Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:11 PM GMT

PDB ID : 4G03
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 : 2.22 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

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.22 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		0.287
Clashscore		6
Ramachandran outliers		1.0%
Sidechain outliers		5.3%
RSRZ outliers		5.4%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
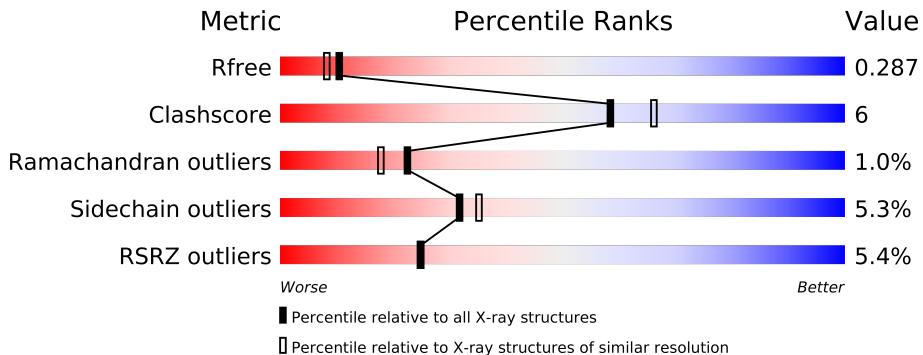
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3340 (2.24-2.20)
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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 9279 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	32	Total	O	0	0
			32	32		
2	B	49	Total	O	0	0
			49	49		

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:
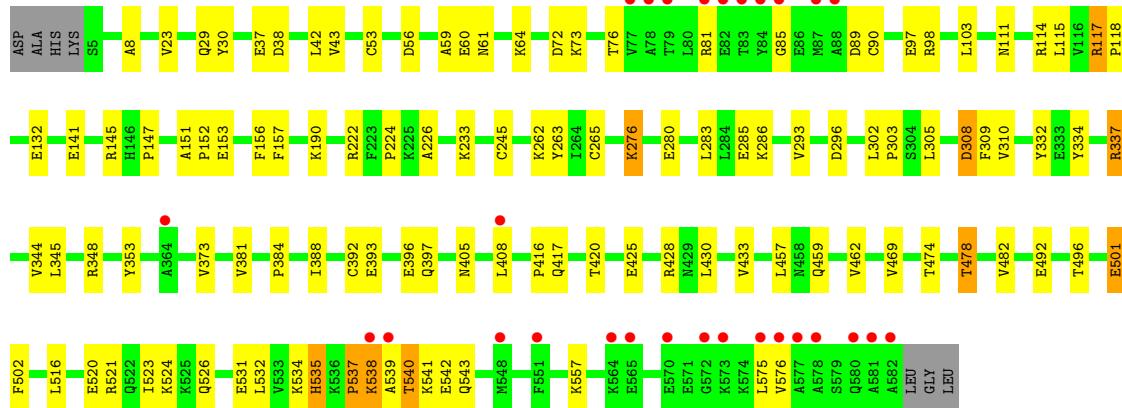
- Molecule 1: Serum albumin

Chain B:
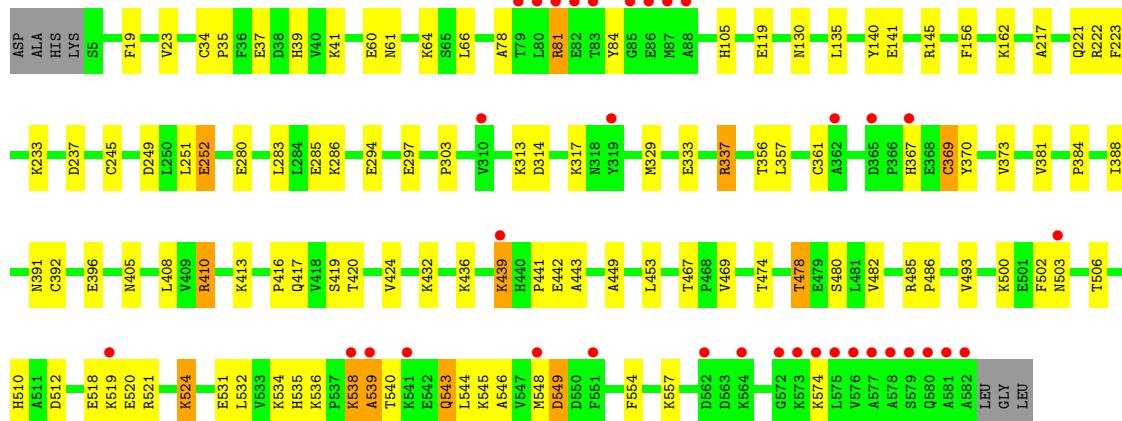
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.57Å 58.67Å 95.67Å 75.71° 88.07° 73.63°	Depositor
Resolution (Å)	47.22 – 2.22 47.22 – 2.22	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.22-2.22) 90.2 (47.22-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.236 , 0.301 0.227 , 0.287	Depositor DCC
R_{free} test set	1852 reflections (3.49%)	DCC
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 56806 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9279	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.41	0/4688	0.54	0/6324
1	B	0.42	0/4688	0.55	0/6324
All	All	0.42	0/9376	0.55	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	57	0
1	B	4599	0	4518	56	0
2	A	32	0	0	0	0
2	B	49	0	0	0	0
All	All	9279	0	9036	113	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 6.

All (113) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:303:PRO:O	1:B:337:ARG:NH1	2.09	0.86

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W O R L D W I D E
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PROTEIN DATA BANK

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:PRO:O	1:A:337:ARG:NH1	2.13	0.80
1:A:502:PHE:HZ	1:A:576:VAL:HB	1.54	0.73
1:A:516:LEU:O	1:A:521:ARG:NH2	2.23	0.70
1:A:405:ASN:HA	1:A:408:LEU:HD12	1.75	0.68
1:B:156:PHE:HE1	1:B:285:GLU:HG3	1.58	0.67
1:A:417:GLN:HB3	1:A:469:VAL:HG12	1.78	0.64
1:B:135:LEU:HD21	1:B:162:LYS:HB2	1.80	0.64
1:B:356:THR:HG21	1:B:373:VAL:HG22	1.82	0.61
1:B:156:PHE:CE1	1:B:285:GLU:HG3	2.36	0.60
1:B:531:GLU:O	1:B:535:HIS:ND1	2.35	0.59
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.85	0.59
1:A:353:TYR:HD1	1:A:373:VAL:HG11	1.68	0.58
1:B:384:PRO:O	1:B:388:ILE:HG12	2.04	0.58
1:B:416:PRO:O	1:B:534:LYS:HE2	2.04	0.58
1:B:313:LYS:HA	1:B:367:HIS:CE1	2.39	0.57
1:B:518:GLU:OE1	1:B:521:ARG:NH1	2.37	0.56
1:A:384:PRO:O	1:A:388:ILE:HG12	2.06	0.56
1:B:540:THR:HB	1:B:544:LEU:HG	1.86	0.56
1:A:392:CYS:O	1:A:396:GLU:HG2	2.05	0.56
1:B:392:CYS:O	1:B:396:GLU:HG2	2.05	0.56
1:A:474:THR:O	1:A:478:THR:OG1	2.20	0.56
1:A:531:GLU:O	1:A:535:HIS:ND1	2.39	0.55
1:B:417:GLN:HB3	1:B:469:VAL:HG12	1.89	0.55
1:B:405:ASN:HA	1:B:408:LEU:HD12	1.88	0.55
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.88	0.54
1:B:369:CYS:SG	1:B:370:TYR:N	2.81	0.54
1:A:276:LYS:O	1:A:280:GLU:HG2	2.08	0.54
1:B:249:ASP:HB3	1:B:252:GLU:CG	2.38	0.53
1:A:540:THR:HA	1:A:543:GLN:HE21	1.74	0.53
1:B:536:LYS:O	1:B:540:THR:HG21	2.09	0.52
1:A:56:ASP:HB3	1:A:59:ALA:HB2	1.92	0.52
1:B:314:ASP:HB3	1:B:317:LYS:HB3	1.92	0.52
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.75	0.51
1:B:520:GLU:O	1:B:524:LYS:HG2	2.10	0.51
1:A:308:ASP:HB2	1:A:309:PHE:CD2	2.46	0.51
1:B:249:ASP:HB3	1:B:252:GLU:HG2	1.94	0.50
1:A:420:THR:OG1	1:A:531:GLU:OE2	2.23	0.50
1:B:546:ALA:HA	1:B:549:ASP:HB2	1.93	0.50
1:B:391:ASN:OD1	1:B:410:ARG:NH2	2.43	0.50
1:A:156:PHE:CE1	1:A:285:GLU:HG3	2.47	0.49
1:A:428:ARG:NE	1:A:526:GLN:OE1	2.45	0.49
1:A:81:ARG:HA	1:A:85:GLY:H	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.42	0.49
1:B:441:PRO:O	1:B:443:ALA:N	2.42	0.49
1:A:233:LYS:HE3	1:A:263:TYR:CZ	2.48	0.49
1:B:502:PHE:HA	1:B:535:HIS:HD2	1.78	0.48
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.95	0.48
1:B:510:HIS:HB3	1:B:512:ASP:OD1	2.13	0.48
1:A:222:ARG:HD3	1:A:293:VAL:HG12	1.96	0.48
1:B:474:THR:O	1:B:478:THR:HB	2.13	0.48
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.29	0.48
1:A:153:GLU:O	1:A:157:PHE:HD1	1.96	0.48
1:B:538:LYS:O	1:B:540:THR:N	2.46	0.48
1:B:329:MET:O	1:B:333:GLU:HG2	2.15	0.47
1:A:353:TYR:CD1	1:A:373:VAL:HG11	2.48	0.47
1:A:42:LEU:HD22	1:A:73:LYS:HG3	1.97	0.47
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.54	0.46
1:B:313:LYS:HG3	1:B:367:HIS:HE1	1.81	0.46
1:B:432:LYS:O	1:B:436:LYS:HG3	2.16	0.46
1:B:370:TYR:O	1:B:373:VAL:HG23	2.16	0.45
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.82	0.45
1:A:61:ASN:HB3	1:A:64:LYS:HE2	1.97	0.45
1:B:217:ALA:O	1:B:221:GLN:HG3	2.16	0.45
1:A:114:ARG:NH2	1:A:520:GLU:OE2	2.48	0.45
1:A:457:LEU:HA	1:A:457:LEU:HD23	1.80	0.45
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.36	0.45
1:A:537:PRO:HB2	1:A:538:LYS:H	1.66	0.45
1:B:233:LYS:NZ	1:B:237:ASP:OD2	2.46	0.45
1:A:416:PRO:O	1:A:534:LYS:HE2	2.16	0.44
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.82	0.44
1:A:90:CYS:O	1:A:98:ARG:HG3	2.17	0.44
1:A:537:PRO:O	1:A:539:ALA:N	2.50	0.44
1:B:19:PHE:O	1:B:23:VAL:HG23	2.18	0.44
1:B:81:ARG:HB2	1:B:81:ARG:HH11	1.83	0.44
1:B:485:ARG:HB3	1:B:486:PRO:HD3	2.00	0.43
1:B:449:ALA:O	1:B:453:LEU:HG	2.18	0.43
1:A:541:LYS:C	1:A:543:GLN:H	2.22	0.43
1:A:345:LEU:HD21	1:A:381:VAL:HG22	1.99	0.43
1:B:439:LYS:O	1:B:439:LYS:NZ	2.39	0.43
1:B:413:LYS:HB3	1:B:493:VAL:HG23	2.00	0.43
1:B:61:ASN:HB3	1:B:64:LYS:HD2	2.01	0.43
1:B:441:PRO:C	1:B:443:ALA:H	2.21	0.43
1:A:501:GLU:O	1:A:535:HIS:HB3	2.18	0.43
1:B:66:LEU:HD13	1:B:251:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:381:VAL:O	1:B:384:PRO:HD2	2.19	0.42
1:A:38:ASP:O	1:A:42:LEU:HG	2.20	0.42
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.42
1:B:544:LEU:C	1:B:546:ALA:H	2.23	0.42
1:A:540:THR:HA	1:A:543:GLN:NE2	2.33	0.42
1:A:393:GLU:O	1:A:397:GLN:HG3	2.20	0.42
1:A:428:ARG:NE	1:A:523:ILE:HG12	2.35	0.42
1:B:39:HIS:HD2	1:B:140:TYR:HE1	1.68	0.42
1:B:503:ASN:HB2	1:B:506:THR:OG1	2.20	0.41
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.79	0.41
1:A:425:GLU:HG2	1:A:459:GLN:NE2	2.36	0.41
1:A:226:ALA:O	1:A:332:TYR:OH	2.34	0.41
1:B:539:ALA:O	1:B:543:GLN:NE2	2.54	0.41
1:B:78:ALA:HA	1:B:84:TYR:CD2	2.55	0.41
1:A:117:ARG:HG3	1:A:117:ARG:O	2.20	0.41
1:A:8:ALA:HB2	1:A:53:CYS:HB3	2.03	0.41
1:B:420:THR:O	1:B:424:VAL:HG23	2.21	0.41
1:A:459:GLN:HA	1:A:462:VAL:HG22	2.03	0.41
1:A:190:LYS:HE2	1:A:190:LYS:HB3	1.88	0.41
1:B:574:LYS:HD3	1:B:574:LYS:HA	1.88	0.40
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.02	0.40
1:B:78:ALA:HA	1:B:84:TYR:HD2	1.87	0.40
1:B:222:ARG:HG2	1:B:223:PHE:CE1	2.56	0.40
1:B:500:LYS:HG2	1:B:535:HIS:CE1	2.57	0.40
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.82	0.40
1:B:141:GLU:OE1	1:B:145:ARG:NH1	2.30	0.40
1:A:430:LEU:O	1:A:433:VAL:HG12	2.21	0.40
1:B:357:LEU:O	1:B:361:CYS:HB2	2.21	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%)	542 (94%)	29 (5%)	5 (1%)	25	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	576/585 (98%)	539 (94%)	31 (5%)	6 (1%)	22	18
All	All	1152/1170 (98%)	1081 (94%)	60 (5%)	11 (1%)	22	18

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	538	LYS
1	B	539	ALA
1	B	60	GLU
1	A	501	GLU
1	A	537	PRO
1	A	542	GLU
1	B	283	LEU
1	B	442	GLU
1	B	538	LYS
1	B	545	LYS

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%)	481 (95%)	25 (5%)	35	39
1	B	506/511 (99%)	477 (94%)	29 (6%)	29	31
All	All	1012/1022 (99%)	958 (95%)	54 (5%)	32	35

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

Mol	Chain	Res	Type
1	A	37	GLU
1	A	89	ASP
1	A	97	GLU
1	A	111	ASN
1	A	117	ARG
1	A	132	GLU
1	A	245	CYS

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Mol	Chain	Res	Type
1	A	262	LYS
1	A	276	LYS
1	A	283	LEU
1	A	305	LEU
1	A	308	ASP
1	A	310	VAL
1	A	334	TYR
1	A	337	ARG
1	A	344	VAL
1	A	478	THR
1	A	492	GLU
1	A	496	THR
1	A	524	LYS
1	A	532	LEU
1	A	535	HIS
1	A	540	THR
1	A	557	LYS
1	A	575	LEU
1	B	37	GLU
1	B	41	LYS
1	B	81	ARG
1	B	105	HIS
1	B	119	GLU
1	B	130	ASN
1	B	245	CYS
1	B	252	GLU
1	B	280	GLU
1	B	286	LYS
1	B	294	GLU
1	B	297	GLU
1	B	337	ARG
1	B	369	CYS
1	B	410	ARG
1	B	419	SER
1	B	439	LYS
1	B	467	THR
1	B	478	THR
1	B	480	SER
1	B	482	VAL
1	B	519	LYS
1	B	524	LYS
1	B	532	LEU

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Mol	Chain	Res	Type
1	B	543	GLN
1	B	548	MET
1	B	549	ASP
1	B	554	PHE
1	B	557	LYS

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	367	HIS

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%)	0.22	28 (4%)	29	29	34, 49, 87, 124	0
1	B	578/585 (98%)	0.19	35 (6%)	21	20	29, 46, 90, 117	0
All	All	1156/1170 (98%)	0.20	63 (5%)	25	25	29, 48, 89, 124	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	ALA	10.5
1	A	577	ALA	10.1
1	B	575	LEU	9.4
1	B	581	ALA	9.3
1	A	83	THR	9.1
1	A	539	ALA	7.8
1	A	79	THR	7.8
1	A	78	ALA	7.2
1	A	81	ARG	7.0
1	B	582	ALA	6.2
1	A	82	GLU	5.8
1	B	564	LYS	5.6
1	A	87	MET	5.3
1	B	574	LYS	5.1
1	B	87	MET	5.0
1	A	575	LEU	4.9
1	A	84	TYR	4.8
1	B	82	GLU	4.8
1	B	577	ALA	4.6
1	B	548	MET	4.6
1	A	582	ALA	4.5
1	A	581	ALA	4.5
1	B	86	GLU	4.4
1	A	573	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	576	VAL	4.1
1	A	576	VAL	4.0
1	A	88	ALA	3.9
1	B	80	LEU	3.9
1	A	77	VAL	3.8
1	B	362	ALA	3.7
1	B	572	GLY	3.7
1	A	580	GLN	3.7
1	B	580	GLN	3.6
1	B	551	PHE	3.5
1	A	538	LYS	3.4
1	B	81	ARG	3.4
1	A	564	LYS	3.2
1	B	83	THR	3.2
1	A	565	GLU	3.2
1	A	570	GLU	3.1
1	A	364	ALA	3.0
1	A	551	PHE	3.0
1	B	79	THR	2.9
1	B	367	HIS	2.9
1	B	365	ASP	2.8
1	B	319	TYR	2.7
1	A	85	GLY	2.7
1	A	578	ALA	2.6
1	B	541	LYS	2.6
1	A	572	GLY	2.5
1	B	578	ALA	2.5
1	B	562	ASP	2.4
1	B	88	ALA	2.4
1	B	579	SER	2.3
1	B	503	ASN	2.3
1	B	439	LYS	2.3
1	B	538	LYS	2.2
1	B	519	LYS	2.2
1	B	573	LYS	2.1
1	B	85	GLY	2.1
1	B	310	VAL	2.1
1	A	548	MET	2.0
1	A	408	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.