



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 AM UTC

PDB ID : 6BFT / pdb_00006bft
Title : Structure of Bevacizumab Fab mutant in complex with VEGF
Authors : Christie, M.; Christ, D.
Deposited on : 2017-10-27
Resolution : 2.55 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:

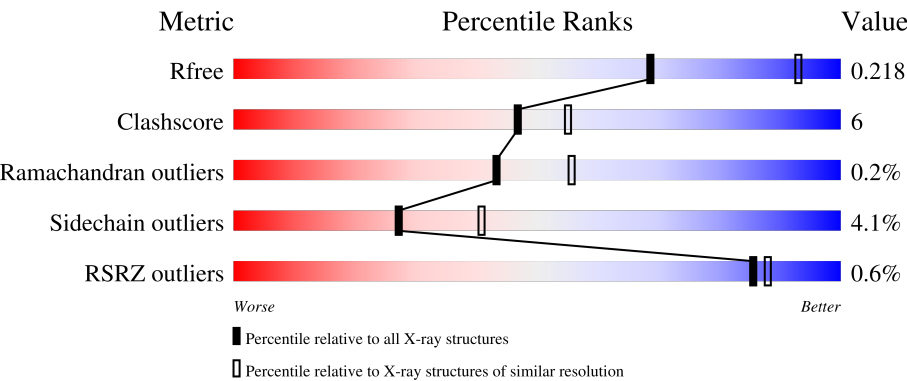
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	B	214	85%15%
1	L	214	85%14%
2	A	231	% 81%14% ••
2	H	231	79%13%6% •
3	C	102	77%15%8%

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Mol	Chain	Length	Quality of chain
3	G	102	2% 79% 14% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8385 atoms, of which 26 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 Avastin Light Chain Fab fragment mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	214	Total	C	N	O	S	0	0	0
			1654	1036	273	339	6			
1	L	213	Total	C	N	O	S	0	0	0
			1648	1033	272	338	5			

- Molecule 2 is a protein called Avastin Heavy Chain Fab fragment mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	224	Total	C	N	O	S	0	0	0
			1705	1087	280	331	7			
2	H	217	Total	C	N	O	S	0	0	0
			1654	1057	271	320	6			

- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	95	Total	C	N	O	S	0	0	0
			771	483	129	146	13			
3	C	94	Total	C	N	O	S	0	0	0
			762	478	128	143	13			

There are 4 discrepancies between the modelled and reference sequences:

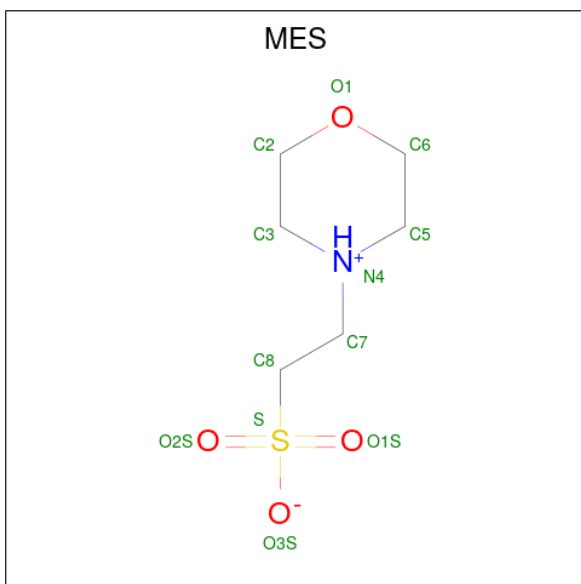
Chain	Residue	Modelled	Actual	Comment	Reference
G	8	GLY	-	cloning artifact	UNP P15692
G	9	PRO	-	cloning artifact	UNP P15692
C	8	GLY	-	cloning artifact	UNP P15692
C	9	PRO	-	cloning artifact	UNP P15692

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



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	20	Total	O		
			20	20	0	0
6	A	24	Total	O		
			24	24	0	0
6	L	36	Total	O		
			36	36	0	0
6	H	35	Total	O		
			35	35	0	0
6	G	8	Total	O		
			8	8	0	0
6	C	8	Total	O		
			8	8	0	0

3 Residue-property plots

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: Avastin Light Chain Fab fragment mutant

Chain B: 



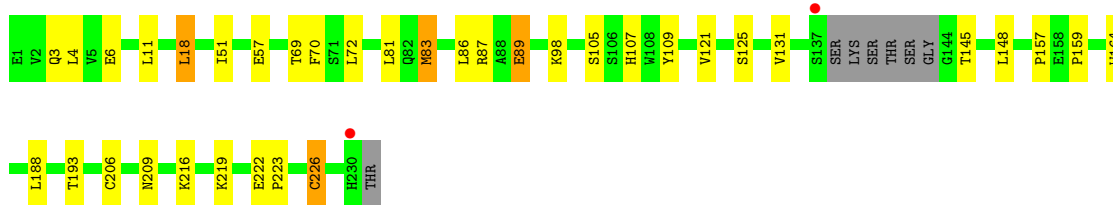
- Molecule 1: Avastin Light Chain Fab fragment mutant

Chain L: 



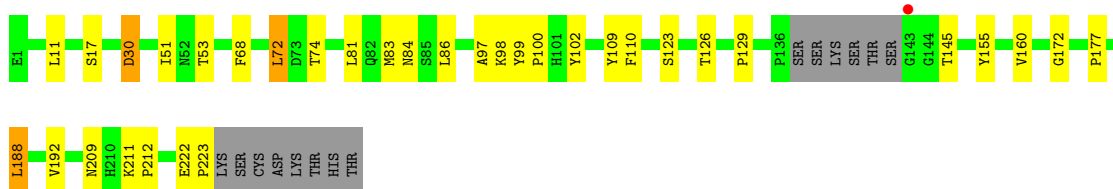
- Molecule 2: Avastin Heavy Chain Fab fragment mutant

Chain A: 

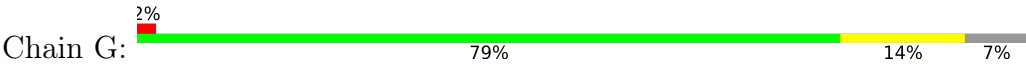


- Molecule 2: Avastin Heavy Chain Fab fragment mutant

Chain H: 



- Molecule 3: Vascular endothelial growth factor A



● Molecule 3: Vascular endothelial growth factor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.28Å 88.75Å 106.68Å 90.00° 111.87° 90.00°	Depositor
Resolution (Å)	45.00 – 2.55 45.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.00-2.55) 99.9 (45.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.170 , 0.220 0.168 , 0.218	Depositor DCC
R_{free} test set	2400 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8385	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: CSO, SO4, MES

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	B	0.40	0/1692	0.60	0/2301
1	L	0.46	0/1686	0.62	0/2293
2	A	0.43	0/1754	0.59	0/2394
2	H	0.44	0/1703	0.63	0/2326
3	C	0.45	0/772	0.67	0/1039
3	G	0.45	0/781	0.63	0/1051
All	All	0.44	0/8388	0.62	0/11404

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	B	1654	0	1588	20	0
1	L	1648	0	1585	17	0
2	A	1705	0	1628	20	0
2	H	1654	0	1580	25	0
3	C	762	0	727	11	0
3	G	771	0	733	10	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	5	0	0	0	0
5	H	24	26	26	1	0
6	A	24	0	0	1	0
6	B	20	0	0	1	0
6	C	8	0	0	0	0
6	G	8	0	0	1	0
6	H	35	0	0	0	0
6	L	36	0	0	1	0
All	All	8359	26	7867	91	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 6.

All (91) 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:189:HIS:O	1:B:211:ARG:NH1	2.01	0.94
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.63	0.81
2:A:57:GLU:O	6:A:301:HOH:O	2.02	0.77
2:H:51:ILE:HD13	2:H:72:LEU:HD13	1.67	0.76
1:B:4:MET:HE3	1:B:23:CYS:SG	2.29	0.72
3:G:59:GLY:N	3:C:32:LEU:HD13	2.10	0.67
2:H:83:MET:HE2	2:H:86:LEU:CD2	2.25	0.65
2:A:83:MET:HB2	2:A:86:LEU:HD21	1.79	0.64
3:G:29:ILE:HD13	3:C:32:LEU:HD12	1.77	0.64
3:G:32:LEU:HD13	3:C:59:GLY:CA	2.27	0.64
1:B:33:LEU:HD22	1:B:71:PHE:CG	2.33	0.63
1:B:191:VAL:HG22	1:B:210:ASN:OD1	2.00	0.61
2:H:51:ILE:CD1	2:H:72:LEU:HD13	2.31	0.61
3:G:59:GLY:CA	3:C:32:LEU:HD13	2.30	0.61
1:L:191:VAL:HG22	1:L:210:ASN:OD1	2.02	0.60
2:H:51:ILE:HD13	2:H:72:LEU:CD1	2.31	0.59
1:B:214:CYS:SG	2:A:226:CYS:HB2	2.43	0.57
3:G:32:LEU:HD13	3:C:59:GLY:HA2	1.85	0.57
1:L:39:LYS:HE2	6:L:405:HOH:O	2.03	0.57
2:A:89:GLU:H	2:A:89:GLU:CD	2.14	0.56
2:A:18:LEU:CD1	2:A:83:MET:HG3	2.35	0.56
1:B:34:ASN:OD1	1:B:49:TYR:HA	2.06	0.56
1:B:175:LEU:C	1:B:175:LEU:HD23	2.31	0.55
2:H:53:THR:HA	2:H:72:LEU:HD21	1.89	0.55
2:H:211:LYS:N	2:H:212:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:SER:HA	1:L:8:PRO:C	2.32	0.54
2:H:188:LEU:C	2:H:188:LEU:HD12	2.32	0.54
3:G:13:GLU:O	6:G:201:HOH:O	2.18	0.53
3:G:16:LYS:O	3:G:20:VAL:HG23	2.08	0.53
2:H:172:GLY:O	2:H:192:VAL:HA	2.09	0.52
2:A:209:ASN:ND2	2:A:216:LYS:HE3	2.24	0.52
1:B:151:ASP:O	1:B:152:ASN:HB2	2.10	0.51
2:A:131:VAL:O	2:A:219:LYS:HE3	2.11	0.51
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.92	0.51
2:H:102:TYR:HB3	3:C:90:HIS:CE1	2.46	0.51
2:H:98:LYS:HE2	2:H:99:TYR:O	2.11	0.50
1:B:11:LEU:HD12	1:B:11:LEU:C	2.37	0.50
2:H:68:PHE:CE2	2:H:83:MET:HG2	2.47	0.50
1:L:4:MET:CE	1:L:23:CYS:SG	3.00	0.49
2:A:148:LEU:C	2:A:148:LEU:HD12	2.37	0.49
1:L:175:LEU:HD23	1:L:176:SER:N	2.27	0.49
1:B:145:LYS:HB3	1:B:197:THR:HB	1.94	0.49
1:L:11:LEU:C	1:L:11:LEU:HD12	2.38	0.49
2:A:70:PHE:CE1	2:A:81:LEU:HD13	2.48	0.49
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.95	0.49
1:B:29:ILE:O	1:B:30:SER:HB2	2.13	0.49
2:A:18:LEU:HD12	2:A:18:LEU:N	2.27	0.49
3:C:35:ILE:HD11	3:C:52:VAL:HG13	1.95	0.48
1:L:80:PRO:HA	1:L:106:ILE:HG12	1.96	0.48
1:B:7:SER:HA	1:B:8:PRO:C	2.39	0.47
2:A:89:GLU:OE1	2:A:89:GLU:N	2.48	0.47
2:H:11:LEU:HD12	2:H:126:THR:HG22	1.96	0.47
1:L:19:VAL:HG21	1:L:78:LEU:HD22	1.97	0.47
2:A:222:GLU:HB2	2:A:223:PRO:CD	2.46	0.46
2:H:222:GLU:HB2	2:H:223:PRO:HD2	1.97	0.46
1:B:34:ASN:ND2	2:A:109:TYR:HB3	2.32	0.45
2:A:51:ILE:HD13	2:A:72:LEU:HD21	1.97	0.45
2:A:164:TRP:CZ3	2:A:206:CYS:HB3	2.52	0.45
1:L:129:THR:HG22	1:L:130:ALA:N	2.31	0.45
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.97	0.45
1:B:50:PHE:CG	2:A:107:HIS:CE1	3.05	0.45
2:H:17:SER:HB3	2:H:84:ASN:HB3	1.98	0.45
2:H:74:THR:HG21	5:H:302:MES:H51	1.98	0.45
3:G:33:VAL:O	3:G:51:CYS:HB2	2.17	0.45
2:A:70:PHE:HE1	2:A:81:LEU:HD13	1.80	0.44
1:B:91:TYR:HA	1:B:96:TRP:CE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:VAL:O	2:H:177:PRO:HG2	2.17	0.44
2:A:87:ARG:O	2:A:121:VAL:HG21	2.18	0.43
3:G:21:TYR:CD2	3:C:49:PRO:HB3	2.53	0.43
2:H:30:ASP:N	2:H:30:ASP:OD1	2.51	0.43
1:L:83:PHE:HZ	1:L:165:GLU:OE2	2.01	0.42
2:H:211:LYS:N	2:H:212:PRO:HD3	2.34	0.42
1:L:175:LEU:HD23	1:L:175:LEU:C	2.44	0.42
2:H:100:PRO:HG3	2:H:109:TYR:CZ	2.54	0.42
1:B:151:ASP:OD2	1:B:189:HIS:HB3	2.20	0.42
2:H:68:PHE:HD2	2:H:81:LEU:HD11	1.84	0.42
2:H:97:ALA:HB1	2:H:110:PHE:HB3	2.01	0.42
1:L:145:LYS:HB3	1:L:197:THR:HB	2.01	0.41
3:C:73:GLU:HB3	3:C:97:LEU:HD11	2.02	0.41
1:L:140:TYR:CD2	1:L:141:PRO:HA	2.56	0.41
3:C:16:LYS:O	3:C:20:VAL:HG23	2.20	0.41
1:L:23:CYS:SG	1:L:88:CYS:SG	3.11	0.41
2:H:100:PRO:HG3	2:H:109:TYR:CE1	2.56	0.41
1:B:45:LYS:NZ	6:B:402:HOH:O	2.53	0.40
1:B:211:ARG:HB3	1:B:211:ARG:CZ	2.51	0.40
1:B:125:LEU:O	1:B:183:LYS:HD2	2.20	0.40
1:L:142:ARG:NH1	1:L:163:VAL:HB	2.37	0.40
3:G:78:MET:HG2	3:C:15:VAL:HB	2.03	0.40
1:B:61:ARG:HD2	1:B:77:SER:O	2.21	0.40
2:A:222:GLU:HB2	2:A:223:PRO:HD3	2.03	0.40
2:A:11:LEU:HG	2:A:157:PRO:HG3	2.03	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	B	212/214 (99%)	204 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
2	A	220/231 (95%)	210 (96%)	10 (4%)	0	100	100
2	H	213/231 (92%)	207 (97%)	6 (3%)	0	100	100
3	C	91/102 (89%)	88 (97%)	2 (2%)	1 (1%)	11	15
3	G	92/102 (90%)	88 (96%)	3 (3%)	1 (1%)	11	15
All	All	1039/1094 (95%)	999 (96%)	38 (4%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	CYS
3	G	26	CYS

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	B	191/191 (100%)	187 (98%)	4 (2%)	47	66
1	L	190/191 (100%)	184 (97%)	6 (3%)	34	51
2	A	186/194 (96%)	171 (92%)	15 (8%)	11	15
2	H	180/194 (93%)	173 (96%)	7 (4%)	28	43
3	C	88/95 (93%)	85 (97%)	3 (3%)	32	48
3	G	89/95 (94%)	86 (97%)	3 (3%)	32	48
All	All	924/960 (96%)	886 (96%)	38 (4%)	27	41

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	THR
1	B	106	ILE
1	B	181	LEU
1	B	190	LYS

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Mol	Chain	Res	Type
2	A	3	GLN
2	A	4	LEU
2	A	6	GLU
2	A	18	LEU
2	A	69	THR
2	A	83	MET
2	A	89	GLU
2	A	98	LYS
2	A	105	SER
2	A	125	SER
2	A	145	THR
2	A	159	PRO
2	A	188	LEU
2	A	193	THR
2	A	226	CYS
1	L	23	CYS
1	L	24	SER
1	L	106	ILE
1	L	143	GLU
1	L	152	ASN
1	L	207	LYS
2	H	30	ASP
2	H	72	LEU
2	H	123	SER
2	H	145	THR
2	H	160	VAL
2	H	188	LEU
2	H	209	ASN
3	G	95	SER
3	G	105	ARG
3	G	107	LYS
3	C	22	GLN
3	C	63	ASP
3	C	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	ASN
1	B	79	GLN
1	B	160	GLN
2	A	202	GLN

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Mol	Chain	Res	Type
1	L	31	ASN
2	H	202	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	CSO	G	60	3	3,6,7	0.82	0	1,6,8	0.95	0
3	CSO	C	60	3	3,6,7	1.05	0	1,6,8	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CSO	G	60	3	-	0/1/5/7	-
3	CSO	C	60	3	-	0/1/5/7	-

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.

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
5	MES	H	302	-	12,12,12	2.31	1 (8%)	15,16,16	1.48	2 (13%)
4	SO4	B	301	-	4,4,4	0.26	0	6,6,6	0.15	0
5	MES	H	301	-	12,12,12	2.09	1 (8%)	15,16,16	1.74	3 (20%)
4	SO4	L	301	-	4,4,4	0.27	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	H	302	-	-	3/6/14/14	0/1/1/1
5	MES	H	301	-	-	4/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	302	MES	C8-S	-7.62	1.66	1.77
5	H	301	MES	C8-S	-6.92	1.67	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	MES	O1S-S-C8	3.64	112.23	106.73
5	H	302	MES	C5-N4-C3	3.52	116.42	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	MES	O2S-S-C8	3.46	111.96	106.73
5	H	301	MES	C5-N4-C3	3.37	116.10	108.84
5	H	302	MES	O3S-S-C8	2.32	110.55	106.00

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	MES	C7-C8-S-O1S
5	H	301	MES	C7-C8-S-O2S
5	H	301	MES	C7-C8-S-O3S
5	H	302	MES	C8-C7-N4-C3
5	H	302	MES	C8-C7-N4-C5
5	H	301	MES	C8-C7-N4-C5
5	H	302	MES	C7-C8-S-O3S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	302	MES	1	0

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	B	214/214 (100%)	-0.40	1 (0%) 87 89	22, 37, 61, 77	0
1	L	213/214 (99%)	-0.57	0 100 100	17, 30, 54, 71	0
2	A	224/231 (96%)	-0.24	2 (0%) 81 83	22, 39, 65, 80	0
2	H	217/231 (93%)	-0.56	1 (0%) 87 89	18, 30, 53, 72	0
3	C	93/102 (91%)	-0.43	0 100 100	20, 33, 52, 71	0
3	G	94/102 (92%)	-0.21	2 (2%) 63 64	25, 37, 66, 89	0
All	All	1055/1094 (96%)	-0.42	6 (0%) 85 88	17, 35, 61, 89	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	143	GLY	4.9
2	A	137	SER	2.8
3	G	13	GLU	2.7
3	G	43	ILE	2.4
1	B	214	CYS	2.4
2	A	230	HIS	2.3

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

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
3	CSO	C	60	7/8	0.96	0.09	26,34,55,61	0
3	CSO	G	60	7/8	0.97	0.09	21,30,51,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	SO4	L	301	5/5	0.88	0.15	76,77,84,88	0
4	SO4	B	301	5/5	0.89	0.16	73,76,79,80	0
5	MES	H	301	12/12	0.96	0.09	49,62,70,71	0
5	MES	H	302	12/12	0.96	0.08	50,61,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.