



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:56 PM UTC

PDB ID : 7KPG / pdb_00007kpg
Title : Blocking Fab 25 anti-SIRP-alpha antibody in complex with SIRP-alpha Variant 1
Authors : Sim, J.; Pons, J.
Deposited on : 2020-11-11
Resolution : 2.27 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

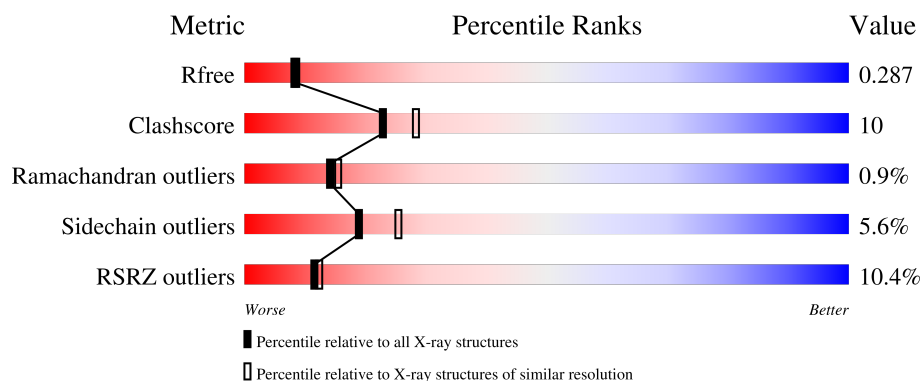
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	H	212	5% 90% 9%
2	L	212	19% 73% 18% 8%
3	S	115	5% 88% 10% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4238 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 Heavy chain of Fab 25 anti-SIRP-alpha antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1587	1000	266	315	6			

- Molecule 2 is a protein called Light chain of Fab 25 anti-SIRP-alpha antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1575	985	256	330	4			

- Molecule 3 is a protein called Tyrosine-protein phosphatase non-receptor type substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	115	Total	C	N	O	S	0	1	0
			885	558	158	166	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	80	ALA	ASN	conflict	UNP P78324

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	54	Total	O	0	0
			54	54		
5	L	67	Total	O	0	0
			67	67		
5	S	45	Total	O	0	0
			45	45		

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.

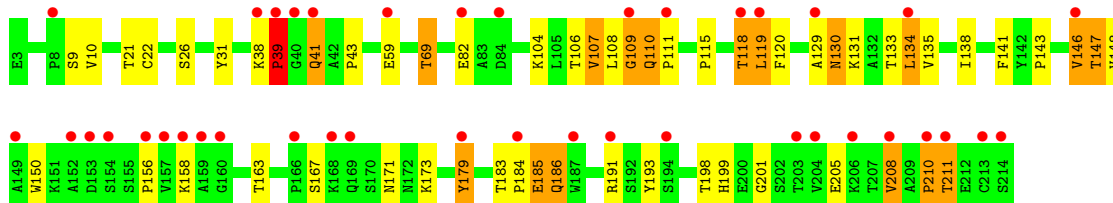
- Molecule 1: Heavy chain of Fab 25 anti-SIRP-alpha antibody

Chain H: 



- Molecule 2: Light chain of Fab 25 anti-SIRP-alpha antibody

Chain L: 



- Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1

Chain S: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	189.16Å 189.16Å 78.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.92 – 2.27 61.92 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.92-2.27) 99.5 (61.92-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.234 , 0.282 0.240 , 0.287	Depositor DCC
R_{free} test set	1972 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4238	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	H	0.81	0/1624	0.98	1/2213 (0.0%)
2	L	0.90	0/1617	1.21	9/2215 (0.4%)
3	S	0.81	0/906	1.02	4/1227 (0.3%)
All	All	0.84	0/4147	1.08	14/5655 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
3	S	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	110	GLN	CB-CA-C	7.79	120.72	109.26
2	L	39	PRO	N-CA-CB	-6.19	96.75	103.25
2	L	143	PRO	CA-C-N	5.92	126.55	119.98
2	L	143	PRO	C-N-CA	5.92	126.55	119.98
2	L	106	THR	CA-C-N	-5.34	113.96	122.50
2	L	106	THR	C-N-CA	-5.34	113.96	122.50
3	S	69	ARG	CA-C-N	5.24	130.31	121.14
3	S	69	ARG	C-N-CA	5.24	130.31	121.14
1	H	105	ASP	CA-CB-CG	5.21	117.81	112.60
3	S	3	GLU	CA-C-N	5.19	128.48	121.05
3	S	3	GLU	C-N-CA	5.19	128.48	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	118	THR	CB-CA-C	5.04	119.91	109.38
2	L	211	THR	CA-C-N	5.00	127.29	120.54
2	L	211	THR	C-N-CA	5.00	127.29	120.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	66	ARG	Sidechain
3	S	77	ARG	Sidechain

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	H	1587	0	1545	17	0
2	L	1575	0	1472	68	0
3	S	885	0	889	8	0
4	H	5	0	0	0	0
4	L	15	0	0	0	0
4	S	5	0	0	1	0
5	H	54	0	0	1	0
5	L	67	0	0	6	0
5	S	45	0	0	0	0
All	All	4238	0	3906	83	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 (83) 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)
2:L:147:THR:HG22	2:L:198:THR:HB	1.19	1.10
2:L:150:TRP:O	2:L:156:PRO:HD2	1.65	0.96
2:L:108:LEU:O	2:L:110:GLN:N	1.99	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:147:THR:CG2	2:L:198:THR:HB	1.98	0.94
2:L:150:TRP:O	2:L:156:PRO:CD	2.18	0.91
3:S:98:SER:HB3	3:S:99:PRO:HD3	1.58	0.83
2:L:138:ILE:HG22	2:L:141:PHE:CD1	2.13	0.83
1:H:171:PRO:O	2:L:163:THR:HG21	1.78	0.83
2:L:147:THR:HG22	2:L:198:THR:CB	2.08	0.81
2:L:115:PRO:CB	2:L:138:ILE:HG23	2.15	0.76
2:L:134:LEU:HD13	2:L:150:TRP:CZ3	2.28	0.68
1:H:171:PRO:HD2	2:L:163:THR:HG22	1.75	0.67
2:L:119:LEU:HD13	2:L:210:PRO:HD3	1.76	0.67
2:L:120:PHE:O	2:L:134:LEU:HD23	1.93	0.67
2:L:138:ILE:HG22	2:L:141:PHE:CE1	2.30	0.66
2:L:193:TYR:O	2:L:210:PRO:HD2	1.95	0.66
2:L:38:LYS:HB2	2:L:39:PRO:HD3	1.76	0.65
2:L:115:PRO:HB2	2:L:138:ILE:HG23	1.78	0.65
2:L:150:TRP:O	2:L:156:PRO:HD3	1.97	0.64
1:H:82:MET:HB3	1:H:85:LEU:HD21	1.79	0.64
2:L:119:LEU:HD23	2:L:120:PHE:H	1.64	0.63
2:L:205:GLU:CD	2:L:205:GLU:N	2.57	0.62
1:H:145:LEU:CD2	2:L:133:THR:HG21	2.31	0.61
2:L:115:PRO:HB3	2:L:138:ILE:HG23	1.82	0.61
2:L:119:LEU:HB2	2:L:208:VAL:CG1	2.31	0.60
2:L:82:GLU:CG	2:L:107:VAL:HG13	2.32	0.59
2:L:115:PRO:HB3	2:L:138:ILE:CG2	2.33	0.59
2:L:205:GLU:CD	2:L:205:GLU:H	2.12	0.58
1:H:149:TYR:CE1	1:H:154:VAL:HG13	2.39	0.58
2:L:119:LEU:HD23	2:L:120:PHE:N	2.19	0.58
1:H:171:PRO:O	2:L:163:THR:CG2	2.52	0.58
2:L:158:LYS:HA	5:L:429:HOH:O	2.04	0.58
2:L:108:LEU:O	2:L:109:GLY:C	2.46	0.57
2:L:129:ALA:O	2:L:130:ASN:CB	2.52	0.57
2:L:134:LEU:HD11	2:L:193:TYR:HB3	1.87	0.56
2:L:69:THR:CG2	5:L:424:HOH:O	2.53	0.56
1:H:145:LEU:HD22	2:L:133:THR:HG21	1.88	0.56
2:L:82:GLU:HG3	2:L:107:VAL:HG13	1.89	0.54
2:L:120:PHE:O	2:L:134:LEU:CD2	2.56	0.53
2:L:141:PHE:CE2	2:L:146:VAL:CG2	2.92	0.53
2:L:141:PHE:CE2	2:L:146:VAL:HG21	2.44	0.53
3:S:77:ARG:NH2	4:S:201:SO4:O2	2.41	0.53
1:H:107:TRP:CD2	2:L:43:PRO:HG2	2.44	0.52
2:L:205:GLU:N	2:L:205:GLU:OE1	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:LEU:C	2:L:110:GLN:N	2.68	0.52
2:L:110:GLN:HG3	2:L:111:PRO:O	2.09	0.51
3:S:98:SER:HB3	3:S:99:PRO:CD	2.38	0.50
2:L:147:THR:CG2	2:L:198:THR:CB	2.80	0.49
2:L:171:ASN:OD1	2:L:173:LYS:HG2	2.13	0.49
2:L:184:PRO:HD2	5:L:456:HOH:O	2.12	0.49
2:L:193:TYR:O	2:L:210:PRO:CD	2.60	0.49
2:L:82:GLU:OE2	2:L:167:SER:OG	2.23	0.49
2:L:185:GLU:HG3	5:L:456:HOH:O	2.12	0.49
1:H:98:GLU:HA	1:H:103:LEU:O	2.15	0.47
1:H:145:LEU:HD21	2:L:133:THR:HG21	1.96	0.47
2:L:69:THR:HG22	5:L:424:HOH:O	2.15	0.47
3:S:31:ILE:HA	3:S:32:PRO:C	2.40	0.47
2:L:130:ASN:O	2:L:184:PRO:HD3	2.14	0.47
2:L:130:ASN:O	2:L:184:PRO:CD	2.63	0.46
2:L:110:GLN:HE21	2:L:111:PRO:HD2	1.80	0.46
1:H:91:ALA:HB3	1:H:93:TYR:CE1	2.52	0.45
2:L:191:ARG:HG3	2:L:211:THR:HG23	1.99	0.45
1:H:6:GLU:HA	1:H:21:SER:O	2.17	0.44
1:H:19:ARG:NH1	5:H:403:HOH:O	2.48	0.44
1:H:56:ASP:OD2	3:S:68:LYS:HD2	2.18	0.44
2:L:138:ILE:HD11	2:L:148:VAL:HG22	2.00	0.44
2:L:39:PRO:HD2	2:L:41:GLN:HB2	1.98	0.44
2:L:131:LYS:HA	2:L:184:PRO:HD3	1.99	0.44
2:L:199:HIS:CD2	2:L:201:GLY:H	2.36	0.43
2:L:108:LEU:O	2:L:110:GLN:O	2.37	0.43
1:H:103:LEU:HD11	2:L:31:TYR:HB3	2.01	0.43
2:L:134:LEU:HD23	2:L:134:LEU:HA	1.80	0.43
2:L:31:TYR:CE1	3:S:96:LYS:HD3	2.53	0.43
2:L:134:LEU:HD13	2:L:150:TRP:HZ3	1.82	0.43
2:L:39:PRO:CD	2:L:41:GLN:HB2	2.49	0.43
1:H:205:LYS:N	1:H:206:PRO:CD	2.81	0.42
3:S:98:SER:CB	3:S:99:PRO:HD3	2.41	0.42
3:S:4:LEU:C	3:S:4:LEU:HD23	2.44	0.42
1:H:154:VAL:HG22	1:H:182:LEU:HD21	2.03	0.41
2:L:183:THR:OG1	2:L:186:GLN:HB2	2.21	0.41
2:L:138:ILE:CG2	2:L:141:PHE:CE1	3.01	0.40
2:L:135:VAL:HG22	2:L:179:TYR:CD1	2.56	0.40
2:L:185:GLU:CG	5:L:456:HOH:O	2.68	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	H	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
2	L	210/212 (99%)	195 (93%)	11 (5%)	4 (2%)	6	5
3	S	114/115 (99%)	111 (97%)	2 (2%)	1 (1%)	14	15
All	All	532/539 (99%)	509 (96%)	18 (3%)	5 (1%)	14	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	39	PRO
2	L	109	GLY
2	L	130	ASN
2	L	210	PRO
3	S	98	SER

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	H	178/178 (100%)	176 (99%)	2 (1%)	65	79
2	L	173/180 (96%)	154 (89%)	19 (11%)	6	6
3	S	95/94 (101%)	91 (96%)	4 (4%)	26	37
All	All	446/452 (99%)	421 (94%)	25 (6%)	19	25

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

Mol	Chain	Res	Type
1	H	147	LYS
1	H	154	VAL
2	L	9	SER
2	L	10	VAL
2	L	21	THR
2	L	22	CYS
2	L	26	SER
2	L	41	GLN
2	L	59	GLU
2	L	69	THR
2	L	104	LYS
2	L	107	VAL
2	L	118	THR
2	L	119	LEU
2	L	134	LEU
2	L	146	VAL
2	L	147	THR
2	L	179	TYR
2	L	185	GLU
2	L	186	GLN
2	L	208	VAL
3	S	15	VAL
3	S	70	ASN
3	S	82	THR
3	S	102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
2	L	36	GLN
2	L	37	GLN
2	L	92	GLN
2	L	110	GLN
2	L	186	GLN
2	L	199	HIS
3	S	70	ASN

5.3.3 RNA ⓘ

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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	L	302	-	4,4,4	0.52	0	6,6,6	0.48	0
4	SO4	L	301	-	4,4,4	0.42	0	6,6,6	0.52	0
4	SO4	L	303	-	4,4,4	0.50	0	6,6,6	0.52	0
4	SO4	S	201	-	4,4,4	0.40	0	6,6,6	0.35	0
4	SO4	H	301	-	4,4,4	0.46	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	201	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	130:PRO	C	137:GLY	N	12.88

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	H	212/212 (100%)	0.35	10 (4%) 36 37	23, 38, 67, 93	0
2	L	212/212 (100%)	0.92	40 (18%) 3 3	22, 38, 68, 82	0
3	S	115/115 (100%)	0.28	6 (5%) 33 33	23, 36, 62, 92	1 (0%)
All	All	539/539 (100%)	0.56	56 (10%) 11 12	22, 37, 67, 93	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	109	GLY	10.6
2	L	152	ALA	6.9
2	L	179	TYR	6.0
2	L	210	PRO	4.9
1	H	137	GLY	4.7
3	S	56[A]	HIS	4.6
2	L	40	GLY	4.4
2	L	159	ALA	4.0
2	L	39	PRO	4.0
3	S	117	LYS	3.9
2	L	213	CYS	3.8
2	L	184	PRO	3.8
2	L	154	SER	3.8
2	L	146	VAL	3.6
3	S	98	SER	3.5
2	L	41	GLN	3.5
2	L	204	VAL	3.4
2	L	156	PRO	3.4
3	S	44	PRO	3.3
1	H	195	THR	3.3
1	H	218	LYS	3.2
2	L	158	LYS	3.2
2	L	129	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	134	LEU	3.0
2	L	194	SER	2.9
2	L	84	ASP	2.9
2	L	187	TRP	2.9
2	L	214	SER	2.8
2	L	169	GLN	2.8
2	L	157	VAL	2.8
2	L	149	ALA	2.8
2	L	8	PRO	2.7
2	L	82	GLU	2.7
2	L	203	THR	2.7
1	H	139	THR	2.6
3	S	99	PRO	2.6
2	L	208	VAL	2.6
2	L	191	ARG	2.6
2	L	118	THR	2.5
2	L	38	LYS	2.4
1	H	191	SER	2.4
2	L	168	LYS	2.3
2	L	59	GLU	2.3
1	H	1	ASP	2.3
2	L	153	ASP	2.3
1	H	9	GLY	2.3
2	L	206	LYS	2.3
2	L	211	THR	2.2
2	L	166	PRO	2.2
1	H	140	ALA	2.2
3	S	70	ASN	2.1
1	H	138	GLY	2.1
2	L	119	LEU	2.1
2	L	160	GLY	2.1
1	H	23	GLU	2.0
2	L	111	PRO	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 oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	H	301	5/5	0.73	0.15	100,101,104,113	0
4	SO4	L	303	5/5	0.76	0.15	78,80,91,95	0
4	SO4	L	302	5/5	0.87	0.15	64,70,85,88	0
4	SO4	L	301	5/5	0.95	0.12	40,45,48,52	0
4	SO4	S	201	5/5	0.95	0.08	49,53,58,58	0

6.5 Other polymers

There are no such residues in this entry.