Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 09:12 PM JST

PDB ID	:	7DJN
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:

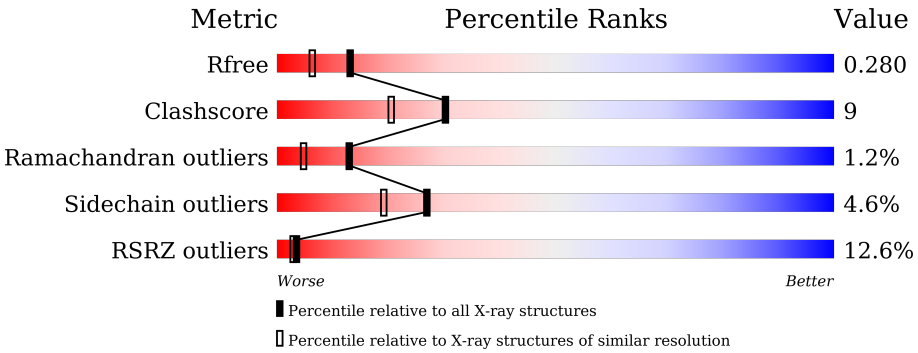
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 <=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	10% 78% 16%
1	B	585	14% 72% 22%

2 Entry composition (i)

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.

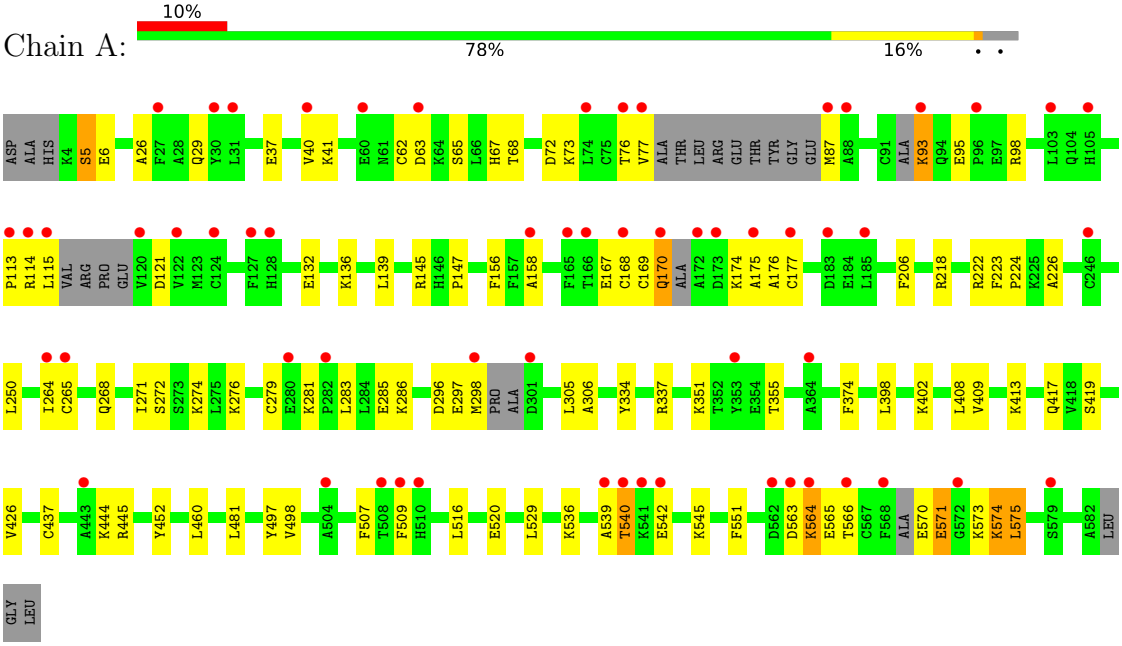
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	92	Total	O	0	0
			92	92		

3 Residue-property plots (i)

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.

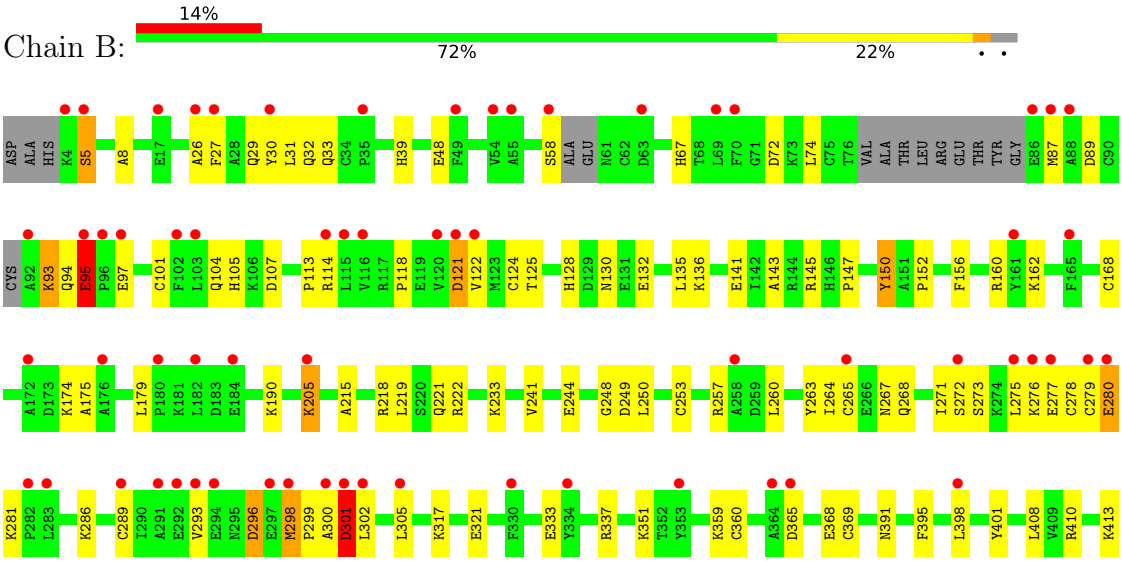
• Molecule 1: Serum albumin

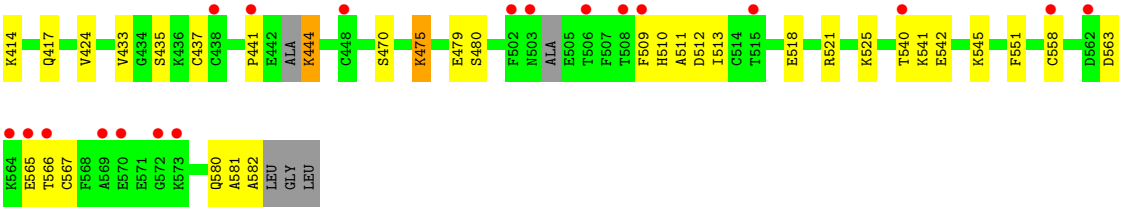
Chain A:



• Molecule 1: Serum albumin

Chain B:




K414
Q417
V424
V433
G434
S435
K436
C437
C438
P441
E442
ALA
K444
C448
S470
K475
E479
S480
F502
N503
ALA
E505
T506
F507
T508
F509
H510
A511
D512
I513
C514
T515
E518
R521
K525
T540
K541
E542
K545
F551
C558
D562
D563
K564
E565
T566
C567
F568
A569
E570
E571
G572
K573
Q580
A581
A582
LEU
GLY
LEU

4 Data and refinement statistics (i)

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) 94.3 (19.34-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.04Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.242 , 0.276 0.246 , 0.280	Depositor DCC
R_{free} test set	1971 reflections (3.04%)	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 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/4555	0.45	0/6130
1	B	0.31	0/4584	0.47	0/6173
All	All	0.30	0/9139	0.46	0/12303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4475	0	4396	70	0
1	B	4502	0	4425	95	0
2	A	95	0	0	4	0
2	B	92	0	0	8	0
All	All	9164	0	8821	165	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 9.

All (165) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:409:VAL:HG12	1:A:413:LYS:HZ3	1.64	0.61
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:A:409:VAL:CG1	1:A:413:LYS:HZ3	2.14	0.60
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:413:LYS:HZ2	1:A:540:THR:CG2	2.20	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: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:A:121:ASP:CG	1:A:175:ALA:HB2	2.29	0.53
1:B:113:PRO:O	1:B:145:ARG:NH1	2.42	0.53
1:A:65:SER:HG	1:A:68:THR:HG1	1.56	0.52
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:281:LYS:HD2	1:A:285:GLU:CD	2.35	0.46
1:A:509:PHE:CE1	1:A:551:PHE:HE1	2.28	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: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:351:LYS:NZ	2:B:607:HOH:O	2.33	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:540:THR:C	1:B:542:GLU:H	2.21	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:413:LYS:HZ2	1:A:540:THR:HG23	1.83	0.43
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:510:HIS:HB3	1:B:565:GLU:CD	2.40	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:B:300:ALA:O	1:B:301:ASP:C	2.59	0.41
1:A:563:ASP:C	1:A:564:LYS:HD2	2.40	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: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: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 (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	547/585 (94%)	512 (94%)	28 (5%)	7 (1%)	12	4
1	B	553/585 (94%)	512 (93%)	35 (6%)	6 (1%)	14	5
All	All	1100/1170 (94%)	1024 (93%)	63 (6%)	13 (1%)	13	5

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
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 (i)

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%)	475 (96%)	20 (4%)	31 24
1	B	497/511 (97%)	471 (95%)	26 (5%)	23 14
All	All	992/1022 (97%)	946 (95%)	46 (5%)	27 19

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	VAL
1	A	87	MET
1	A	93	LYS
1	A	169	CYS
1	A	170	GLN
1	A	272	SER
1	A	276	LYS
1	A	297	GLU
1	A	298	MET
1	A	334	TYR
1	A	419	SER
1	A	444	LYS
1	A	452	TYR
1	A	507	PHE
1	A	564	LYS
1	A	570	GLU
1	A	571	GLU
1	A	573	LYS
1	A	574	LYS
1	A	575	LEU
1	B	5	SER
1	B	48	GLU
1	B	58	SER
1	B	72	ASP
1	B	87	MET
1	B	89	ASP
1	B	93	LYS
1	B	94	GLN
1	B	95	GLU
1	B	114	ARG
1	B	121	ASP
1	B	130	ASN
1	B	150	TYR
1	B	205	LYS
1	B	253	CYS

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Mol	Chain	Res	Type
1	B	267	ASN
1	B	296	ASP
1	B	298	MET
1	B	301	ASP
1	B	305	LEU
1	B	359	LYS
1	B	398	LEU
1	B	444	LYS
1	B	475	LYS
1	B	480	SER
1	B	512	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	543	GLN
1	B	39	HIS
1	B	61	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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%)	0.66	59 (10%)	6 6	29, 58, 104, 140	0
1	B	565/585 (96%)	0.86	83 (14%)	2 2	29, 64, 107, 136	0
All	All	1126/1170 (96%)	0.76	142 (12%)	3 3	29, 61, 105, 140	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	ALA	4.9
1	B	573	LYS	4.9
1	B	88	ALA	4.8
1	B	298	MET	4.8
1	A	124	CYS	4.8
1	A	96	PRO	4.7
1	A	566	THR	4.4
1	A	60	GLU	4.3
1	B	280	GLU	4.3
1	B	506	THR	4.3
1	B	276	LYS	4.2
1	A	540	THR	4.2
1	B	297	GLU	4.2
1	B	502	PHE	4.2
1	A	120	VAL	4.2
1	B	301	ASP	4.1
1	A	443	ALA	4.1
1	B	258	ALA	4.1
1	A	114	ARG	4.0
1	B	277	GLU	4.0
1	B	116	VAL	4.0
1	A	562	ASP	3.9
1	B	87	MET	3.9
1	B	5	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	3.8
1	A	31	LEU	3.7
1	A	168	CYS	3.7
1	B	30	TYR	3.6
1	B	300	ALA	3.6
1	A	185	LEU	3.6
1	B	330	PHE	3.5
1	B	540	THR	3.5
1	B	63	ASP	3.5
1	A	364	ALA	3.5
1	A	170	GLN	3.5
1	A	122	VAL	3.5
1	B	97	GLU	3.4
1	A	88	ALA	3.4
1	A	509	PHE	3.4
1	A	508	THR	3.4
1	B	96	PRO	3.4
1	B	95	GLU	3.4
1	B	565	GLU	3.4
1	A	564	LYS	3.3
1	B	58	SER	3.3
1	A	264	ILE	3.3
1	A	353	TYR	3.2
1	B	282	PRO	3.2
1	B	503	ASN	3.2
1	B	302	LEU	3.2
1	A	298	MET	3.2
1	B	564	LYS	3.2
1	B	508	THR	3.2
1	B	115	LEU	3.2
1	A	173	ASP	3.2
1	A	541	LYS	3.1
1	A	175	ALA	3.1
1	B	265	CYS	3.1
1	B	279	CYS	3.1
1	B	161	TYR	3.0
1	B	283	LEU	3.0
1	B	54	VAL	3.0
1	B	70	PHE	3.0
1	B	305	LEU	3.0
1	B	364	ALA	3.0
1	B	103	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	17	GLU	2.9
1	A	172	ALA	2.9
1	B	441	PRO	2.9
1	B	275	LEU	2.9
1	B	122	VAL	2.8
1	B	172	ALA	2.8
1	A	30	TYR	2.7
1	B	562	ASP	2.7
1	B	291	ALA	2.7
1	B	121	ASP	2.7
1	A	76	THR	2.7
1	A	165	PHE	2.7
1	A	280	GLU	2.6
1	B	294	GLU	2.6
1	A	177	CYS	2.6
1	A	166	THR	2.6
1	A	542	GLU	2.6
1	B	184	GLU	2.6
1	B	509	PHE	2.6
1	A	113	PRO	2.6
1	B	398	LEU	2.6
1	B	165	PHE	2.5
1	A	265	CYS	2.5
1	B	515	THR	2.5
1	A	63	ASP	2.5
1	B	114	ARG	2.5
1	B	365	ASP	2.5
1	B	353	TYR	2.5
1	B	569	ALA	2.5
1	A	539	ALA	2.4
1	A	27	PHE	2.3
1	B	289	CYS	2.3
1	A	77	VAL	2.3
1	B	49	PHE	2.3
1	B	176	ALA	2.3
1	B	438	CYS	2.3
1	A	105	HIS	2.3
1	B	26	ALA	2.3
1	B	448	CYS	2.3
1	B	558	CYS	2.3
1	A	510	HIS	2.2
1	A	127	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	40	VAL	2.2
1	A	563	ASP	2.2
1	B	566	THR	2.2
1	A	103	LEU	2.2
1	A	504	ALA	2.2
1	A	579	SER	2.2
1	B	4	LYS	2.2
1	A	87	MET	2.2
1	B	570	GLU	2.2
1	A	282	PRO	2.2
1	B	180	PRO	2.2
1	B	55	ALA	2.2
1	B	182	LEU	2.1
1	B	102	PHE	2.1
1	B	205	LYS	2.1
1	B	69	LEU	2.1
1	A	128	HIS	2.1
1	A	301	ASP	2.1
1	B	120	VAL	2.1
1	A	568	PHE	2.1
1	A	572	GLY	2.1
1	A	93	LYS	2.1
1	A	183	ASP	2.1
1	B	293	VAL	2.1
1	B	572	GLY	2.1
1	A	158	ALA	2.1
1	B	86	GLU	2.1
1	B	292	GLU	2.1
1	B	334	TYR	2.1
1	B	35	PRO	2.0
1	A	246	CYS	2.0
1	A	74	LEU	2.0
1	B	27	PHE	2.0
1	B	272	SER	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 monosaccharides 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.