VAL:HA	1.93	0.49
1:B:273:SER:O	1:B:273:SER:OG	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:LYS:NZ	2:B:606:HOH:O	2.31	0.49
1:A:305:LEU:HD13	1:A:337:ARG:NH2	2.28	0.49
1:A:398:LEU:HB3	1:A:402:LYS:HB2	1.95	0.49
1:B:156:PHE:CE2	1:B:160:ARG:HD2	2.48	0.48
1:B:302:LEU:HB3	1:B:337:ARG:NH2	2.28	0.48
1:A:121:ASP:OD2	1:A:175:ALA:CB	2.60	0.48
1:B:260:LEU:O	1:B:264:ILE:HG13	2.13	0.48
1:B:540:THR:C	1:B:542:GLU:H	2.21	0.48
1:A:413:LYS:HZ2	1:A:540:THR:HG23	1.77	0.48
1:B:510:HIS:HB3	1:B:565:GLU:OE1	2.13	0.48
1:B:511:ALA:H	1:B:565:GLU:HG2	1.78	0.48
1:B:8:ALA:N	2:B:611:HOH:O	2.40	0.48
1:A:168:CYS:HB3	1:A:177:CYS:HB3	1.54	0.48
1:B:558:CYS:HB3	1:B:567:CYS:HB3	1.74	0.48
1:B:278:CYS:O	1:B:281:LYS:HG3	2.15	0.47
1:B:413:LYS:HE3	1:B:541:LYS:HE2	1.97	0.47
1:B:132:GLU:HB3	1:B:136:LYS:NZ	2.30	0.47
1:B:510:HIS:HB3	1:B:565:GLU:CD	2.40	0.46
1:A:413:LYS:NZ	1:A:540:THR:CG2	2.78	0.46
1:A:426:VAL:HG21	1:A:460:LEU:HB2	1.96	0.46
1:B:580:GLN:O	1:B:582:ALA:N	2.48	0.46
1:B:241:VAL:HG21	1:B:257:ARG:HB2	1.96	0.46
1:A:72:ASP:N	1:A:98:ARG:NH2	2.63	0.46
1:A:509:PHE:CE1	1:A:551:PHE:HE1	2.28	0.46
1:B:300:ALA:O	1:B:301:ASP:C	2.59	0.46
1:A:563:ASP:C	1:A:564:LYS:HD2	2.40	0.46
1:B:205:LYS:HD3	1:B:205:LYS:HA	1.54	0.46
1:B:317:LYS:O	1:B:321:GLU:HG3	2.16	0.46
1:B:410:ARG:HG2	1:B:414:LYS:HE2	1.97	0.46
1:A:264:ILE:HG22	1:A:265:CYS:H	1.80	0.46
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.90	0.46
1:A:6:GLU:N	2:A:612:HOH:O	2.47	0.46
1:A:26:ALA:HB2	1:A:250:LEU:HD22	1.97	0.46
1:B:298:MET:HE2	1:B:298:MET:HB3	1.77	0.45
1:B:26:ALA:HB2	1:B:250:LEU:HD13	1.97	0.45
1:B:279:CYS:HA	1:B:286:LYS:HG3	1.98	0.45
1:A:222:ARG:HG2	1:A:223:PHE:CE1	2.52	0.45
1:B:565:GLU:N	2:B:603:HOH:O	2.30	0.45
1:B:518:GLU:N	1:B:518:GLU:OE2	2.49	0.45
1:B:27:PHE:HB3	1:B:39:HIS:CD2	2.47	0.45
1:B:93:LYS:HB2	1:B:93:LYS:HE2	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:N	1:B:286:LYS:HE2	2.31	0.44
1:B:218:ARG:HE	1:B:222:ARG:NH2	2.15	0.44
1:B:333:GLU:OE1	1:B:337:ARG:NH1	2.51	0.44
1:A:95:GLU:HA	1:A:98:ARG:HG2	2.00	0.44
1:B:395:PHE:CZ	1:B:435:SER:HA	2.53	0.44
1:B:563:ASP:CB	1:B:566:THR:HB	2.48	0.44
1:B:446:MET:HE3	1:B:446:MET:HB3	1.81	0.43
1:A:132:GLU:O	1:A:136:LYS:HD2	2.17	0.43
1:B:351:LYS:HE3	1:B:351:LYS:HB3	1.68	0.43
1:B:278:CYS:SG	2:B:673:HOH:O	2.61	0.43
1:B:509:PHE:CE2	1:B:551:PHE:HE2	2.37	0.43
1:B:27:PHE:CD1	1:B:74:LEU:HD13	2.51	0.43
1:B:365:ASP:O	1:B:368:GLU:HG2	2.18	0.43
1:A:93:LYS:HD3	1:A:93:LYS:HA	1.44	0.43
1:B:30:TYR:OH	1:B:248:GLY:HA3	2.18	0.43
1:A:139:LEU:HD21	1:A:158:ALA:HB2	2.01	0.43
1:A:123:MET:C	1:A:125:THR:N	2.77	0.42
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.01	0.42
1:A:575:LEU:HD22	1:A:575:LEU:HA	1.83	0.42
1:B:150:TYR:OH	1:B:257:ARG:HD2	2.19	0.42
1:B:417:GLN:HB2	1:B:470:SER:HB2	2.00	0.42
1:B:118:PRO:HB2	1:B:122:VAL:CG1	2.49	0.42
1:B:175:ALA:O	1:B:179:LEU:HD23	2.19	0.42
1:B:441:PRO:HG2	1:B:444:LYS:HB2	2.01	0.42
1:B:104:GLN:NE2	2:B:617:HOH:O	2.51	0.42
1:B:190:LYS:O	1:B:190:LYS:HD3	2.19	0.42
1:B:276:LYS:HB3	1:B:276:LYS:HE3	1.80	0.42
1:A:281:LYS:HG3	1:A:285:GLU:HB3	2.01	0.42
1:A:170:GLN:HE21	1:A:170:GLN:HB3	1.50	0.42
1:A:437:CYS:O	1:A:445:ARG:HG3	2.20	0.42
1:A:542:GLU:O	1:A:545:LYS:HB3	2.20	0.42
1:B:29:GLN:HG2	1:B:147:PRO:HA	2.02	0.41
1:B:31:LEU:HA	1:B:31:LEU:HD12	1.80	0.41
1:B:124:CYS:O	1:B:128:HIS:N	2.49	0.41
1:A:306:ALA:HB2	1:A:374:PHE:HE2	1.85	0.41
1:A:37:GLU:HA	1:A:40:VAL:HG12	2.01	0.41
1:A:132:GLU:OE2	1:A:132:GLU:N	2.54	0.41
1:B:360:CYS:HB3	1:B:369:CYS:HB3	1.83	0.41
1:A:206:PHE:CD2	1:A:481:LEU:HD12	2.56	0.41
1:A:409:VAL:O	1:A:413:LYS:HG3	2.21	0.41
1:B:190:LYS:HD3	1:B:190:LYS:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:O	1:B:219:LEU:HB2	2.20	0.41
1:B:218:ARG:NH1	1:B:221:GLN:OE1	2.54	0.41
1:B:272:SER:HB3	1:B:296:ASP:OD2	2.21	0.41
1:A:417:GLN:HE21	1:A:497:TYR:HD1	1.68	0.40
1:A:564:LYS:O	1:A:566:THR:N	2.54	0.40
1:B:87:MET:HE2	1:B:87:MET:HB3	1.60	0.40
1:A:509:PHE:HE1	1:A:551:PHE:HZ	1.51	0.40
1:B:299:PRO:HB2	1:B:302:LEU:HD11	2.03	0.40
1:A:67:HIS:HB3	1:A:95:GLU:OE2	2.21	0.40
1:B:74:LEU:HD12	1:B:74:LEU:HA	1.85	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	547/585 (94%)	512 (94%)	28 (5%)	7 (1%)	9	3
1	B	553/585 (94%)	512 (93%)	35 (6%)	6 (1%)	11	5
All	All	1100/1170 (94%)	1024 (93%)	63 (6%)	13 (1%)	10	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	A	114	ARG
1	A	565	GLU
1	B	301	ASP
1	A	540	THR
1	B	95	GLU
1	A	5	SER
1	A	167	GLU

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Mol	Chain	Res	Type
1	A	274	LYS
1	B	5	SER
1	B	280	GLU
1	B	298	MET
1	B	581	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	495/511 (97%)	482 (97%)	13 (3%)	40	37
1	B	497/511 (97%)	485 (98%)	12 (2%)	43	40
All	All	992/1022 (97%)	967 (98%)	25 (2%)	42	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	VAL
1	A	93	LYS
1	A	97	GLU
1	A	169	CYS
1	A	170	GLN
1	A	298	MET
1	A	444	LYS
1	A	570	GLU
1	A	571	GLU
1	A	573	LYS
1	A	574	LYS
1	A	575	LEU
1	A	576	VAL
1	B	48	GLU
1	B	58	SER
1	B	87	MET
1	B	89	ASP
1	B	93	LYS

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Mol	Chain	Res	Type
1	B	94	GLN
1	B	205	LYS
1	B	301	ASP
1	B	305	LEU
1	B	398	LEU
1	B	444	LYS
1	B	475	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	295	ASN
1	A	543	GLN
1	B	61	ASN
1	B	580	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	561/585 (95%)	0.63	53 (9%)	14 14	29, 58, 104, 140	0
1	B	565/585 (96%)	0.81	64 (11%)	10 9	29, 64, 107, 136	0
All	All	1126/1170 (96%)	0.72	117 (10%)	11 11	29, 61, 105, 140	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	PRO	4.8
1	B	92	ALA	4.4
1	A	539	ALA	4.3
1	A	540	THR	4.2
1	B	258	ALA	3.8
1	A	77	VAL	3.8
1	B	305	LEU	3.8
1	A	172	ALA	3.7
1	B	58	SER	3.7
1	B	293	VAL	3.7
1	B	103	LEU	3.6
1	B	275	LEU	3.6
1	A	161	TYR	3.6
1	B	509	PHE	3.5
1	A	31	LEU	3.5
1	A	509	PHE	3.4
1	B	569	ALA	3.4
1	A	576	VAL	3.3
1	A	298	MET	3.3
1	A	168	CYS	3.3
1	A	575	LEU	3.3
1	A	74	LEU	3.2
1	B	87	MET	3.2
1	B	302	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	122	VAL	3.2
1	A	113	PRO	3.2
1	B	261	ALA	3.2
1	B	205	LYS	3.2
1	A	115	LEU	3.1
1	B	398	LEU	3.1
1	A	551	PHE	3.1
1	A	40	VAL	3.1
1	A	582	ALA	3.0
1	A	120	VAL	3.0
1	B	74	LEU	2.9
1	B	448	CYS	2.9
1	B	298	MET	2.9
1	B	300	ALA	2.9
1	A	185	LEU	2.9
1	A	164	ALA	2.9
1	B	446	MET	2.8
1	B	161	TYR	2.8
1	B	279	CYS	2.8
1	B	560	LYS	2.8
1	A	124	CYS	2.8
1	B	61	ASN	2.7
1	A	102	PHE	2.7
1	A	502	PHE	2.7
1	A	271	ILE	2.7
1	A	226	ALA	2.7
1	A	568	PHE	2.7
1	B	265	CYS	2.7
1	B	31	LEU	2.6
1	B	115	LEU	2.6
1	B	299	PRO	2.6
1	B	508	THR	2.6
1	A	121	ASP	2.6
1	A	166	THR	2.6
1	A	272	SER	2.6
1	B	30	TYR	2.5
1	B	226	ALA	2.5
1	B	169	CYS	2.5
1	A	283	LEU	2.5
1	B	172	ALA	2.5
1	B	102	PHE	2.5
1	B	502	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	125	THR	2.4
1	B	5	SER	2.4
1	A	175	ALA	2.4
1	A	284	LEU	2.4
1	B	503	ASN	2.4
1	A	562	ASP	2.4
1	B	55	ALA	2.4
1	A	127	PHE	2.4
1	B	272	SER	2.4
1	B	567	CYS	2.4
1	A	30	TYR	2.4
1	A	59	ALA	2.4
1	B	34	CYS	2.4
1	B	339	PRO	2.4
1	A	182	LEU	2.3
1	B	558	CYS	2.3
1	B	204	GLN	2.3
1	B	581	ALA	2.3
1	A	246	CYS	2.3
1	B	438	CYS	2.3
1	A	151	ALA	2.3
1	B	121	ASP	2.3
1	A	94	GLN	2.3
1	B	283	LEU	2.3
1	B	7	VAL	2.2
1	A	176	ALA	2.2
1	B	289	CYS	2.2
1	B	437	CYS	2.2
1	A	302	LEU	2.2
1	B	396	GLU	2.2
1	A	114	ARG	2.2
1	B	573	LYS	2.2
1	A	301	ASP	2.2
1	A	305	LEU	2.2
1	B	434	GLY	2.1
1	A	8	ALA	2.1
1	A	91	CYS	2.1
1	B	301	ASP	2.1
1	A	275	LEU	2.1
1	B	178	LEU	2.1
1	B	86	GLU	2.1
1	B	442	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	369	CYS	2.1
1	B	94	GLN	2.1
1	A	128	HIS	2.1
1	B	447	PRO	2.1
1	B	70	PHE	2.1
1	B	551	PHE	2.1
1	B	532	LEU	2.0
1	A	360	CYS	2.0
1	B	135	LEU	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.