



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:54 PM UTC

PDB ID : 8TS5 / pdb_00008ts5
Title : Structure of the apo FabS1C_C1
Authors : Singer, A.U.; Bruce, H.A.; Blazer, L.L.; Adams, J.J.; Sicheri, F.; Sidhu, S.S.
Deposited on : 2023-08-10
Resolution : 2.10 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

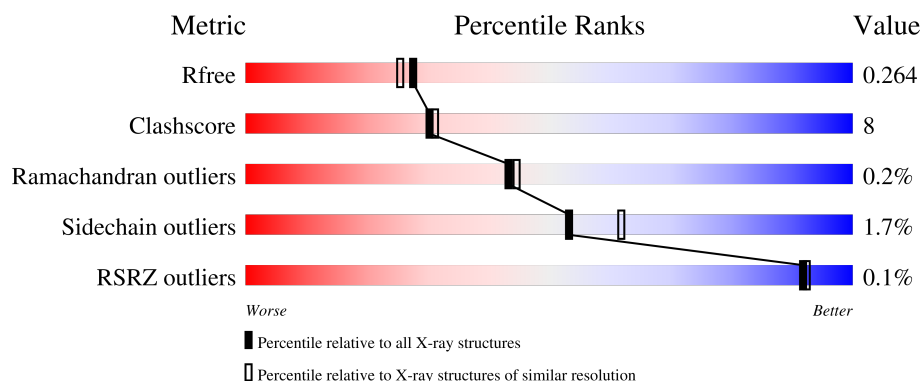
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

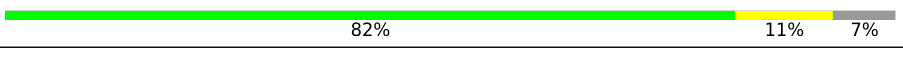
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	A	223	 79% 17% .
1	B	223	 82% 11% 7%
2	C	215	 79% 19% ..
2	G	215	 82% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	302	-	-	X	-
4	PEG	A	307	-	-	X	-
5	EDO	A	309	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7063 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.

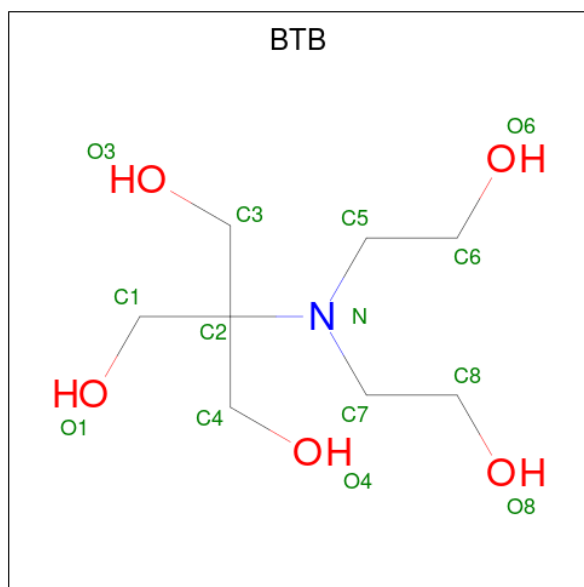
- Molecule 1 is a protein called S1C variant of Fab C1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1603	1018	261	317	7			
1	B	208	Total	C	N	O	S	0	0	0
			1551	987	251	306	7			

- Molecule 2 is a protein called S1C variant of Fab C1 light chain.

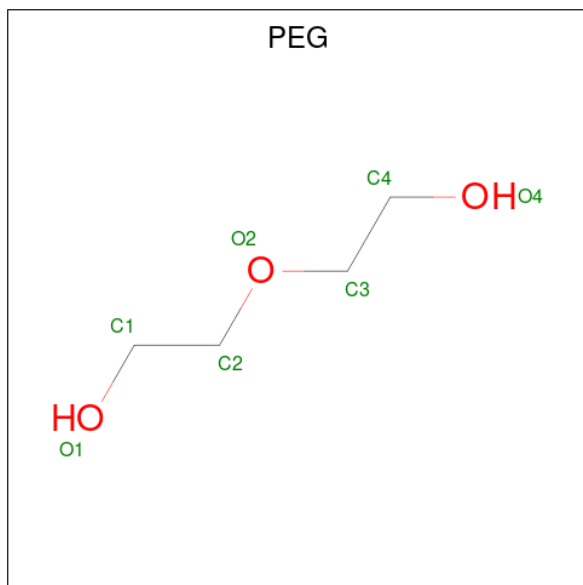
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	213	Total	C	N	O	S	0	1	0
			1629	1021	267	336	5			
2	C	211	Total	C	N	O	S	0	2	0
			1618	1010	266	336	6			

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	1
			14	8	6		
4	G	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	1
			8	4	4		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total Na 4 4	0	0
7	G	2	Total Na 2 2	0	0
7	B	2	Total Na 2 2	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	G	1	Total Cl 1 1	0	0

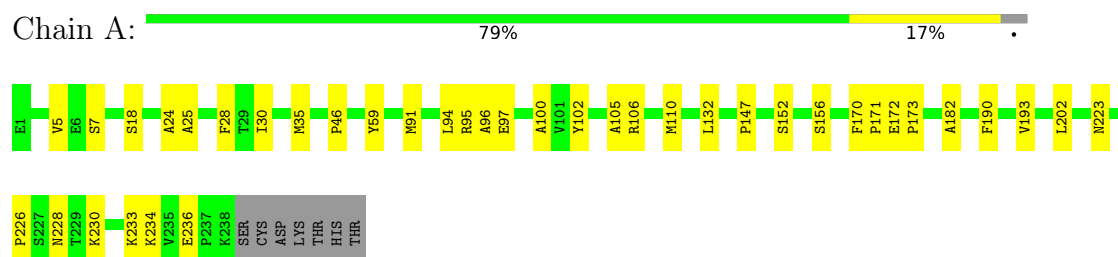
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	146	Total 151	O 151	0	5
9	G	142	Total 145	O 145	0	3
9	B	98	Total 99	O 99	0	1
9	C	90	Total 92	O 92	0	2

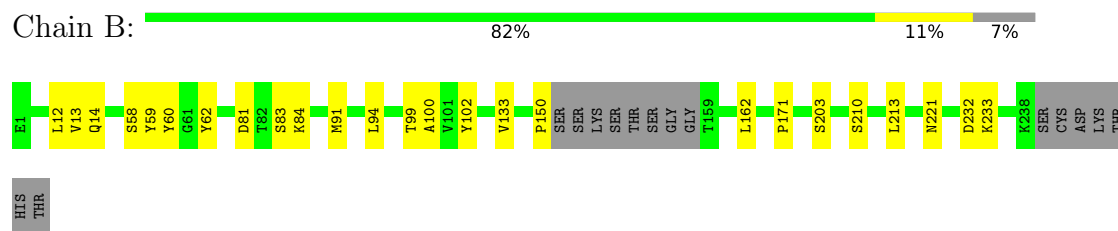
3 Residue-property plots

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.

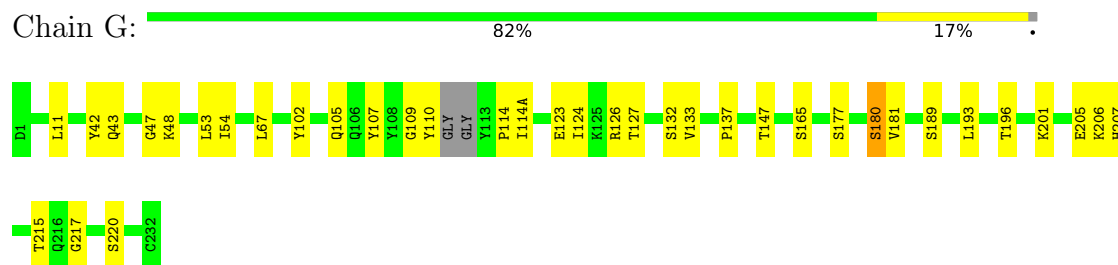
- Molecule 1: S1C variant of Fab C1 heavy chain



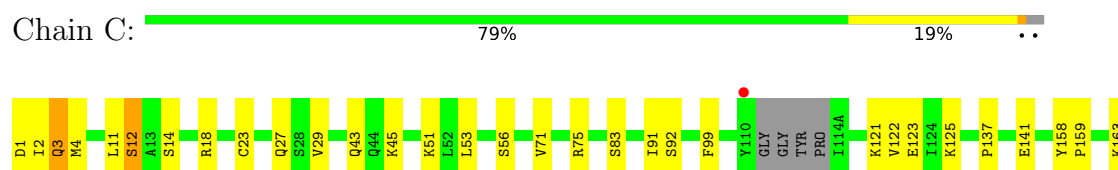
- Molecule 1: S1C variant of Fab C1 heavy chain



- Molecule 2: S1C variant of Fab C1 light chain



- Molecule 2: S1C variant of Fab C1 light chain



Y167	V168	D169	E163	K201	E205	K206	H207	A211	K225	S226	F227	N228	E231	C232
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.69Å 73.79Å 174.20Å 90.00° 96.37° 90.00°	Depositor
Resolution (Å)	86.56 – 2.10 86.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (86.56-2.10) 92.6 (86.56-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.220 , 0.264 0.223 , 0.264	Depositor DCC
R_{free} test set	3649 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.129 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7063	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 4.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NA, EDO, ACT, CL, BTB

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	0.38	0/1645	0.58	0/2248
1	B	0.29	0/1591	0.50	0/2176
2	C	0.28	0/1650	0.49	0/2241
2	G	0.36	0/1663	0.58	0/2261
All	All	0.33	0/6549	0.54	0/8926

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 [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	A	1603	0	1538	36	0
1	B	1551	0	1478	15	0
2	C	1618	0	1536	25	0
2	G	1629	0	1557	29	0
3	A	14	0	19	1	0
3	G	14	0	19	5	0
4	A	28	0	40	9	0
4	B	7	0	10	1	0
4	G	42	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	24	0	36	6	0
5	C	4	0	6	0	0
5	G	16	0	24	4	0
6	A	8	0	6	1	0
6	B	8	0	6	0	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	G	2	0	0	0	0
8	A	1	0	0	0	0
8	G	1	0	0	1	0
9	A	151	0	0	7	0
9	B	99	0	0	0	0
9	C	92	0	0	3	0
9	G	145	0	0	3	0
All	All	7063	0	6335	109	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 8.

All (109) 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:C:12:SER:HB2	2:C:125:LYS:HE3	1.52	0.89
2:G:215:THR:HG1	2:G:220:SER:HG	1.36	0.73
2:C:2:ILE:HD12	2:C:27:GLN:HG3	1.69	0.73
2:C:43:GLN:HB2	2:C:53:LEU:HD11	1.70	0.72
2:G:206:LYS:NZ	9:G:402:HOH:O	2.24	0.70
1:A:172:GLU:HG3	4:A:302:PEG:H41	1.74	0.69
1:A:91:MET:HE2	1:A:94:LEU:HD21	1.77	0.67
1:B:13:VAL:HG11	1:B:94:LEU:HD13	1.76	0.66
1:A:182:ALA:HB2	6:A:311:ACT:H2	1.78	0.64
2:G:132:SER:HA	3:G:302:BTB:H72	1.79	0.64
2:G:109:GLY:HA2	2:G:114:PRO:HA	1.80	0.64
1:A:96:ALA:N	5:A:309:EDO:H11	2.13	0.64
1:A:147:PRO:HD3	1:A:233:LYS:HE3	1.81	0.61
2:G:165:SER:HA	5:G:305:EDO:H21	1.82	0.61
1:A:30:ILE:HD11	1:A:35:MET:HG3	1.83	0.61
1:A:171:PRO:HG3	5:A:310:EDO:H21	1.83	0.60
1:A:95:ARG:NH1	5:A:309:EDO:H21	2.17	0.60
2:G:47:GLY:C	2:G:48:LYS:HE2	2.28	0.59
1:A:95:ARG:NH1	9:A:407:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:304:PEG:H22	2:G:137:PRO:HG2	1.85	0.58
1:A:228:ASN:ND2	9:A:402:HOH:O	2.28	0.58
1:A:172:GLU:OE2	4:A:302:PEG:H32	2.03	0.57
2:G:47:GLY:O	2:G:48:LYS:HE2	2.03	0.57
2:C:75:ARG:HB2	9:C:418:HOH:O	2.04	0.57
2:G:110:TYR:CZ	2:G:114:PRO:HD3	2.39	0.57
2:G:123:GLU:HG2	2:G:124:ILE:N	2.18	0.57
2:C:51:LYS:NZ	9:C:401:HOH:O	2.26	0.57
1:A:96:ALA:H	5:A:309:EDO:H11	1.69	0.56
1:B:210:SER:HA	1:B:213:LEU:HD13	1.86	0.56
2:C:2:ILE:HD11	2:C:29:VAL:HG12	1.87	0.56
2:G:126:ARG:HH11	2:G:126:ARG:HG3	1.71	0.56
1:A:132:LEU:HD22	4:A:307:PEG:H22	1.88	0.55
2:G:105:GLN:HE21	2:G:114(A):ILE:HG23	1.72	0.55
1:A:5:VAL:HG23	1:A:24:ALA:HB3	1.89	0.55
2:G:147:THR:HB	8:G:312:CL:CL	2.42	0.55
2:C:18:ARG:HG2	2:C:92:SER:O	2.07	0.55
1:A:234:LYS:NZ	9:A:404:HOH:O	2.31	0.54
2:C:201:LYS:O	2:C:205:GLU:HG2	2.06	0.54
1:B:150:PRO:HG3	1:B:162:LEU:HB3	1.90	0.54
1:A:234:LYS:HE2	1:A:236:GLU:OE2	2.08	0.53
1:A:100:ALA:HB3	1:A:102:TYR:CE1	2.44	0.53
5:A:309:EDO:H22	9:A:485:HOH:O	2.09	0.53
5:G:305:EDO:H22	9:G:527:HOH:O	2.09	0.53
2:C:163:LYS:O	2:C:163:LYS:HE2	2.09	0.52
1:A:190:PHE:HB3	2:G:180:SER:OG	2.09	0.52
1:B:100:ALA:HB3	1:B:102:TYR:CE1	2.45	0.51
2:C:4:MET:HE3	2:C:23:CYS:SG	2.50	0.51
2:G:126:ARG:NH1	2:G:127:THR:O	2.43	0.51
2:C:45:LYS:NZ	2:C:99:PHE:O	2.36	0.50
1:A:5:VAL:CG2	1:A:24:ALA:HB3	2.41	0.50
1:B:62:TYR:HA	4:B:301:PEG:H42	1.92	0.50
1:A:46:PRO:HB2	4:A:302:PEG:H12	1.94	0.50
2:C:121:LYS:NZ	2:C:183[A]:GLU:OE1	2.32	0.49
1:A:173:PRO:HG3	4:A:307:PEG:H21	1.94	0.49
2:G:217:GLY:H	5:G:309:EDO:H21	1.78	0.49
2:C:11:LEU:HD11	2:C:122:VAL:HG13	1.94	0.48
2:G:181:VAL:HG22	2:G:193:LEU:HD12	1.96	0.47
2:G:201:LYS:O	2:G:205:GLU:HG2	2.14	0.47
2:C:225:LYS:HB3	2:C:225:LYS:HE2	1.67	0.47
2:G:132:SER:HA	3:G:302:BTB:H62	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:O	1:A:110:MET:HA	2.15	0.47
1:B:233:LYS:NZ	2:C:141:GLU:OE1	2.48	0.46
1:B:91:MET:HE3	1:B:91:MET:HB2	1.75	0.46
2:G:133:VAL:H	3:G:302:BTB:C7	2.28	0.46
3:A:301:BTB:H32	3:A:301:BTB:H71	1.71	0.46
3:G:302:BTB:O8	3:G:302:BTB:H41	2.16	0.46
2:G:217:GLY:H	5:G:309:EDO:C2	2.29	0.46
1:B:99:THR:HA	1:B:133:VAL:O	2.16	0.46
1:B:221:ASN:ND2	1:B:232:ASP:OD1	2.31	0.45
1:A:25:ALA:HB1	1:A:28:PHE:CE1	2.51	0.45
1:A:132:LEU:CB	4:A:307:PEG:H31	2.46	0.45
1:A:230:LYS:NZ	9:A:415:HOH:O	2.49	0.45
4:G:313:PEG:H41	4:G:313:PEG:H22	1.53	0.45
2:C:163:LYS:HE2	2:C:163:LYS:C	2.42	0.45
2:C:228:ASN:HB2	2:C:231:GLU:HG2	1.99	0.45
1:A:132:LEU:HB2	4:A:307:PEG:H31	1.99	0.45
1:A:105:ALA:HB1	1:A:110:MET:HB3	1.99	0.44
1:A:18:SER:HA	1:A:91:MET:O	2.17	0.44
2:C:169:ASP:OD2	2:C:207:HIS:HB3	2.17	0.44
1:B:81:ASP:OD1	1:B:84:LYS:HD3	2.18	0.44
2:C:137:PRO:HG3	2:C:227:PHE:CD2	2.53	0.44
2:G:206:LYS:HG3	2:G:207:HIS:CD2	2.52	0.43
2:G:43:GLN:HB2	2:G:53:LEU:HD11	2.00	0.43
1:B:81:ASP:CG	1:B:84:LYS:HD3	2.43	0.43
2:G:126:ARG:HD2	2:G:189:SER:HB2	2.00	0.43
1:A:202:LEU:C	1:A:202:LEU:HD12	2.44	0.43
2:C:167:TYR:HB2	2:C:211:ALA:HB3	2.01	0.43
1:A:46:PRO:HG3	4:A:302:PEG:H42	2.01	0.42
1:A:193:VAL:HG12	4:G:308[A]:PEG:H42	2.01	0.42
2:C:83:SER:HB2	9:C:406:HOH:O	2.19	0.42
2:C:1:ASP:O	2:C:3:GLN:HG3	2.20	0.42
3:G:302:BTB:H12	3:G:302:BTB:H52	1.61	0.42
1:B:12:LEU:HB2	1:B:171:PRO:HG3	2.02	0.41
2:G:54:ILE:HD13	2:G:67:LEU:HA	2.03	0.41
1:B:91:MET:HB3	1:B:94:LEU:HD21	2.02	0.41
2:C:158:TYR:CG	2:C:159:PRO:HA	2.56	0.41
1:A:233:LYS:HA	1:A:233:LYS:HD3	1.87	0.41
1:A:223:ASN:ND2	9:A:418:HOH:O	2.53	0.41
2:G:107:TYR:O	9:G:401:HOH:O	2.22	0.41
2:G:177:SER:HA	2:G:196:THR:O	2.21	0.41
1:B:58:SER:O	1:B:60:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:LYS:HZ1	2:C:71:VAL:HG22	1.86	0.41
1:A:170:PHE:HA	1:A:171:PRO:HA	1.84	0.41
2:G:126:ARG:HG3	2:G:126:ARG:NH1	2.35	0.41
2:G:42:TYR:O	2:G:102:TYR:HA	2.21	0.41
1:A:152:SER:N	9:A:410:HOH:O	2.43	0.40
2:C:91:ILE:HD12	2:C:91:ILE:N	2.36	0.40
1:B:14:GLN:H	1:B:14:GLN:HG3	1.72	0.40
1:A:226:PRO:HB3	5:A:310:EDO:H12	2.02	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	A	214/223 (96%)	209 (98%)	4 (2%)	1 (0%)	24	22
1	B	204/223 (92%)	199 (98%)	4 (2%)	1 (0%)	24	22
2	C	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
2	G	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
All	All	837/876 (96%)	816 (98%)	19 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	TYR
1	A	59	TYR

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	A	174/186 (94%)	171 (98%)	3 (2%)	53	62
1	B	167/186 (90%)	165 (99%)	2 (1%)	63	72
2	C	181/187 (97%)	176 (97%)	5 (3%)	38	43
2	G	183/187 (98%)	181 (99%)	2 (1%)	65	74
All	All	705/746 (94%)	693 (98%)	12 (2%)	53	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	97	GLU
1	A	156	SER
2	G	11	LEU
2	G	180	SER
1	B	83	SER
1	B	203	SER
2	C	3	GLN
2	C	12	SER
2	C	14	SER
2	C	56	SER
2	C	123	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	92	ASN
2	G	155	ASN
2	G	216	GLN

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 ⓘ

Of 38 ligands modelled in this entry, 10 are monoatomic - leaving 28 for Mogul analysis.

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	PEG	G	308[A]	-	6,6,6	0.20	0	5,5,5	0.07	0
5	EDO	G	305	-	3,3,3	0.54	0	2,2,2	0.12	0
5	EDO	C	301	-	3,3,3	0.47	0	2,2,2	0.21	0
4	PEG	G	308[B]	-	6,6,6	0.13	0	5,5,5	0.12	0
4	PEG	A	304	-	6,6,6	0.12	0	5,5,5	0.12	0
4	PEG	A	303	-	6,6,6	0.18	0	5,5,5	0.07	0
5	EDO	A	309	-	3,3,3	0.35	0	2,2,2	0.44	0
5	EDO	G	309	-	3,3,3	0.48	0	2,2,2	0.26	0
6	ACT	A	312	-	3,3,3	1.45	1 (33%)	3,3,3	1.35	0
5	EDO	A	310	-	3,3,3	0.55	0	2,2,2	0.12	0
5	EDO	G	306	-	3,3,3	0.36	0	2,2,2	0.50	0
5	EDO	G	307	-	3,3,3	0.71	0	2,2,2	0.13	0
5	EDO	A	306	-	3,3,3	0.58	0	2,2,2	0.12	0
5	EDO	A	305	-	3,3,3	0.45	0	2,2,2	0.40	0
4	PEG	G	303	-	6,6,6	0.13	0	5,5,5	0.13	0
6	ACT	B	303	-	3,3,3	1.58	1 (33%)	3,3,3	1.31	0
4	PEG	A	302	-	6,6,6	0.21	0	5,5,5	0.22	0
4	PEG	A	307	-	6,6,6	0.16	0	5,5,5	0.16	0
4	PEG	G	304	-	6,6,6	0.20	0	5,5,5	0.19	0
4	PEG	G	313	-	6,6,6	0.16	0	5,5,5	0.10	0
4	PEG	G	301	-	6,6,6	0.19	0	5,5,5	0.15	0
6	ACT	B	302	-	3,3,3	1.47	1 (33%)	3,3,3	1.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BTB	G	302	-	13,13,13	0.91	0	7,16,16	1.79	2 (28%)
5	EDO	A	308[A]	-	3,3,3	0.43	0	2,2,2	0.41	0
4	PEG	B	301	-	6,6,6	0.14	0	5,5,5	0.10	0
3	BTB	A	301	-	13,13,13	0.86	1 (7%)	7,16,16	0.77	0
5	EDO	A	308[B]	-	3,3,3	0.44	0	2,2,2	0.43	0
6	ACT	A	311	-	3,3,3	1.44	1 (33%)	3,3,3	1.34	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
4	PEG	G	308[A]	-	-	2/4/4/4	-
5	EDO	G	305	-	-	1/1/1/1	-
5	EDO	C	301	-	-	0/1/1/1	-
4	PEG	G	308[B]	-	-	0/4/4/4	-
4	PEG	A	304	-	-	2/4/4/4	-
4	PEG	A	303	-	-	3/4/4/4	-
5	EDO	A	309	-	-	1/1/1/1	-
5	EDO	G	309	-	-	1/1/1/1	-
5	EDO	A	310	-	-	1/1/1/1	-
5	EDO	G	306	-	-	1/1/1/1	-
5	EDO	G	307	-	-	1/1/1/1	-
5	EDO	A	306	-	-	1/1/1/1	-
5	EDO	A	305	-	-	1/1/1/1	-
4	PEG	G	303	-	-	2/4/4/4	-
4	PEG	A	302	-	-	2/4/4/4	-
4	PEG	A	307	-	-	3/4/4/4	-
4	PEG	G	304	-	-	1/4/4/4	-
4	PEG	G	313	-	-	3/4/4/4	-
4	PEG	G	301	-	-	1/4/4/4	-
3	BTB	G	302	-	-	13/21/21/21	-
5	EDO	A	308[A]	-	-	1/1/1/1	-
4	PEG	B	301	-	-	2/4/4/4	-
3	BTB	A	301	-	-	2/21/21/21	-
5	EDO	A	308[B]	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	303	ACT	CH3-C	2.44	1.58	1.49
6	A	311	ACT	CH3-C	2.22	1.57	1.49
6	A	312	ACT	CH3-C	2.16	1.57	1.49
6	B	302	ACT	CH3-C	2.15	1.57	1.49
3	A	301	BTB	C3-C2	2.12	1.55	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	BTB	O3-C3-C2	3.53	119.69	111.40
3	G	302	BTB	C6-C5-N	2.23	120.31	111.59

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	BTB	C6-C5-N-C7
3	G	302	BTB	O1-C1-C2-C3
3	G	302	BTB	O1-C1-C2-C4
3	G	302	BTB	O1-C1-C2-N
3	G	302	BTB	C1-C2-C3-O3
3	G	302	BTB	C4-C2-C3-O3
3	G	302	BTB	N-C2-C3-O3
3	G	302	BTB	C3-C2-N-C7
3	G	302	BTB	C6-C5-N-C7
3	G	302	BTB	C8-C7-N-C2
4	G	313	PEG	C4-C3-O2-C2
4	A	307	PEG	O2-C3-C4-O4
4	G	308[A]	PEG	O1-C1-C2-O2
4	G	303	PEG	O2-C3-C4-O4
4	G	313	PEG	O2-C3-C4-O4
4	B	301	PEG	O1-C1-C2-O2
3	G	302	BTB	N-C5-C6-O6
4	A	303	PEG	O2-C3-C4-O4
4	A	304	PEG	O1-C1-C2-O2
3	G	302	BTB	N-C7-C8-O8
3	A	301	BTB	N-C7-C8-O8
4	G	303	PEG	O1-C1-C2-O2
5	A	305	EDO	O1-C1-C2-O2
5	A	310	EDO	O1-C1-C2-O2
5	G	309	EDO	O1-C1-C2-O2
4	A	302	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	A	303	PEG	O1-C1-C2-O2
5	A	306	EDO	O1-C1-C2-O2
4	G	301	PEG	O2-C3-C4-O4
5	A	308[A]	EDO	O1-C1-C2-O2
3	G	302	BTB	C1-C2-N-C7
3	G	302	BTB	C4-C2-N-C7
4	A	302	PEG	C1-C2-O2-C3
4	G	304	PEG	C4-C3-O2-C2
5	G	306	EDO	O1-C1-C2-O2
4	A	304	PEG	O2-C3-C4-O4
4	A	303	PEG	C1-C2-O2-C3
4	G	308[A]	PEG	C1-C2-O2-C3
5	A	309	EDO	O1-C1-C2-O2
4	G	313	PEG	C1-C2-O2-C3
5	A	308[B]	EDO	O1-C1-C2-O2
5	G	307	EDO	O1-C1-C2-O2
4	A	307	PEG	C1-C2-O2-C3
4	B	301	PEG	O2-C3-C4-O4
5	G	305	EDO	O1-C1-C2-O2
4	A	307	PEG	C4-C3-O2-C2

There are no ring outliers.

13 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	308[A]	PEG	1	0
5	G	305	EDO	2	0
4	A	304	PEG	1	0
5	A	309	EDO	4	0
5	G	309	EDO	2	0
5	A	310	EDO	2	0
4	A	302	PEG	4	0
4	A	307	PEG	4	0
4	G	313	PEG	1	0
3	G	302	BTB	5	0
4	B	301	PEG	1	0
3	A	301	BTB	1	0
6	A	311	ACT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	216/223 (96%)	-1.19	0	100 100	18, 28, 46, 61	0
1	B	208/223 (93%)	-1.08	0	100 100	28, 37, 57, 76	0
2	C	211/215 (98%)	-0.87	1 (0%)	87 88	23, 44, 66, 83	2 (0%)
2	G	213/215 (99%)	-1.18	0	100 100	19, 34, 52, 80	1 (0%)
All	All	848/876 (96%)	-1.08	1 (0%)	92 92	18, 36, 58, 83	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	110	TYR	2.1

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 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(Å ²)	Q<0.9
4	PEG	A	307	7/7	0.96	0.09	36,38,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	312	4/4	0.96	0.09	48,51,54,54	0
6	ACT	B	302	4/4	0.96	0.08	45,50,52,52	0
5	EDO	A	305	4/4	0.97	0.06	34,42,48,51	0
5	EDO	G	309	4/4	0.97	0.08	36,38,43,44	0
4	PEG	A	303	7/7	0.97	0.06	39,48,50,51	0
4	PEG	A	302	7/7	0.97	0.06	34,39,45,46	0
6	ACT	B	303	4/4	0.97	0.09	39,41,45,50	0
7	NA	B	305	1/1	0.97	0.05	45,45,45,45	0
4	PEG	G	308[B]	7/7	0.98	0.06	32,39,41,43	7
4	PEG	B	301	7/7	0.98	0.06	54,62,66,66	0
3	BTB	G	302	14/14	0.98	0.07	26,37,43,44	0
5	EDO	A	306	4/4	0.98	0.06	40,48,51,52	0
5	EDO	A	308[A]	4/4	0.98	0.05	30,32,32,35	4
5	EDO	A	308[B]	4/4	0.98	0.05	28,31,32,32	4
5	EDO	G	307	4/4	0.98	0.05	34,34,43,44	0
4	PEG	A	304	7/7	0.98	0.05	30,39,49,59	0
3	BTB	A	301	14/14	0.98	0.06	29,40,54,66	0
4	PEG	G	303	7/7	0.98	0.07	38,44,55,55	0
4	PEG	G	304	7/7	0.98	0.05	36,41,46,49	0
7	NA	A	315	1/1	0.98	0.07	37,37,37,37	0
7	NA	G	310	1/1	0.98	0.06	50,50,50,50	0
4	PEG	G	308[A]	7/7	0.98	0.06	25,34,39,44	7
5	EDO	C	301	4/4	0.99	0.04	47,51,53,55	0
6	ACT	A	311	4/4	0.99	0.05	27,36,37,38	0
5	EDO	A	309	4/4	0.99	0.04	32,36,39,45	0
5	EDO	A	310	4/4	0.99	0.04	34,39,43,44	0
5	EDO	G	305	4/4	0.99	0.04	25,31,37,41	0
7	NA	A	313	1/1	0.99	0.04	39,39,39,39	0
7	NA	A	314	1/1	0.99	0.04	37,37,37,37	0
5	EDO	G	306	4/4	0.99	0.04	40,42,42,46	0
7	NA	A	316	1/1	0.99	0.04	43,43,43,43	0
4	PEG	G	313	7/7	0.99	0.06	27,37,41,45	0
7	NA	G	311	1/1	0.99	0.04	48,48,48,48	0
4	PEG	G	301	7/7	0.99	0.04	25,28,37,44	0
8	CL	A	317	1/1	0.99	0.04	46,46,46,46	0
8	CL	G	312	1/1	0.99	0.04	56,56,56,56	0
7	NA	B	304	1/1	1.00	0.10	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.