



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2025 – 10:04 AM EST

PDB ID : 9CQA
Title : Structure of antibody 1G1 bound to the central conserved region of RSV G
Authors : Juarez, M.G.; DuBois, R.M.
Deposited on : 2024-07-19
Resolution : 1.74 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

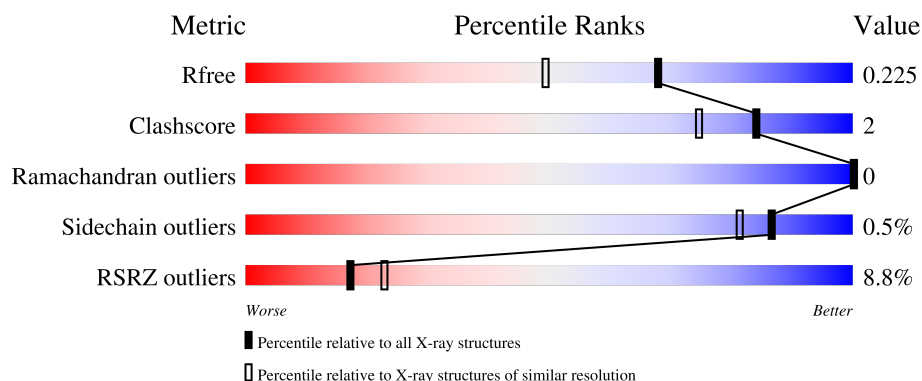
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	164625	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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	D	264	<div> <div>7%</div> <div>78%</div> <div>18%</div> </div>
1	E	264	<div> <div>6%</div> <div>80%</div> <div>18%</div> </div>
2	F	215	<div> <div>9%</div> <div>92%</div> <div>7%</div> </div>
2	G	215	<div> <div>8%</div> <div>93%</div> <div>6%</div> </div>
3	A	49	<div> <div>8%</div> <div>49%</div> <div>6%</div> <div>43%</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	49	<p>10% 49% 6% 43%</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7451 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 Fab 1G1 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	217	Total	C	N	O	S	0	0	0
			1665	1056	283	318	8			
1	D	217	Total	C	N	O	S	0	0	0
			1665	1056	283	318	8			

- Molecule 2 is a protein called Fab1G1 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	213	Total	C	N	O	S	0	0	0
			1625	1018	268	335	4			
2	G	213	Total	C	N	O	S	0	0	0
			1625	1018	268	335	4			

- Molecule 3 is a protein called Mature secreted glycoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	28	Total	C	N	O	S	0	0	0
			229	147	39	39	4			
3	B	28	Total	C	N	O	S	0	0	0
			229	147	39	39	4			

There are 16 discrepancies between the modelled and reference sequences:

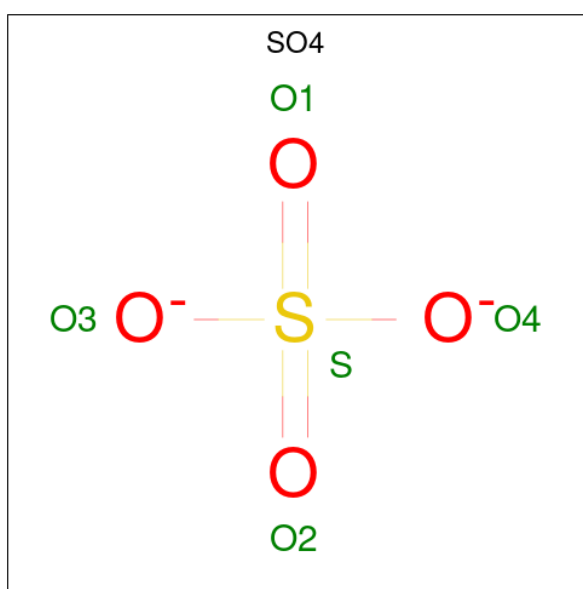
Chain	Residue	Modelled	Actual	Comment	Reference
A	155	MET	-	initiating methionine	UNP P03423
A	156	GLY	-	expression tag	UNP P03423
A	198	HIS	-	expression tag	UNP P03423
A	199	HIS	-	expression tag	UNP P03423
A	200	HIS	-	expression tag	UNP P03423
A	201	HIS	-	expression tag	UNP P03423
A	202	HIS	-	expression tag	UNP P03423
A	203	HIS	-	expression tag	UNP P03423

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Chain	Residue	Modelled	Actual	Comment	Reference
B	155	MET	-	initiating methionine	UNP P03423
B	156	GLY	-	expression tag	UNP P03423
B	198	HIS	-	expression tag	UNP P03423
B	199	HIS	-	expression tag	UNP P03423
B	200	HIS	-	expression tag	UNP P03423
B	201	HIS	-	expression tag	UNP P03423
B	202	HIS	-	expression tag	UNP P03423
B	203	HIS	-	expression tag	UNP P03423

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	102	Total	O	0	0
			102	102		

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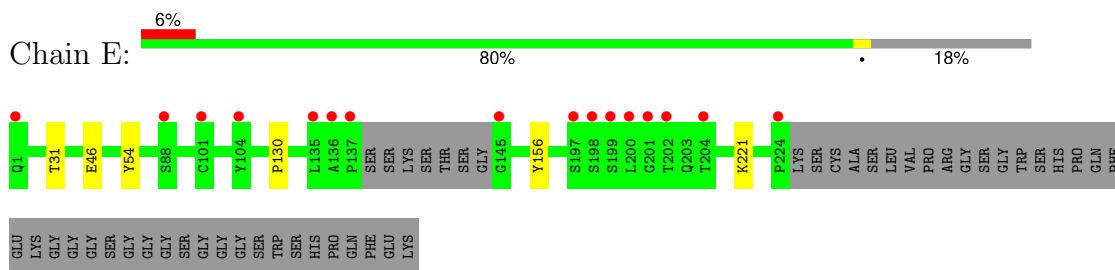
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	98	Total 98	O 98	0	0
5	D	88	Total 88	O 88	0	0
5	G	93	Total 93	O 93	0	0
5	A	6	Total 6	O 6	0	0
5	B	6	Total 6	O 6	0	0

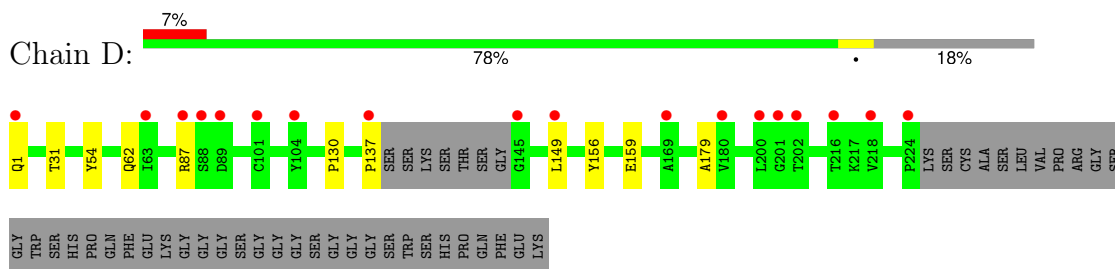
3 Residue-property plots [i](#)

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.

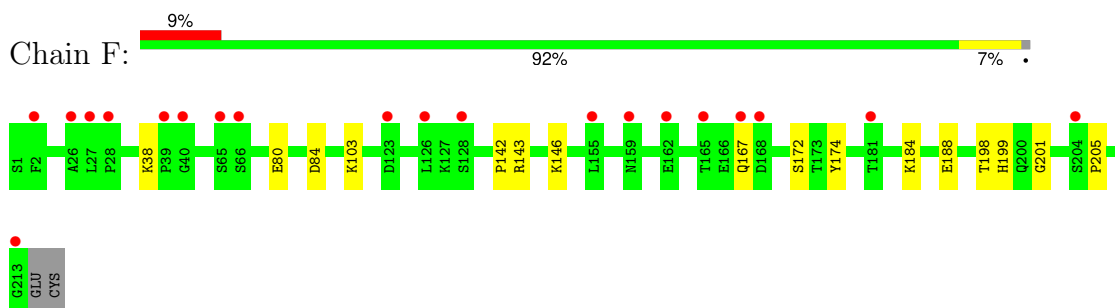
• Molecule 1: Fab 1G1 Heavy Chain



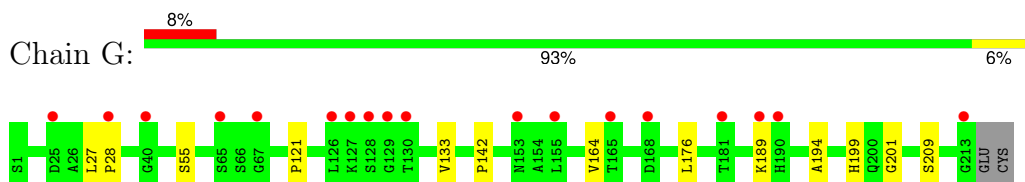
• Molecule 1: Fab 1G1 Heavy Chain



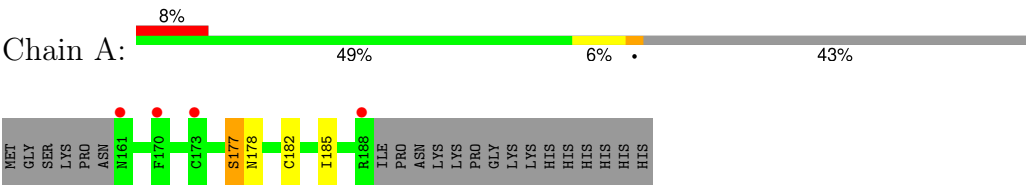
• Molecule 2: Fab1G1 Light Chain



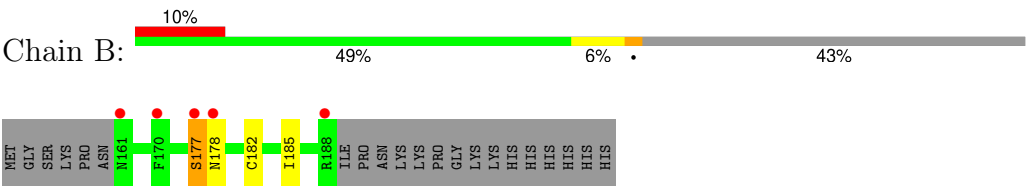
• Molecule 2: Fab1G1 Light Chain



● Molecule 3: Mature secreted glycoprotein G



● Molecule 3: Mature secreted glycoprotein G



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.42Å 80.75Å 175.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 1.74 47.32 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.32-1.74) 99.1 (47.32-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: 000)	Depositor
R, R_{free}	0.211 , 0.225 0.211 , 0.225	Depositor DCC
R_{free} test set	109738 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4440e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	D	0.42	0/1712	0.63	0/2339
1	E	0.41	0/1712	0.61	0/2339
2	F	0.43	0/1661	0.63	0/2264
2	G	0.41	0/1661	0.64	0/2264
3	A	0.41	0/237	0.56	0/322
3	B	0.41	0/237	0.54	0/322
All	All	0.42	0/7220	0.62	0/9850

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	D	1665	0	1606	7	0
1	E	1665	0	1606	5	0
2	F	1625	0	1575	9	0
2	G	1625	0	1575	8	0
3	A	229	0	204	3	0
3	B	229	0	204	3	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	D	88	0	0	1	0
5	E	102	0	0	0	0
5	F	98	0	0	0	0
5	G	93	0	0	0	0
All	All	7451	0	6770	30	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 2.

All (30) 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:D:137:PRO:HG3	1:D:149:LEU:HB3	1.68	0.75
2:G:199:HIS:CD2	2:G:201:GLY:H	2.12	0.67
2:F:199:HIS:CD2	2:F:201:GLY:H	2.12	0.67
3:A:177:SER:OG	3:A:178:ASN:N	2.22	0.66
2:F:184:LYS:NZ	2:F:188:GLU:OE2	2.31	0.53
2:G:142:PRO:O	2:G:199:HIS:HE1	1.95	0.49
2:G:27:LEU:N	2:G:28:PRO:HD2	2.29	0.48
2:F:142:PRO:O	2:F:199:HIS:HE1	1.96	0.47
2:G:164:VAL:HG22	2:G:176:LEU:HD12	1.98	0.46
1:D:54:TYR:O	3:B:182:CYS:HB2	2.15	0.46
1:E:54:TYR:O	3:A:182:CYS:HB2	2.16	0.45
2:F:84:ASP:OD1	2:F:103:LYS:HD3	2.17	0.45
2:F:143:ARG:HB2	2:F:174:TYR:CE2	2.53	0.44
1:D:1:GLN:HB3	5:D:304:HOH:O	2.18	0.44
2:G:194:ALA:HB2	2:G:209:SER:HB3	1.99	0.43
1:D:31:THR:HG22	3:B:185:ILE:HD13	1.99	0.43
2:F:146:LYS:HB3	2:F:198:THR:OG1	2.19	0.43
2:F:38:LYS:HE2	2:F:80:GLU:O	2.18	0.43
2:G:199:HIS:HD2	2:G:201:GLY:H	1.64	0.43
2:G:121:PRO:HD3	2:G:133:VAL:HG22	2.00	0.42
2:F:198:THR:HG22	2:F:205:PRO:HG3	2.01	0.42
2:G:189:LYS:HB3	2:G:189:LYS:HE2	1.84	0.42
1:E:130:PRO:HB3	1:E:156:TYR:HB3	2.03	0.41
1:D:130:PRO:HB3	1:D:156:TYR:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:GLU:HG3	1:D:62:GLN:NE2	2.36	0.41
1:E:31:THR:HG22	3:A:185:ILE:HD13	2.03	0.41
1:E:221:LYS:HB2	1:E:221:LYS:HE3	1.99	0.40
1:D:159:GLU:OE2	1:D:179:ALA:HB3	2.21	0.40
2:F:167:GLN:NE2	2:F:172:SER:OG	2.55	0.40
3:B:177:SER:HB3	3:B:178:ASN:H	1.58	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	D	213/264 (81%)	211 (99%)	2 (1%)	0	100	100
1	E	213/264 (81%)	211 (99%)	2 (1%)	0	100	100
2	F	211/215 (98%)	207 (98%)	4 (2%)	0	100	100
2	G	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
3	A	26/49 (53%)	25 (96%)	1 (4%)	0	100	100
3	B	26/49 (53%)	25 (96%)	1 (4%)	0	100	100
All	All	900/1056 (85%)	887 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	D	185/219 (84%)	184 (100%)	1 (0%)	86	81
1	E	185/219 (84%)	185 (100%)	0	100	100
2	F	186/188 (99%)	186 (100%)	0	100	100
2	G	186/188 (99%)	185 (100%)	1 (0%)	86	81
3	A	27/46 (59%)	26 (96%)	1 (4%)	29	7
3	B	27/46 (59%)	26 (96%)	1 (4%)	29	7
All	All	796/906 (88%)	792 (100%)	4 (0%)	86	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	87	ARG
2	G	55	SER
3	A	177	SER
3	B	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	36	GLN
2	F	167	GLN
2	F	199	HIS
1	D	62	GLN
2	G	36	GLN
2	G	199	HIS
3	B	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	G	301	-	4,4,4	0.42	0	6,6,6	0.12	0
4	SO4	A	301	-	4,4,4	0.41	0	6,6,6	0.07	0
4	SO4	E	301	-	4,4,4	0.44	0	6,6,6	0.08	0
4	SO4	B	301	-	4,4,4	0.42	0	6,6,6	0.08	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.

No monomer is involved in short contacts.

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, 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	D	217/264 (82%)	0.69	18 (8%)	19 24	21, 36, 53, 65	0
1	E	217/264 (82%)	0.56	16 (7%)	22 28	21, 34, 52, 66	0
2	F	213/215 (99%)	0.58	20 (9%)	15 21	21, 33, 48, 55	0
2	G	213/215 (99%)	0.62	18 (8%)	18 24	20, 33, 55, 62	0
3	A	28/49 (57%)	0.90	4 (14%)	7 10	25, 34, 50, 58	0
3	B	28/49 (57%)	1.00	5 (17%)	4 5	25, 35, 51, 56	0
All	All	916/1056 (86%)	0.63	81 (8%)	17 23	20, 34, 52, 66	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	145	GLY	4.8
1	E	137	PRO	4.7
1	D	1	GLN	4.7
1	E	104	TYR	4.3
1	D	145	GLY	4.0
2	G	213	GLY	4.0
2	G	25	ASP	3.9
1	D	104	TYR	3.9
1	E	200	LEU	3.7
1	D	137	PRO	3.7
2	F	213	GLY	3.6
1	E	202	THR	3.6
1	D	224	PRO	3.6
1	E	136	ALA	3.4
2	F	65	SER	3.3
3	B	170	PHE	3.3
2	G	126	LEU	3.3
1	D	202	THR	3.2
1	E	224	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	2	PHE	3.1
3	A	188	ARG	3.1
3	A	170	PHE	3.1
1	D	89	ASP	3.0
1	D	201	GLY	3.0
1	D	101	CYS	3.0
1	D	87	ARG	2.8
1	D	149	LEU	2.8
3	B	178	ASN	2.8
2	G	155	LEU	2.7
3	B	177	SER	2.7
1	D	200	LEU	2.7
2	F	167	GLN	2.7
2	G	153	ASN	2.7
2	F	27	LEU	2.6
2	F	126	LEU	2.6
1	E	198	SER	2.6
2	G	128	SER	2.6
1	E	135	LEU	2.6
2	F	159	ASN	2.6
2	F	168	ASP	2.6
1	E	1	GLN	2.6
3	A	161	ASN	2.6
1	E	204	THR	2.6
3	B	161	ASN	2.5
1	D	216	THR	2.5
2	G	65	SER	2.5
2	F	204	SER	2.5
2	F	40	GLY	2.5
2	G	40	GLY	2.5
1	D	88	SER	2.4
2	G	28	PRO	2.4
3	B	188	ARG	2.4
2	F	165	THR	2.4
2	G	165	THR	2.4
2	G	67	GLY	2.4
1	E	88	SER	2.4
1	D	169	ALA	2.4
2	F	123	ASP	2.3
1	D	63	ILE	2.3
2	G	189	LYS	2.3
2	G	130	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	181	THR	2.3
1	E	199	SER	2.3
1	E	101	CYS	2.2
3	A	173	CYS	2.2
1	D	180	VAL	2.2
1	E	197	SER	2.2
2	F	155	LEU	2.2
2	G	168	ASP	2.2
2	F	162	GLU	2.1
2	F	181	THR	2.1
2	F	28	PRO	2.1
2	G	190	HIS	2.1
2	G	127	LYS	2.1
2	F	39	PRO	2.1
2	F	66	SER	2.1
2	F	128	SER	2.1
1	D	218	VAL	2.1
2	G	129	GLY	2.0
2	F	26	ALA	2.0
1	E	201	GLY	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](#)

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	G	301	5/5	0.88	0.26	30,30,30,30	0
4	SO4	A	301	5/5	0.88	0.31	30,30,30,30	0
4	SO4	B	301	5/5	0.89	0.34	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	E	301	5/5	0.93	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.