



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 04:55 PM EDT

PDB ID : 7KGU  
Title : Structure of 2Q1-Fab, an antibody selective for IDH2R140Q-HLA-B\*07:02  
Authors : Miller, M.S.; Aytenfisu, T.Y.; Wright, K.M.; Gabelli, S.B.  
Deposited on : 2020-10-18  
Resolution : 2.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

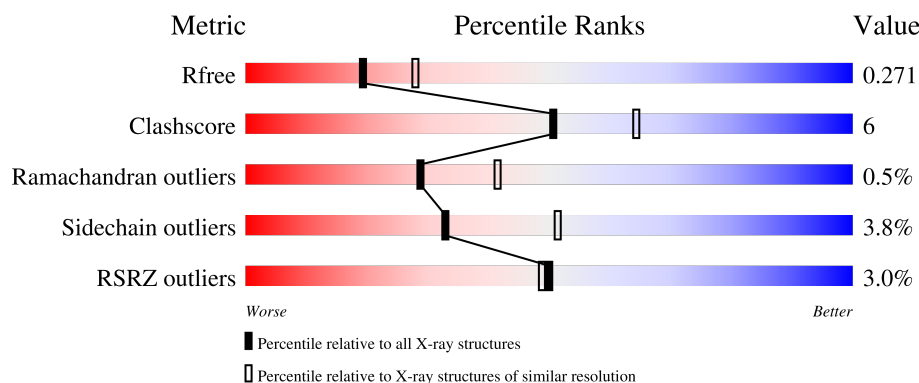
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	214	<div> <div>%</div> <div>87% 11% ..</div> </div>
1	C	214	<div> <div>2%</div> <div>89% 10% .</div> </div>
1	E	214	<div> <div>7%</div> <div>89% 8% ..</div> </div>
1	L	214	<div> <div>5%</div> <div>85% 11% ..</div> </div>
2	B	218	<div> <div>%</div> <div>84% 12% ..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	218	 2% 85% 11% . .
2	F	218	 2% 85% 11% . .
2	H	218	 3% 86% 11% .

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	BTB	A	302	-	-	X	-
5	SO4	D	304	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13756 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.

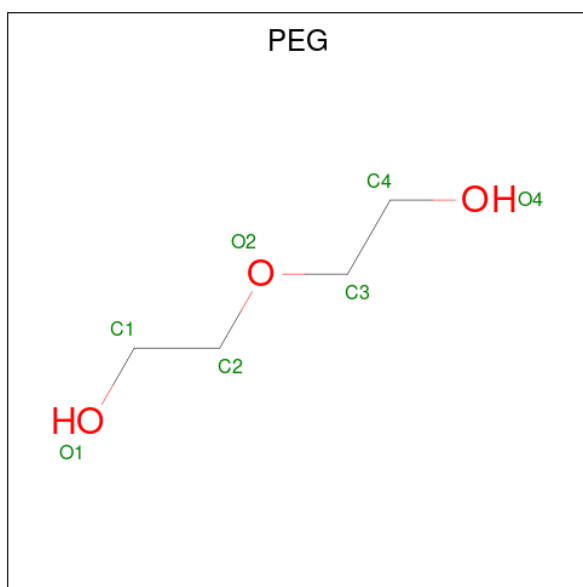
- Molecule 1 is a protein called Light Chain, Fab fragment, IGG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1633	1025	273	330	5			
1	C	212	Total	C	N	O	S	0	0	0
			1633	1025	273	330	5			
1	E	210	Total	C	N	O	S	0	0	0
			1625	1021	271	328	5			
1	L	211	Total	C	N	O	S	0	0	0
			1629	1023	272	329	5			

- Molecule 2 is a protein called Heavy Chain, Fab, IGG, Fab.

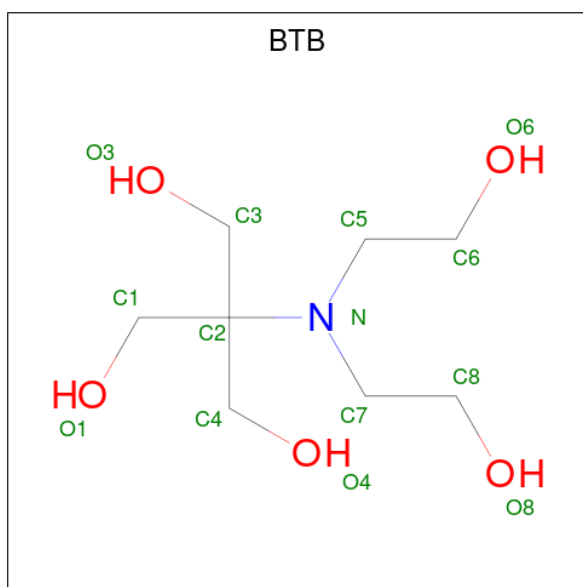
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1600	1018	265	310	7			
2	D	212	Total	C	N	O	S	0	0	0
			1597	1016	265	309	7			
2	F	210	Total	C	N	O	S	0	0	0
			1592	1014	263	308	7			
2	H	211	Total	C	N	O	S	0	0	0
			1591	1013	264	307	7			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



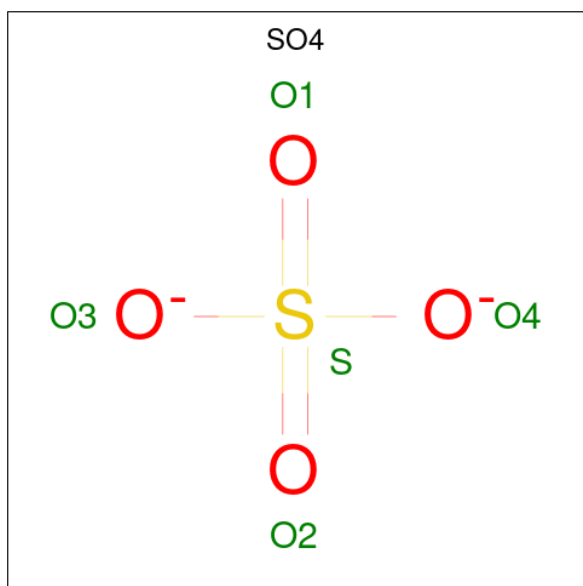
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		
3	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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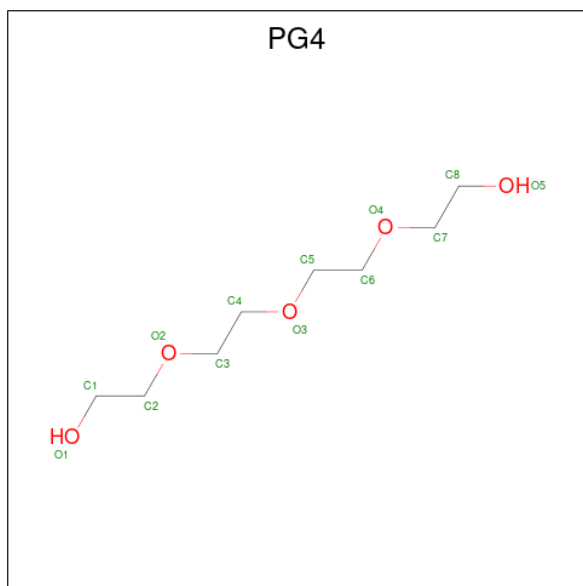
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		



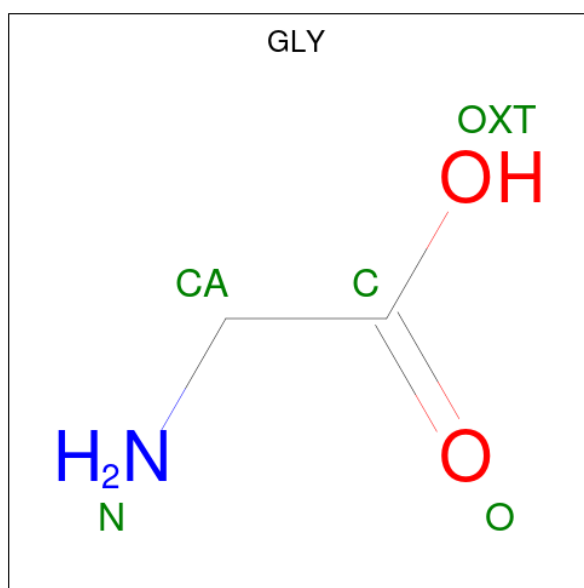
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total Cl 1 1	0	0
7	L	1	Total Cl 1 1	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total K 1 1	0	0

- Molecule 9 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C N O 4 2 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	67	Total O 67 67	0	0
10	B	84	Total O 84 84	0	0
10	C	65	Total O 65 65	0	0

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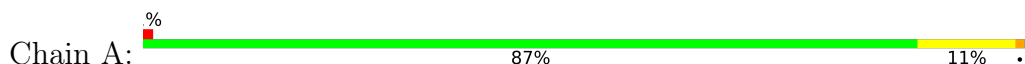
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	100	Total 100	O 100	0	0
10	E	46	Total 46	O 46	0	0
10	F	82	Total 82	O 82	0	0
10	H	91	Total 91	O 91	0	0
10	L	60	Total 60	O 60	0	0

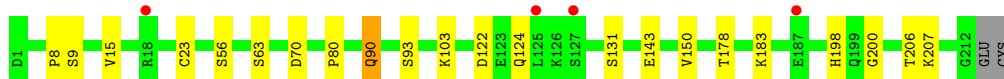
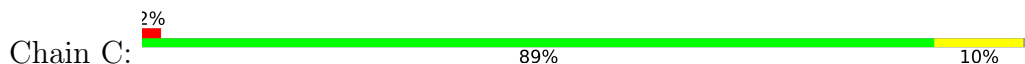
### 3 Residue-property plots [i](#)

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.

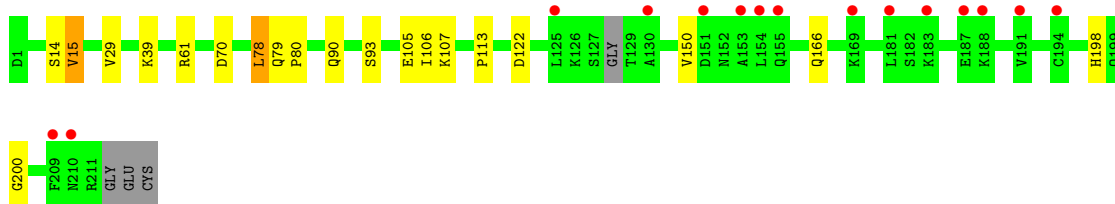
- Molecule 1: Light Chain, Fab fragment, IGG



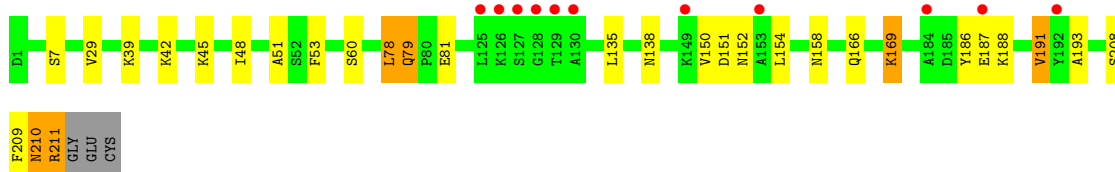
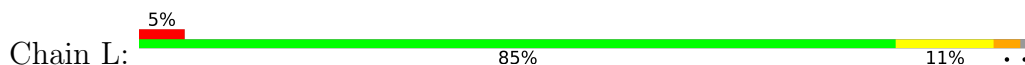
- Molecule 1: Light Chain, Fab fragment, IGG



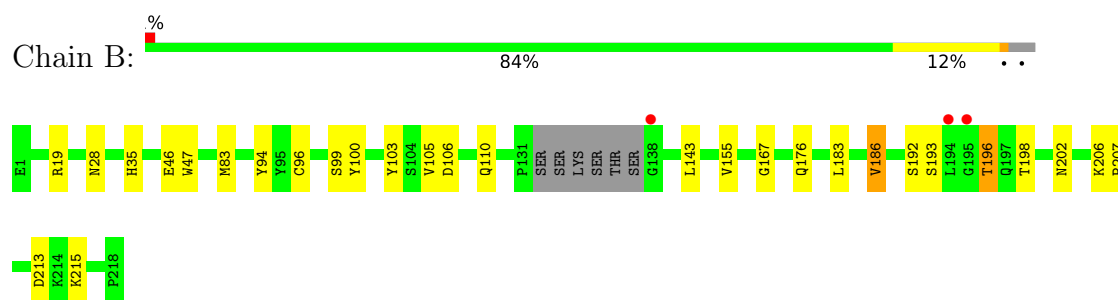
- Molecule 1: Light Chain, Fab fragment, IGG



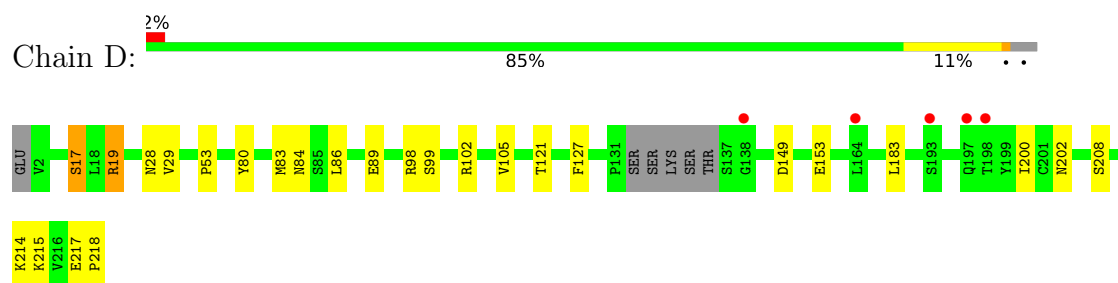
- Molecule 1: Light Chain, Fab fragment, IGG



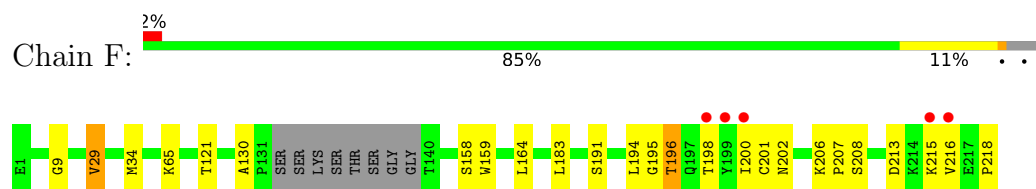
- Molecule 2: Heavy Chain, Fab, IGG, Fab



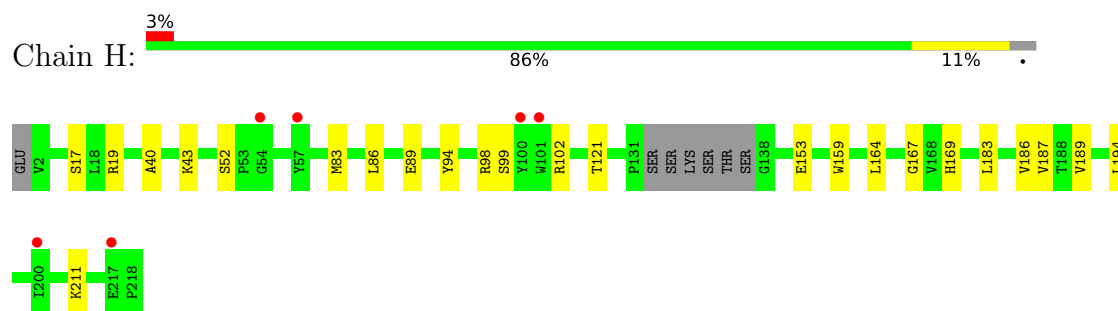
- Molecule 2: Heavy Chain, Fab, IGG, Fab



- Molecule 2: Heavy Chain, Fab, IGG, Fab



- Molecule 2: Heavy Chain, Fab, IGG, Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.46Å 263.95Å 91.24Å 90.00° 99.53° 90.00°	Depositor
Resolution (Å)	45.53 – 2.40 45.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.53-2.40) 98.8 (45.53-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.208 , 0.269 0.213 , 0.271	Depositor DCC
$R_{free}$ test set	3437 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BTB, PG4, SO4, PEG, CL, K

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	0.79	0/1669	0.96	0/2267
1	C	0.82	1/1669 (0.1%)	1.02	0/2267
1	E	0.75	0/1660	0.97	0/2254
1	L	0.79	1/1665 (0.1%)	1.03	0/2262
2	B	0.80	0/1642	0.96	0/2241
2	D	0.88	3/1639 (0.2%)	0.98	0/2237
2	F	0.83	1/1634 (0.1%)	1.01	0/2231
2	H	0.86	2/1633 (0.1%)	0.99	1/2229 (0.0%)
All	All	0.81	8/13211 (0.1%)	0.99	1/17988 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	130	ALA	C-N	8.19	1.49	1.34
2	D	89	GLU	CD-OE1	6.46	1.32	1.25
1	L	81	GLU	CD-OE2	6.25	1.32	1.25
2	D	153	GLU	CD-OE1	6.22	1.32	1.25
2	D	89	GLU	CD-OE2	6.22	1.32	1.25
2	H	153	GLU	CD-OE1	5.60	1.31	1.25
1	C	143	GLU	CD-OE1	5.11	1.31	1.25
2	H	89	GLU	CD-OE1	5.06	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	ARG	NE-CZ-NH2	-7.02	116.79	120.30

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	A	1633	0	1589	21	1
1	C	1633	0	1589	17	0
1	E	1625	0	1582	15	0
1	L	1629	0	1586	26	1
2	B	1600	0	1557	24	0
2	D	1597	0	1553	14	0
2	F	1592	0	1550	17	0
2	H	1591	0	1548	19	0
3	A	7	0	10	0	0
3	C	7	0	10	3	0
3	D	14	0	20	0	0
3	F	7	0	10	0	0
3	H	7	0	10	0	0
3	L	7	0	10	3	0
4	A	14	0	19	11	0
5	A	20	0	0	0	0
5	B	30	0	0	2	0
5	C	15	0	0	0	0
5	D	40	0	0	2	0
5	F	30	0	0	1	0
5	H	25	0	0	1	0
5	L	5	0	0	0	0
6	B	26	0	36	5	0
7	F	1	0	0	0	0
7	L	1	0	0	1	0
8	H	1	0	0	0	0
9	L	4	0	2	0	0
10	A	67	0	0	1	0
10	B	84	0	0	1	0
10	C	65	0	0	5	0
10	D	100	0	0	1	0
10	E	46	0	0	1	0
10	F	82	0	0	0	0
10	H	91	0	0	1	0
10	L	60	0	0	2	0
All	All	13756	0	12681	146	1

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 (146) 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:F:194:LEU:HD11	2:F:218:PRO:CG	1.80	1.09
2:F:194:LEU:CD1	2:F:218:PRO:HG3	1.84	1.08
2:F:194:LEU:HD21	2:F:218:PRO:HG2	1.42	0.97
1:L:151:ASP:OD1	1:L:191:VAL:HG23	1.64	0.97
1:C:9:SER:H	3:C:301:PEG:H21	1.33	0.92
1:A:123:GLU:HB3	10:A:455:HOH:O	1.70	0.90
2:F:194:LEU:HD21	2:F:218:PRO:CG	2.12	0.80
2:F:194:LEU:HD11	2:F:218:PRO:HG3	0.90	0.79
1:L:211:ARG:NH1	1:L:211:ARG:HG3	1.97	0.79
1:A:43:ALA:HB3	4:A:302:BTB:H61	1.65	0.79
1:C:8:PRO:HA	3:C:301:PEG:H31	1.67	0.77
1:L:211:ARG:HG3	1:L:211:ARG:HH11	1.51	0.76
1:L:211:ARG:CD	1:L:211:ARG:H	1.97	0.75
1:A:42:LYS:HA	4:A:302:BTB:H82	1.69	0.73
1:E:80:PRO:HA	1:E:106:ILE:HD13	1.70	0.73
1:C:178:THR:HG22	10:C:435:HOH:O	1.88	0.72
1:L:211:ARG:H	1:L:211:ARG:HD2	1.54	0.72
2:D:28:ASN:N	5:D:304:SO4:O2	2.23	0.72
2:F:194:LEU:CD2	2:F:218:PRO:HG2	2.20	0.72
2:H:194:LEU:HD13	2:H:194:LEU:O	1.93	0.69
1:E:79:GLN:HB3	1:E:80:PRO:HD2	1.74	0.69
1:C:198:HIS:CD2	1:C:200:GLY:H	2.11	0.69
4:A:302:BTB:H71	2:B:110:GLN:HG2	1.75	0.68
1:L:45:LYS:HE3	3:L:302:PEG:H42	1.74	0.68
1:L:187:GLU:HA	1:L:187:GLU:OE1	1.94	0.67
2:H:40:ALA:HB3	2:H:43:LYS:HD2	1.77	0.67
1:A:190:LYS:HD2	1:A:210:ASN:HB3	1.77	0.66
1:L:187:GLU:HA	1:L:211:ARG:HH22	1.61	0.65
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.79	0.64
1:A:78:LEU:O	1:A:82:ASP:OD2	2.17	0.64
1:L:210:ASN:ND2	1:L:210:ASN:H	1.96	0.61
2:H:211:LYS:NZ	5:H:406:SO4:O4	2.31	0.60
1:E:90:GLN:HE21	1:E:93:SER:H	1.50	0.59
1:E:198:HIS:CD2	1:E:200:GLY:H	2.19	0.59
2:B:183:LEU:HD12	2:B:183:LEU:C	2.24	0.58
1:E:15:VAL:HG22	1:E:15:VAL:O	2.04	0.57
1:L:211:ARG:HD2	1:L:211:ARG:N	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LYS:CG	10:C:424:HOH:O	2.52	0.57
2:D:29:VAL:HG22	2:D:53:PRO:HG2	1.87	0.56
2:B:83:MET:HE1	2:B:94:TYR:CZ	2.40	0.56
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.54	0.56
6:B:502:PG4:H41	2:H:17:SER:N	2.22	0.55
1:C:103:LYS:HD2	10:C:425:HOH:O	2.05	0.55
1:E:106:ILE:H	1:E:166:GLN:HE22	1.53	0.55
2:H:186:VAL:HG11	1:L:135:LEU:HD22	1.88	0.55
1:A:135:LEU:CD2	2:B:186:VAL:HG11	2.36	0.55
2:D:83:MET:HE2	2:D:86:LEU:HD21	1.88	0.53
1:E:106:ILE:N	1:E:166:GLN:HE22	2.06	0.53
1:E:15:VAL:O	1:E:15:VAL:HG13	2.08	0.53
2:F:183:LEU:HD12	2:F:183:LEU:C	2.29	0.53
2:H:159:TRP:HB3	2:H:164:LEU:HD21	1.91	0.52
1:C:124:GLN:HE22	1:C:131:SER:HB2	1.74	0.52
1:A:135:LEU:HD22	2:B:186:VAL:HG11	1.90	0.52
1:C:15:VAL:HG21	1:C:80:PRO:HG3	1.91	0.52
2:F:195:GLY:O	2:F:196:THR:HG23	2.10	0.52
1:L:45:LYS:CE	3:L:302:PEG:H42	2.39	0.52
2:H:189:VAL:HG12	10:H:521:HOH:O	2.10	0.52
6:B:502:PG4:H41	2:H:17:SER:H	1.74	0.52
1:C:103:LYS:HG2	10:C:424:HOH:O	2.09	0.52
1:A:109:THR:HG22	1:A:110:VAL:O	2.10	0.51
1:A:42:LYS:HB3	4:A:302:BTB:H42	1.93	0.51
2:F:206:LYS:N	2:F:207:PRO:CD	2.74	0.51
2:H:183:LEU:C	2:H:183:LEU:HD12	2.31	0.51
6:B:502:PG4:C4	2:H:17:SER:HB2	2.41	0.51
6:B:502:PG4:H41	2:H:17:SER:HB2	1.93	0.51
1:C:9:SER:N	3:C:301:PEG:H21	2.14	0.51
1:L:152:ASN:HB2	10:L:421:HOH:O	2.11	0.51
1:L:150:VAL:HA	1:L:191:VAL:O	2.10	0.51
1:A:150:VAL:HA	1:A:191:VAL:O	2.10	0.50
2:F:9:GLY:N	5:F:307:SO4:O3	2.45	0.50
1:E:106:ILE:H	1:E:166:GLN:NE2	2.09	0.50
1:L:211:ARG:HH11	1:L:211:ARG:CG	2.21	0.50
2:B:206:LYS:N	2:B:207:PRO:CD	2.75	0.49
4:A:302:BTB:H52	2:B:110:GLN:HG2	1.94	0.49
1:C:206:THR:O	1:C:207:LYS:HE2	2.11	0.49
2:D:17:SER:OG	2:D:84:ASN:OD1	2.30	0.49
2:D:99:SER:HB3	2:D:105:VAL:HG12	1.94	0.49
2:B:193:SER:HA	2:B:196:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HA	1:A:106:ILE:HG12	1.93	0.49
4:A:302:BTB:H71	2:B:110:GLN:HE21	1.78	0.49
1:C:103:LYS:HG3	10:C:424:HOH:O	2.13	0.48
2:D:183:LEU:C	2:D:183:LEU:HD12	2.33	0.48
1:E:90:GLN:NE2	1:E:93:SER:H	2.11	0.48
1:A:46:LEU:HD22	2:B:106:ASP:HA	1.95	0.48
1:C:124:GLN:HA	2:D:127:PHE:CE1	2.49	0.48
4:A:302:BTB:C7	2:B:110:GLN:HE21	2.27	0.47
1:A:190:LYS:O	1:A:210:ASN:HA	2.15	0.47
4:A:302:BTB:H52	2:B:110:GLN:HA	1.95	0.47
2:F:159:TRP:CZ3	2:F:201:CYS:HB3	2.49	0.47
2:B:35:HIS:HE1	2:B:99:SER:HB3	1.79	0.47
2:F:159:TRP:CH2	2:F:201:CYS:HB3	2.49	0.47
1:L:169:LYS:NZ	10:L:401:HOH:O	2.48	0.47
2:D:19:ARG:HD3	2:D:80:TYR:HB3	1.97	0.47
1:L:42:LYS:HD3	3:L:302:PEG:H32	1.97	0.46
1:L:210:ASN:ND2	1:L:210:ASN:N	2.59	0.46
2:B:28:ASN:N	5:D:304:SO4:O1	2.41	0.46
1:A:90:GLN:HE21	1:A:93:SER:H	1.64	0.46
2:H:40:ALA:CB	2:H:43:LYS:HD2	2.45	0.46
2:H:169:HIS:HE1	1:L:138:ASN:HD21	1.63	0.46
2:B:35:HIS:O	2:B:96:CYS:HA	2.17	0.45
2:D:83:MET:HB3	2:D:86:LEU:HD21	2.00	0.44
2:D:83:MET:HE2	2:D:86:LEU:CD2	2.48	0.44
1:E:113:PRO:HD3	1:E:198:HIS:CD2	2.53	0.44
1:A:106:ILE:N	1:A:106:ILE:HD12	2.32	0.44
4:A:302:BTB:C5	2:B:110:GLN:HG2	2.47	0.43
1:A:160:GLN:HE22	2:B:176:GLN:HA	1.83	0.43
2:B:167:GLY:HA2	5:B:506:SO4:O2	2.18	0.43
2:H:83:MET:CE	2:H:94:TYR:CZ	3.01	0.43
1:A:13:ALA:HB3	1:A:78:LEU:HD22	2.00	0.43
1:L:193:ALA:HB2	1:L:208:SER:HB3	1.99	0.43
2:D:19:ARG:NH1	10:D:407:HOH:O	2.51	0.43
2:F:121:THR:HG21	2:F:208:SER:HA	2.00	0.43
2:B:100:TYR:O	2:B:103:TYR:HB2	2.18	0.43
1:E:105:GLU:HB3	10:E:334:HOH:O	2.19	0.42
2:F:29:VAL:HG23	2:F:34:MET:SD	2.60	0.42
2:F:158:SER:OG	2:F:202:ASN:HB2	2.19	0.42
6:B:502:PG4:H41	2:H:17:SER:CB	2.48	0.42
2:D:217:GLU:HB2	2:D:218:PRO:HD2	2.01	0.42
2:F:194:LEU:CD1	2:F:218:PRO:CG	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:PHE:CD1	1:L:209:PHE:C	2.92	0.42
2:D:121:THR:HG22	2:D:208:SER:HB3	2.01	0.42
1:C:198:HIS:HD2	1:C:200:GLY:H	1.61	0.42
1:A:90:GLN:NE2	1:A:93:SER:O	2.53	0.41
2:H:167:GLY:O	2:H:187:VAL:HA	2.20	0.41
2:D:200:ILE:HA	2:D:214:LYS:O	2.19	0.41
1:E:78:LEU:HD11	1:E:106:ILE:HG12	2.01	0.41
1:A:149:LYS:HA	1:A:153:ALA:O	2.20	0.41
1:A:42:LYS:HD3	4:A:302:BTB:O1	2.21	0.41
1:C:90:GLN:NE2	1:C:93:SER:H	2.18	0.41
2:B:198:THR:HB	2:B:215:LYS:NZ	2.36	0.41
1:C:15:VAL:CG2	1:C:80:PRO:HG3	2.49	0.41
1:C:124:GLN:HE22	1:C:131:SER:CB	2.34	0.41
1:E:29:VAL:HG11	1:E:90:GLN:HG3	2.03	0.41
2:H:83:MET:HE3	2:H:94:TYR:CZ	2.56	0.41
2:B:46:GLU:HA	5:B:507:SO4:O3	2.21	0.41
1:E:150:VAL:O	1:E:150:VAL:HG23	2.20	0.41
4:A:302:BTB:H11	4:A:302:BTB:H72	1.89	0.40
1:L:51:ALA:O	7:L:304:CL:CL	2.76	0.40
2:F:159:TRP:HB3	2:F:164:LEU:HD21	2.02	0.40
2:H:186:VAL:HG11	1:L:135:LEU:CD2	2.49	0.40
1:L:188:LYS:HB3	1:L:188:LYS:HE2	1.95	0.40
2:B:155:VAL:CG1	2:B:183:LEU:HD21	2.51	0.40
1:L:48:ILE:HA	1:L:53:PHE:O	2.20	0.40
1:L:186:TYR:O	1:L:211:ARG:NH2	2.55	0.40
1:A:29:VAL:HG11	1:A:90:GLN:HG3	2.04	0.40
2:B:28:ASN:ND2	10:B:606:HOH:O	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:CG2	1:L:79:GLN:NE2[1_556]	1.68	0.52

## 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	210/214 (98%)	199 (95%)	9 (4%)	2 (1%)	15	23
1	C	210/214 (98%)	200 (95%)	9 (4%)	1 (0%)	29	41
1	E	206/214 (96%)	197 (96%)	8 (4%)	1 (0%)	29	41
1	L	209/214 (98%)	197 (94%)	10 (5%)	2 (1%)	15	23
2	B	208/218 (95%)	200 (96%)	7 (3%)	1 (0%)	29	41
2	D	208/218 (95%)	204 (98%)	3 (1%)	1 (0%)	29	41
2	F	206/218 (94%)	198 (96%)	7 (3%)	1 (0%)	29	41
2	H	207/218 (95%)	201 (97%)	6 (3%)	0	100	100
All	All	1664/1728 (96%)	1596 (96%)	59 (4%)	9 (0%)	29	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	15	VAL
2	B	196	THR
1	C	122	ASP
1	A	78	LEU
2	D	149	ASP
2	F	196	THR
1	A	79	GLN
1	L	78	LEU
1	L	79	GLN

### 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	187/189 (99%)	184 (98%)	3 (2%)	62	79
1	C	187/189 (99%)	180 (96%)	7 (4%)	34	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	187/189 (99%)	180 (96%)	7 (4%)	34	53
1	L	187/189 (99%)	175 (94%)	12 (6%)	17	28
2	B	176/182 (97%)	169 (96%)	7 (4%)	31	49
2	D	176/182 (97%)	170 (97%)	6 (3%)	37	56
2	F	176/182 (97%)	168 (96%)	8 (4%)	27	44
2	H	175/182 (96%)	170 (97%)	5 (3%)	42	62
All	All	1451/1484 (98%)	1396 (96%)	55 (4%)	33	51

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	47	LEU
1	A	90	GLN
2	B	19	ARG
2	B	105	VAL
2	B	143	LEU
2	B	186	VAL
2	B	192	SER
2	B	202	ASN
2	B	213	ASP
1	C	23	CYS
1	C	56	SER
1	C	63	SER
1	C	70	ASP
1	C	90	GLN
1	C	150	VAL
1	C	183	LYS
2	D	17	SER
2	D	19	ARG
2	D	98	ARG
2	D	102	ARG
2	D	202	ASN
2	D	215	LYS
1	E	14	SER
1	E	39	LYS
1	E	61	ARG
1	E	70	ASP
1	E	78	LEU
1	E	107	LYS

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Mol	Chain	Res	Type
1	E	122	ASP
2	F	29	VAL
2	F	65	LYS
2	F	191	SER
2	F	198	THR
2	F	200	ILE
2	F	213	ASP
2	F	215	LYS
2	F	216	VAL
2	H	52	SER
2	H	98	ARG
2	H	99	SER
2	H	102	ARG
2	H	121	THR
1	L	7	SER
1	L	29	VAL
1	L	39	LYS
1	L	60	SER
1	L	78	LEU
1	L	154	LEU
1	L	158	ASN
1	L	166	GLN
1	L	169	LYS
1	L	191	VAL
1	L	210	ASN
1	L	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	210	ASN
2	B	13	GLN
2	B	28	ASN
2	B	35	HIS
2	B	110	GLN
2	B	197	GLN
1	C	90	GLN
1	C	124	GLN
1	C	152	ASN
1	C	198	HIS
2	D	3	GLN

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Mol	Chain	Res	Type
1	E	79	GLN
1	E	198	HIS
2	H	3	GLN
2	H	110	GLN
1	L	137	ASN
1	L	138	ASN
1	L	158	ASN
1	L	210	ASN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 3 are monoatomic - leaving 44 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	$\# Z  > 2$
5	SO4	C	303	-	4,4,4	0.36	0	6,6,6	0.08	0
5	SO4	C	302	-	4,4,4	0.35	0	6,6,6	0.06	0
5	SO4	H	404	-	4,4,4	0.36	0	6,6,6	0.10	0
6	PG4	B	501	-	12,12,12	0.23	0	11,11,11	0.21	0
5	SO4	B	504	-	4,4,4	0.32	0	6,6,6	0.13	0
3	PEG	L	302	-	6,6,6	0.16	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	F	303	-	4,4,4	0.34	0	6,6,6	0.11	0
5	SO4	H	402	-	4,4,4	0.32	0	6,6,6	0.05	0
4	BTB	A	302	-	13,13,13	1.56	3 (23%)	7,16,16	1.12	0
3	PEG	C	301	-	6,6,6	0.21	0	5,5,5	0.32	0
5	SO4	F	306	-	4,4,4	0.28	0	6,6,6	0.11	0
5	SO4	C	304	-	4,4,4	0.36	0	6,6,6	0.11	0
5	SO4	H	405	-	4,4,4	0.46	0	6,6,6	0.12	0
5	SO4	F	304	-	4,4,4	0.34	0	6,6,6	0.07	0
5	SO4	H	403	-	4,4,4	0.32	0	6,6,6	0.07	0
6	PG4	B	502	-	12,12,12	0.32	0	11,11,11	0.14	0
5	SO4	B	506	-	4,4,4	0.33	0	6,6,6	0.11	0
5	SO4	B	508	-	4,4,4	0.34	0	6,6,6	0.07	0
9	GLY	L	301	-	3,3,4	0.71	0	0,2,4	0.00	-
5	SO4	F	302	-	4,4,4	0.52	0	6,6,6	0.11	0
5	SO4	B	505	-	4,4,4	0.32	0	6,6,6	0.07	0
5	SO4	A	304	-	4,4,4	0.33	0	6,6,6	0.13	0
5	SO4	B	503	-	4,4,4	0.45	0	6,6,6	0.18	0
5	SO4	D	309	-	4,4,4	0.32	0	6,6,6	0.14	0
3	PEG	D	302	-	6,6,6	0.21	0	5,5,5	0.17	0
5	SO4	A	303	-	4,4,4	0.38	0	6,6,6	0.11	0
5	SO4	B	507	-	4,4,4	0.42	0	6,6,6	0.09	0
5	SO4	D	303	-	4,4,4	0.35	0	6,6,6	0.20	0
5	SO4	D	308	-	4,4,4	0.36	0	6,6,6	0.07	0
5	SO4	D	310	-	4,4,4	0.37	0	6,6,6	0.06	0
5	SO4	D	304	-	4,4,4	0.45	0	6,6,6	0.10	0
5	SO4	A	306	-	4,4,4	0.37	0	6,6,6	0.05	0
5	SO4	D	306	-	4,4,4	0.28	0	6,6,6	0.11	0
3	PEG	A	301	-	6,6,6	0.26	0	5,5,5	0.18	0
3	PEG	D	301	-	6,6,6	0.17	0	5,5,5	0.28	0
5	SO4	F	305	-	4,4,4	0.39	0	6,6,6	0.06	0
5	SO4	F	307	-	4,4,4	0.37	0	6,6,6	0.09	0
5	SO4	A	305	-	4,4,4	0.37	0	6,6,6	0.06	0
5	SO4	H	406	-	4,4,4	0.33	0	6,6,6	0.05	0
3	PEG	H	401	-	6,6,6	0.16	0	5,5,5	0.13	0
3	PEG	F	301	-	6,6,6	0.20	0	5,5,5	0.14	0
5	SO4	D	305	-	4,4,4	0.43	0	6,6,6	0.07	0
5	SO4	L	303	-	4,4,4	0.40	0	6,6,6	0.07	0
5	SO4	D	307	-	4,4,4	0.32	0	6,6,6	0.06	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	PEG	A	301	-	-	2/4/4/4	-
3	PEG	D	301	-	-	0/4/4/4	-
3	PEG	D	302	-	-	0/4/4/4	-
6	PG4	B	501	-	-	4/10/10/10	-
6	PG4	B	502	-	-	6/10/10/10	-
3	PEG	L	302	-	-	0/4/4/4	-
3	PEG	H	401	-	-	0/4/4/4	-
3	PEG	F	301	-	-	0/4/4/4	-
9	GLY	L	301	-	-	0/0/1/2	-
4	BTB	A	302	-	-	8/21/21/21	-
3	PEG	C	301	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	BTB	C2-N	4.15	1.56	1.48
4	A	302	BTB	C5-N	2.43	1.51	1.48
4	A	302	BTB	C7-N	2.19	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	BTB	C1-C2-C4-O4
4	A	302	BTB	C3-C2-C4-O4
4	A	302	BTB	N-C2-C4-O4
4	A	302	BTB	C1-C2-N-C7
4	A	302	BTB	C3-C2-N-C7
4	A	302	BTB	C4-C2-N-C7
4	A	302	BTB	C6-C5-N-C2
6	B	501	PG4	O2-C3-C4-O3
3	A	301	PEG	O2-C3-C4-O4
3	C	301	PEG	O2-C3-C4-O4
6	B	501	PG4	O1-C1-C2-O2
6	B	502	PG4	O4-C7-C8-O5
6	B	502	PG4	O1-C1-C2-O2
3	A	301	PEG	O1-C1-C2-O2
3	C	301	PEG	C4-C3-O2-C2
6	B	502	PG4	C1-C2-O2-C3
6	B	502	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	A	302	BTB	C4-C2-N-C5
6	B	501	PG4	O3-C5-C6-O4
6	B	501	PG4	O4-C7-C8-O5
6	B	502	PG4	C6-C5-O3-C4
6	B	502	PG4	C3-C4-O3-C5

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	302	PEG	3	0
4	A	302	BTB	11	0
3	C	301	PEG	3	0
6	B	502	PG4	5	0
5	B	506	SO4	1	0
5	B	507	SO4	1	0
5	D	304	SO4	2	0
5	F	307	SO4	1	0
5	H	406	SO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	212/214 (99%)	-0.14	2 (0%) 84 82	23, 41, 65, 80	0
1	C	212/214 (99%)	-0.06	4 (1%) 66 64	20, 41, 73, 88	0
1	E	210/214 (98%)	0.41	15 (7%) 16 14	29, 57, 95, 119	0
1	L	211/214 (98%)	-0.06	11 (5%) 27 26	22, 39, 81, 96	0
2	B	212/218 (97%)	-0.12	3 (1%) 75 73	16, 30, 72, 92	0
2	D	212/218 (97%)	-0.16	5 (2%) 59 57	17, 29, 72, 93	0
2	F	210/218 (96%)	-0.07	5 (2%) 59 57	17, 33, 87, 105	0
2	H	211/218 (96%)	-0.04	6 (2%) 53 51	16, 31, 77, 94	0
All	All	1690/1728 (97%)	-0.03	51 (3%) 50 49	16, 38, 79, 119	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	181	LEU	5.1
1	E	154	LEU	4.8
1	E	187	GLU	4.6
1	E	125	LEU	4.2
1	E	183	LYS	4.2
2	F	216	VAL	4.2
1	L	184	ALA	4.0
2	B	194	LEU	3.7
1	C	127	SER	3.6
2	H	57	TYR	3.4
2	F	198	THR	3.4
1	E	210	ASN	3.3
2	H	100	TYR	3.2
1	E	151	ASP	3.2
1	E	169	LYS	3.2
1	E	153	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	188	LYS	3.2
2	D	164	LEU	3.1
1	L	125	LEU	3.0
1	E	155	GLN	3.0
2	H	200	ILE	2.9
1	L	129	THR	2.9
2	D	197	GLN	2.9
1	C	187	GLU	2.9
1	L	187	GLU	2.9
2	B	138	GLY	2.9
2	B	195	GLY	2.7
1	E	130	ALA	2.7
2	F	199	TYR	2.7
1	C	18	ARG	2.6
1	L	128	GLY	2.5
1	A	187	GLU	2.5
2	F	215	LYS	2.5
2	H	101	TRP	2.5
2	F	200	ILE	2.4
1	L	130	ALA	2.3
1	A	128	GLY	2.3
2	H	217	GLU	2.3
2	D	198	THR	2.3
1	E	209	PHE	2.2
2	H	54	GLY	2.2
2	D	193	SER	2.2
1	L	126	LYS	2.2
1	C	125	LEU	2.2
1	L	153	ALA	2.1
1	L	192	TYR	2.1
2	D	138	GLY	2.1
1	L	149	LYS	2.0
1	E	191	VAL	2.0
1	L	127	SER	2.0
1	E	194	CYS	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	BTB	A	302	14/14	0.68	0.35	68,72,85,85	0
5	SO4	F	306	5/5	0.68	0.20	76,80,83,92	0
3	PEG	A	301	7/7	0.73	0.27	67,73,76,76	0
3	PEG	C	301	7/7	0.77	0.21	53,58,60,60	0
3	PEG	F	301	7/7	0.81	0.34	62,65,69,69	0
3	PEG	D	301	7/7	0.81	0.24	49,56,66,73	0
3	PEG	D	302	7/7	0.81	0.23	49,53,58,62	0
6	PG4	B	501	13/13	0.81	0.22	51,58,71,71	0
6	PG4	B	502	13/13	0.82	0.23	44,68,78,78	0
3	PEG	L	302	7/7	0.84	0.20	62,65,70,71	0
5	SO4	B	507	5/5	0.84	0.44	83,85,94,106	0
5	SO4	D	309	5/5	0.84	0.28	74,77,84,88	0
9	GLY	L	301	4/5	0.84	0.17	73,75,75,76	0
5	SO4	H	404	5/5	0.87	0.16	71,80,83,84	0
5	SO4	B	506	5/5	0.87	0.19	65,71,78,82	0
5	SO4	A	306	5/5	0.88	0.18	87,90,93,96	0
5	SO4	H	406	5/5	0.89	0.17	64,69,71,81	0
5	SO4	D	307	5/5	0.89	0.26	72,84,86,87	0
5	SO4	C	302	5/5	0.90	0.17	85,86,92,93	0
5	SO4	A	305	5/5	0.90	0.27	87,91,94,95	0
5	SO4	A	304	5/5	0.90	0.17	68,73,76,77	0
5	SO4	D	310	5/5	0.91	0.25	90,91,94,95	0
5	SO4	F	303	5/5	0.91	0.20	63,65,70,74	0
3	PEG	H	401	7/7	0.91	0.17	49,51,52,57	0
5	SO4	H	402	5/5	0.91	0.18	67,73,80,81	0
5	SO4	H	403	5/5	0.91	0.15	70,70,77,77	0
5	SO4	B	504	5/5	0.93	0.11	53,57,62,66	0
5	SO4	C	304	5/5	0.93	0.18	74,79,80,84	0
5	SO4	D	306	5/5	0.93	0.21	62,62,63,65	0
5	SO4	B	508	5/5	0.94	0.15	79,81,90,91	0
5	SO4	F	307	5/5	0.94	0.24	79,83,87,88	0
5	SO4	F	304	5/5	0.94	0.10	55,60,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	L	304	1/1	0.95	0.17	62,62,62,62	0
5	SO4	D	308	5/5	0.96	0.14	64,66,68,74	0
5	SO4	C	303	5/5	0.96	0.27	51,56,62,65	0
8	K	H	407	1/1	0.96	0.12	52,52,52,52	0
5	SO4	B	505	5/5	0.96	0.13	56,62,63,65	0
5	SO4	A	303	5/5	0.97	0.17	51,53,55,58	0
5	SO4	D	305	5/5	0.97	0.11	54,56,58,61	0
5	SO4	D	304	5/5	0.98	0.34	37,50,57,59	0
5	SO4	F	305	5/5	0.98	0.17	74,76,77,82	0
5	SO4	F	302	5/5	0.98	0.13	33,34,34,38	0
5	SO4	D	303	5/5	0.98	0.14	29,31,34,35	0
5	SO4	L	303	5/5	0.98	0.10	49,49,53,54	0
5	SO4	B	503	5/5	0.99	0.15	31,33,36,37	0
5	SO4	H	405	5/5	0.99	0.13	39,39,42,46	0
7	CL	F	308	1/1	0.99	0.10	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.