Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:17 AM GMT

PDB ID : 4G04
Title : High-resolution Crystal Structural Variance Analysis between Recombinant and Wild-type Human Serum Albumin
Authors : Cao, H.L.; Yin, D.C.
Deposited on : 2012-07-09
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

---
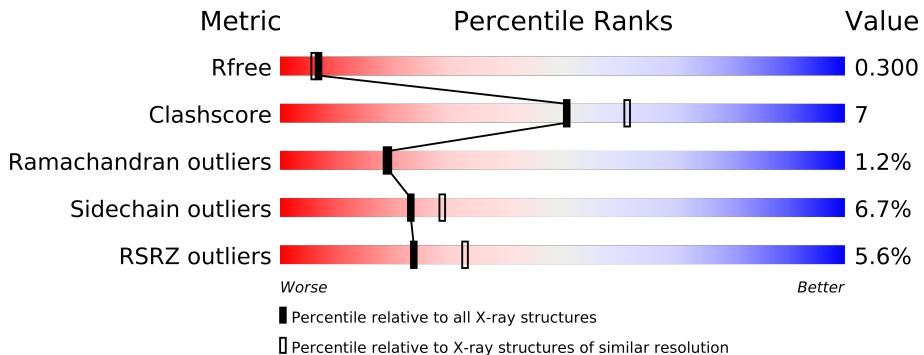
1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.300
Clashscore		7
Ramachandran outliers		1.2%
Sidechain outliers		6.7%
RSRZ outliers		5.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9259 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			4599	2903	776	879	41			
1	B	578	Total	C	N	O	S	0	0	0
			4599	2903	776	879	41			

- Molecule 2 is water.
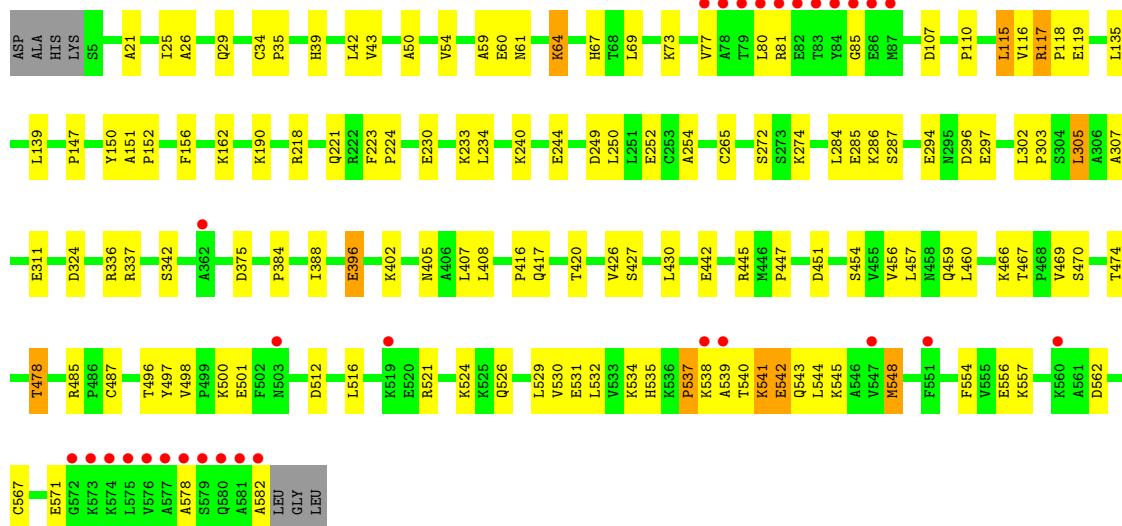
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	32	Total	O	0	0
			32	32		

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 errors 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.
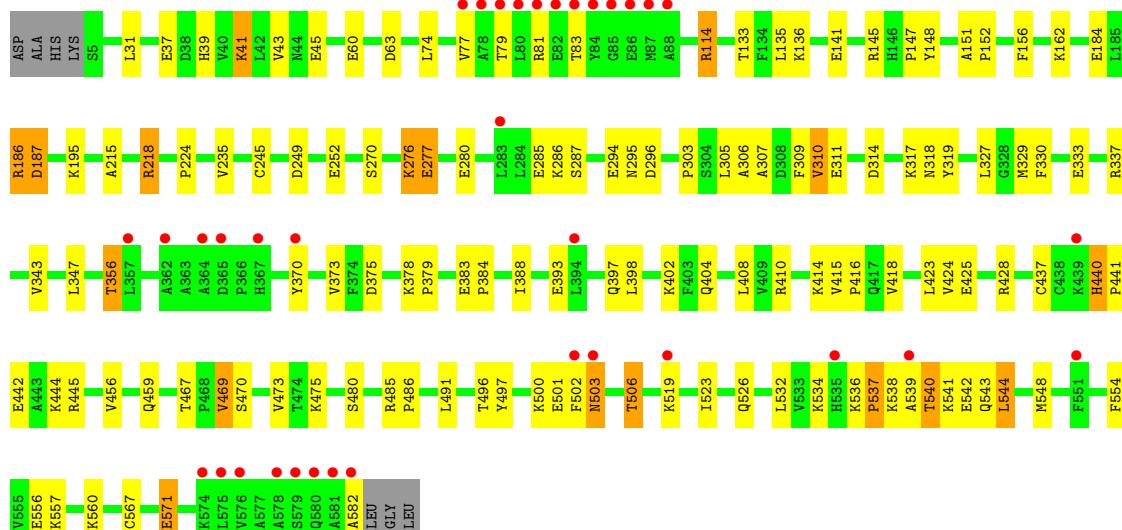
• Molecule 1: Serum albumin

Chain A:

• Molecule 1: Serum albumin

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.74Å 58.66Å 95.73Å 87.85° 75.92° 73.47°	Depositor
Resolution (Å)	47.37 – 2.30 47.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (47.37-2.30) 82.7 (47.37-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.240 , 0.317 0.229 , 0.300	Depositor DCC
R_{free} test set	1834 reflections (4.21%)	DCC
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 47433 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9259	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

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	0.44	0/4688	0.57	0/6324
1	B	0.47	0/4688	0.57	0/6324
All	All	0.45	0/9376	0.57	0/12648

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4599	0	4518	69	0
1	B	4599	0	4518	65	0
2	A	29	0	0	0	0
2	B	32	0	0	1	0
All	All	9259	0	9036	134	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (134) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:PRO:O	1:A:337:ARG:NH1	2.11	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:303:PRO:O	1:B:337:ARG:NH1	2.11	0.82
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.68	0.75
1:A:474:THR:O	1:A:478:THR:OG1	2.07	0.72
1:A:516:LEU:O	1:A:521:ARG:NH2	2.23	0.70
1:B:540:THR:HA	1:B:543:GLN:HE21	1.58	0.69
1:A:537:PRO:O	1:A:539:ALA:N	2.24	0.69
1:A:531:GLU:O	1:A:535:HIS:ND1	2.26	0.68
1:B:114:ARG:HH11	1:B:114:ARG:HB3	1.59	0.67
1:A:578:ALA:HA	1:A:582:ALA:HB3	1.77	0.66
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.79	0.65
1:B:384:PRO:O	1:B:388:ILE:HG12	1.99	0.63
1:B:437:CYS:O	1:B:440:HIS:HB2	2.00	0.61
1:B:156:PHE:HE1	1:B:285:GLU:HG3	1.64	0.61
1:B:414:LYS:HD3	1:B:491:LEU:HB2	1.84	0.60
1:B:156:PHE:CE1	1:B:285:GLU:HG3	2.37	0.59
1:A:427:SER:HA	1:A:430:LEU:HD12	1.84	0.59
1:A:305:LEU:HD11	1:A:337:ARG:HD2	1.85	0.59
1:A:540:THR:HA	1:A:543:GLN:HE21	1.67	0.59
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.68	0.58
1:B:416:PRO:O	1:B:534:LYS:HE2	2.04	0.58
1:B:306:ALA:HA	1:B:310:VAL:HG23	1.86	0.57
1:B:329:MET:O	1:B:333:GLU:HG2	2.04	0.57
1:A:384:PRO:O	1:A:388:ILE:HG12	2.05	0.56
1:A:296:ASP:OD1	1:A:297:GLU:N	2.33	0.56
1:A:156:PHE:CE1	1:A:285:GLU:HG3	2.41	0.56
1:B:314:ASP:HB3	1:B:317:LYS:HB3	1.87	0.56
1:A:42:LEU:HD22	1:A:73:LYS:HG3	1.88	0.56
1:B:276:LYS:O	1:B:280:GLU:HG2	2.05	0.56
1:B:195:LYS:NZ	2:B:631:HOH:O	2.40	0.55
1:B:519:LYS:O	1:B:523:ILE:HG13	2.06	0.55
1:B:141:GLU:OE1	1:B:145:ARG:NH1	2.30	0.54
1:B:276:LYS:HG3	1:B:277:GLU:N	2.22	0.54
1:A:61:ASN:HB3	1:A:64:LYS:HE2	1.90	0.53
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.90	0.52
1:A:554:PHE:CE1	1:A:571:GLU:HB2	2.44	0.52
1:B:567:CYS:O	1:B:571:GLU:HG2	2.10	0.51
1:B:393:GLU:HG2	1:B:397:GLN:NE2	2.25	0.51
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.46	0.51
1:B:415:VAL:HG11	1:B:473:VAL:HG23	1.91	0.51
1:B:428:ARG:NE	1:B:526:GLN:OE1	2.44	0.51
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.93	0.51
1:A:416:PRO:O	1:A:534:LYS:HE2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:356:THR:HG21	1:B:373:VAL:HG22	1.94	0.50
1:B:503:ASN:HB2	1:B:506:THR:OG1	2.12	0.50
1:A:240:LYS:HE2	1:A:244:GLU:OE2	2.11	0.50
1:B:186:ARG:NH1	1:B:187:ASP:OD1	2.45	0.50
1:B:218:ARG:NH2	1:B:295:ASN:OD1	2.45	0.50
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.94	0.49
1:A:408:LEU:HD12	1:A:529:LEU:HD23	1.94	0.49
1:A:223:PHE:HD1	1:A:272:SER:HB2	1.75	0.49
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.94	0.49
1:A:61:ASN:O	1:A:64:LYS:HB2	2.13	0.49
1:A:152:PRO:HG3	1:A:254:ALA:HA	1.95	0.48
1:B:410:ARG:O	1:B:414:LYS:HG3	2.14	0.48
1:A:64:LYS:HB3	1:A:69:LEU:HG	1.94	0.48
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.95	0.48
1:A:21:ALA:O	1:A:25:ILE:HG13	2.14	0.48
1:B:404:GLN:HG2	1:B:428:ARG:HA	1.96	0.47
1:A:405:ASN:ND2	1:A:548:MET:SD	2.87	0.47
1:A:537:PRO:C	1:A:539:ALA:H	2.18	0.47
1:B:135:LEU:HD11	1:B:162:LYS:HG3	1.96	0.47
1:A:50:ALA:O	1:A:54:VAL:HG23	2.14	0.47
1:B:441:PRO:HG2	1:B:444:LYS:HD3	1.96	0.46
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.44	0.46
1:A:426:VAL:HG21	1:A:460:LEU:HB2	1.96	0.46
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.56	0.46
1:B:456:VAL:O	1:B:459:GLN:HB3	2.16	0.46
1:A:540:THR:HA	1:A:543:GLN:NE2	2.30	0.45
1:A:420:THR:OG1	1:A:531:GLU:OE2	2.21	0.45
1:B:538:LYS:HB2	1:B:539:ALA:H	1.45	0.45
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.32	0.45
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.99	0.45
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.52	0.45
1:A:218:ARG:HH21	1:A:221:GLN:HB2	1.82	0.44
1:B:63:ASP:OD1	1:B:63:ASP:N	2.39	0.44
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.99	0.44
1:A:67:HIS:NE2	1:A:249:ASP:OD1	2.51	0.44
1:B:41:LYS:O	1:B:45:GLU:HG3	2.18	0.44
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.81	0.44
1:B:310:VAL:HG12	1:B:370:TYR:O	2.18	0.43
1:B:39:HIS:O	1:B:43:VAL:HG23	2.18	0.43
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.99	0.43
1:A:342:SER:HA	1:A:447:PRO:HA	1.99	0.43
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:343:VAL:O	1:B:347:LEU:HG	2.17	0.43
1:A:230:GLU:O	1:A:234:LEU:HG	2.19	0.43
1:B:307:ALA:HA	1:B:311:GLU:HB2	1.99	0.43
1:B:133:THR:HA	1:B:136:LYS:HE3	2.00	0.43
1:A:402:LYS:HD3	1:A:545:LYS:HE3	2.00	0.43
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.01	0.43
1:B:309:PHE:CZ	1:B:330:PHE:HA	2.54	0.43
1:A:540:THR:HG21	1:A:544:LEU:HD21	2.01	0.43
1:B:428:ARG:NE	1:B:523:ILE:HG12	2.34	0.43
1:B:424:VAL:HG12	1:B:428:ARG:HD2	2.01	0.43
1:A:39:HIS:O	1:A:43:VAL:HG23	2.18	0.42
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.99	0.42
1:B:536:LYS:HE3	1:B:582:ALA:O	2.20	0.42
1:B:501:GLU:HG3	1:B:502:PHE:H	1.84	0.42
1:B:249:ASP:HB3	1:B:252:GLU:CG	2.50	0.42
1:A:107:ASP:O	1:A:110:PRO:HD3	2.19	0.42
1:A:396:GLU:HG2	1:A:396:GLU:H	1.70	0.42
1:A:567:CYS:O	1:A:571:GLU:HG2	2.20	0.42
1:B:319:TYR:HE1	1:B:327:LEU:HD11	1.84	0.42
1:A:417:GLN:HB3	1:A:469:VAL:HG12	2.02	0.42
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.76	0.42
1:B:393:GLU:HG2	1:B:397:GLN:HE21	1.85	0.42
1:B:537:PRO:HB2	1:B:538:LYS:H	1.62	0.42
1:B:541:LYS:HB2	1:B:542:GLU:H	1.73	0.42
1:B:467:THR:O	1:B:469:VAL:N	2.53	0.42
1:A:274:LYS:HE2	1:A:296:ASP:HA	2.01	0.41
1:B:31:LEU:HG	1:B:74:LEU:HD22	2.02	0.41
1:B:215:ALA:HB3	1:B:235:VAL:HG13	2.02	0.41
1:A:541:LYS:HB3	1:A:542:GLU:H	1.54	0.41
1:A:457:LEU:HA	1:A:457:LEU:HD23	1.84	0.41
1:A:485:ARG:HD2	1:A:485:ARG:O	2.20	0.41
1:A:307:ALA:HA	1:A:311:GLU:HB2	2.02	0.41
1:B:416:PRO:HB2	1:B:497:TYR:CD1	2.55	0.41
1:A:451:ASP:O	1:A:454:SER:HB2	2.20	0.41
1:B:544:LEU:HA	1:B:544:LEU:HD22	1.77	0.41
1:B:548:MET:HE3	1:B:548:MET:HA	2.02	0.41
1:B:428:ARG:CZ	1:B:523:ILE:HG12	2.51	0.41
1:A:81:ARG:HG3	1:A:85:GLY:O	2.21	0.41
1:A:407:LEU:HD13	1:A:430:LEU:HB3	2.02	0.41
1:A:526:GLN:O	1:A:530:VAL:HG23	2.21	0.41
1:A:456:VAL:O	1:A:459:GLN:HB3	2.21	0.41
1:A:284:LEU:HA	1:A:284:LEU:HD23	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:418:VAL:HG12	1:B:423:LEU:HG	2.02	0.40
1:B:378:LYS:HB3	1:B:379:PRO:HD3	2.03	0.40
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.86	0.40
1:A:115:LEU:HA	1:A:115:LEU:HD13	1.87	0.40
1:A:442:GLU:HA	1:A:445:ARG:HB2	2.02	0.40
1:B:442:GLU:HG2	1:B:445:ARG:HD2	2.03	0.40
1:B:147:PRO:HG2	1:B:148:TYR:CD1	2.57	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%)	543 (94%)	24 (4%)	9 (2%)	14	12
1	B	576/585 (98%)	538 (93%)	33 (6%)	5 (1%)	25	26
All	All	1152/1170 (98%)	1081 (94%)	57 (5%)	14 (1%)	19	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	537	PRO
1	A	538	LYS
1	B	276	LYS
1	A	501	GLU
1	A	541	LYS
1	B	60	GLU
1	B	537	PRO
1	A	80	LEU
1	B	83	THR
1	B	560	LYS
1	A	59	ALA
1	A	466	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	TYR

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	506/511 (99%)	476 (94%)	30 (6%)	28	35
1	B	506/511 (99%)	468 (92%)	38 (8%)	19	23
All	All	1012/1022 (99%)	944 (93%)	68 (7%)	23	29

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	77	VAL
1	A	115	LEU
1	A	116	VAL
1	A	117	ARG
1	A	119	GLU
1	A	190	LYS
1	A	233	LYS
1	A	287	SER
1	A	294	GLU
1	A	305	LEU
1	A	324	ASP
1	A	336	ARG
1	A	375	ASP
1	A	396	GLU
1	A	467	THR
1	A	470	SER
1	A	478	THR
1	A	487	CYS
1	A	496	THR
1	A	498	VAL
1	A	500	LYS
1	A	512	ASP
1	A	524	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	532	LEU
1	A	542	GLU
1	A	548	MET
1	A	556	GLU
1	A	557	LYS
1	A	562	ASP
1	B	37	GLU
1	B	41	LYS
1	B	77	VAL
1	B	79	THR
1	B	81	ARG
1	B	114	ARG
1	B	184	GLU
1	B	186	ARG
1	B	187	ASP
1	B	218	ARG
1	B	245	CYS
1	B	270	SER
1	B	277	GLU
1	B	286	LYS
1	B	287	SER
1	B	294	GLU
1	B	305	LEU
1	B	310	VAL
1	B	318	ASN
1	B	356	THR
1	B	375	ASP
1	B	425	GLU
1	B	440	HIS
1	B	469	VAL
1	B	470	SER
1	B	475	LYS
1	B	480	SER
1	B	496	THR
1	B	500	LYS
1	B	503	ASN
1	B	506	THR
1	B	532	LEU
1	B	540	THR
1	B	544	LEU
1	B	554	PHE
1	B	556	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	557	LYS
1	B	571	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	543	GLN
1	B	543	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	578/585 (98%)	0.37	30 (5%)	26	36	32, 50, 89, 127	0
1	B	578/585 (98%)	0.34	35 (6%)	21	29	29, 49, 90, 121	0
All	All	1156/1170 (98%)	0.36	65 (5%)	24	33	29, 49, 90, 127	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	LEU	11.6
1	B	582	ALA	10.4
1	A	581	ALA	10.2
1	A	575	LEU	10.2
1	A	85	GLY	9.5
1	A	576	VAL	8.8
1	A	78	ALA	8.8
1	A	577	ALA	7.8
1	A	83	THR	7.1
1	B	82	GLU	7.1
1	A	79	THR	6.9
1	B	578	ALA	6.5
1	B	576	VAL	6.4
1	A	580	GLN	6.3
1	A	82	GLU	6.1
1	A	582	ALA	6.0
1	B	581	ALA	5.5
1	B	83	THR	5.3
1	A	87	MET	4.8
1	B	80	LEU	4.7
1	B	362	ALA	4.2
1	A	80	LEU	4.2
1	B	579	SER	4.1
1	B	85	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	84	TYR	3.8
1	B	81	ARG	3.8
1	A	574	LYS	3.8
1	A	81	ARG	3.7
1	B	88	ALA	3.5
1	B	364	ALA	3.4
1	A	578	ALA	3.4
1	B	574	LYS	3.3
1	B	84	TYR	3.3
1	A	362	ALA	3.3
1	A	539	ALA	3.2
1	B	79	THR	3.1
1	B	365	ASP	3.0
1	A	86	GLU	2.9
1	A	579	SER	2.9
1	B	86	GLU	2.8
1	B	77	VAL	2.8
1	B	367	HIS	2.8
1	B	535	HIS	2.7
1	B	283	LEU	2.7
1	B	551	PHE	2.6
1	A	572	GLY	2.5
1	A	547	VAL	2.4
1	A	519	LYS	2.4
1	B	370	TYR	2.3
1	A	503	ASN	2.3
1	A	538	LYS	2.3
1	B	539	ALA	2.3
1	A	551	PHE	2.2
1	B	87	MET	2.2
1	B	580	GLN	2.2
1	B	502	PHE	2.2
1	B	519	LYS	2.2
1	A	77	VAL	2.2
1	A	560	LYS	2.1
1	A	573	LYS	2.1
1	B	78	ALA	2.1
1	B	439	LYS	2.1
1	B	394	LEU	2.0
1	B	503	ASN	2.0
1	B	357	LEU	2.0

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 carbohydrates in this entry.

6.4　Ligands ⓘ

There are no ligands in this entry.

6.5　Other polymers ⓘ

There are no such residues in this entry.