Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 06:25 PM EDT

PDB ID	:	3QM3
Title	:	1.85 Angstrom Resolution Crystal Structure of Fructose-bisphosphate Aldolase (Fba) from Campylobacter jejuni
Authors	:	Minasov, G.; Wawrzak, Z.; Skarina, T.; Onopriyenko, O.; Papazisi, L.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2011-02-03
Resolution	:	1.85 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 (i) 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 (i)) were used in the production of this report:

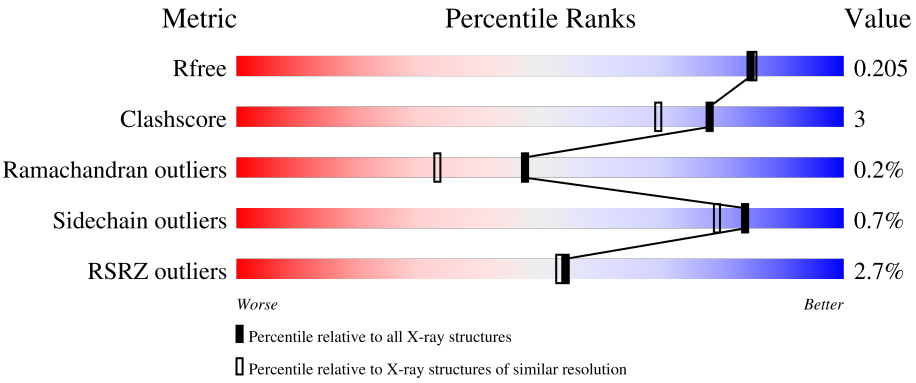
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	357	92% 6%
1	B	357	3% 89% 8%
1	C	357	92%
1	D	357	4% 89% 8%

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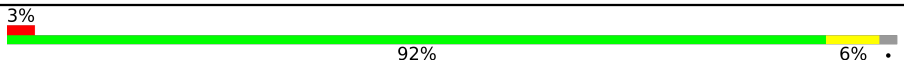
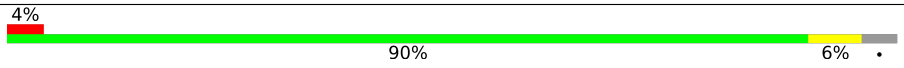
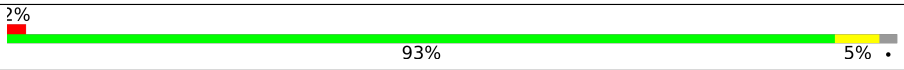
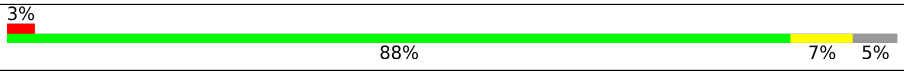
Mol	Chain	Length	Quality of chain
1	E	357	
1	F	357	
1	G	357	
1	H	357	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25480 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	6	0
			2748	1747	464	529	8			
1	B	344	Total	C	N	O	S	0	6	0
			2695	1713	455	518	9			
1	C	344	Total	C	N	O	S	0	4	0
			2685	1705	454	518	8			
1	D	344	Total	C	N	O	S	0	5	0
			2694	1710	456	519	9			
1	E	350	Total	C	N	O	S	0	6	0
			2750	1746	465	531	8			
1	F	343	Total	C	N	O	S	0	7	0
			2702	1718	459	517	8			
1	G	350	Total	C	N	O	S	0	2	0
			2716	1724	458	526	8			
1	H	339	Total	C	N	O	S	0	9	0
			2693	1714	454	516	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q0PAS0
A	-1	ASN	-	expression tag	UNP Q0PAS0
A	0	ALA	-	expression tag	UNP Q0PAS0
B	-2	SER	-	expression tag	UNP Q0PAS0
B	-1	ASN	-	expression tag	UNP Q0PAS0
B	0	ALA	-	expression tag	UNP Q0PAS0
C	-2	SER	-	expression tag	UNP Q0PAS0
C	-1	ASN	-	expression tag	UNP Q0PAS0
C	0	ALA	-	expression tag	UNP Q0PAS0
D	-2	SER	-	expression tag	UNP Q0PAS0
D	-1	ASN	-	expression tag	UNP Q0PAS0
D	0	ALA	-	expression tag	UNP Q0PAS0
E	-2	SER	-	expression tag	UNP Q0PAS0

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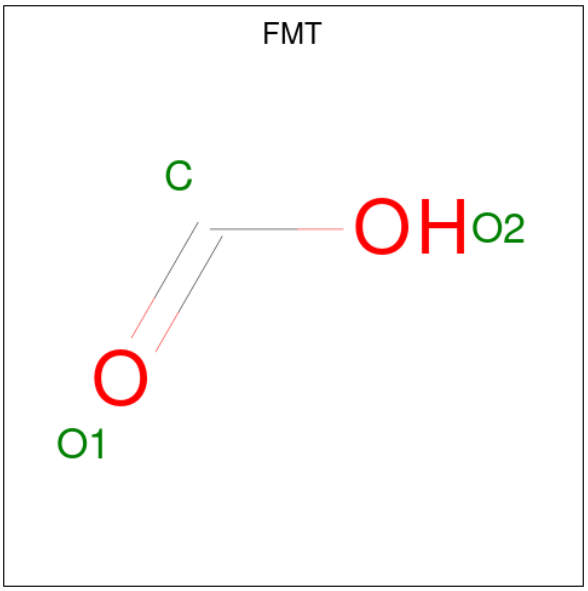
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q0PAS0
E	0	ALA	-	expression tag	UNP Q0PAS0
F	-2	SER	-	expression tag	UNP Q0PAS0
F	-1	ASN	-	expression tag	UNP Q0PAS0
F	0	ALA	-	expression tag	UNP Q0PAS0
G	-2	SER	-	expression tag	UNP Q0PAS0
G	-1	ASN	-	expression tag	UNP Q0PAS0
G	0	ALA	-	expression tag	UNP Q0PAS0
H	-2	SER	-	expression tag	UNP Q0PAS0
H	-1	ASN	-	expression tag	UNP Q0PAS0
H	0	ALA	-	expression tag	UNP Q0PAS0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

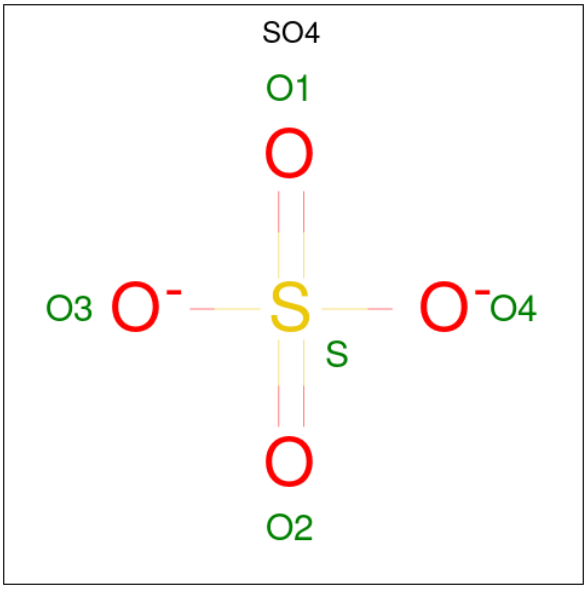
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



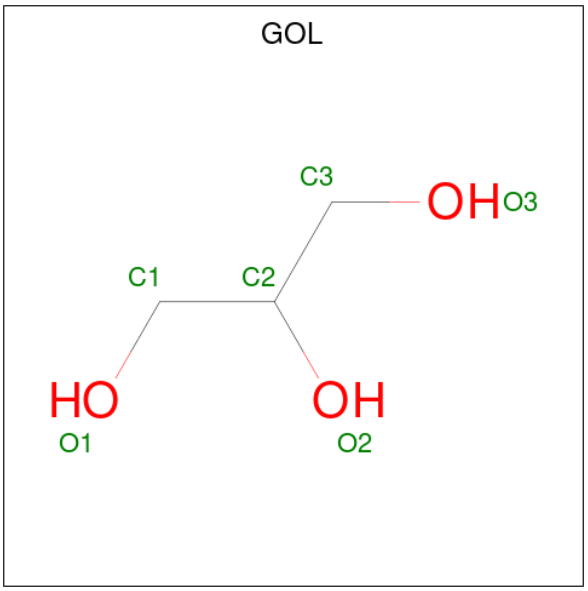
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	1

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	547	Total O 561 561	0	16
7	B	356	Total O 362 362	0	6
7	C	514	Total O 524 524	0	10

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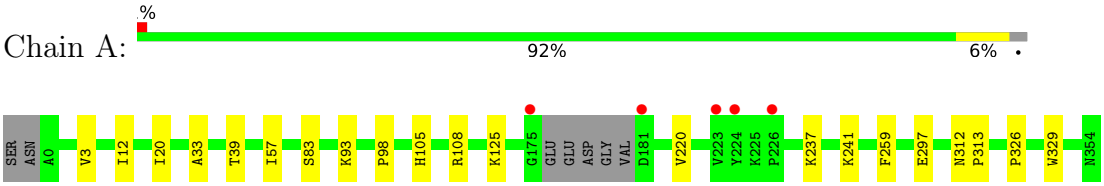
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	390	Total O 400 400	0	12
7	E	499	Total O 506 506	0	8
7	F	342	Total O 347 347	0	7
7	G	546	Total O 560 560	0	14
7	H	368	Total O 378 378	0	11

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.

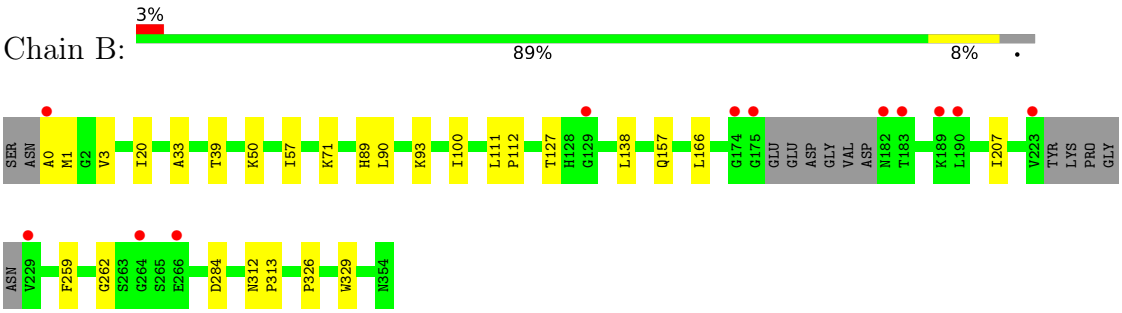
• Molecule 1: Fructose-bisphosphate aldolase

Chain A:



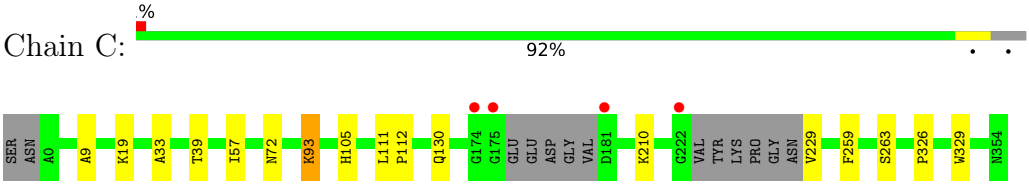
• Molecule 1: Fructose-bisphosphate aldolase

Chain B:



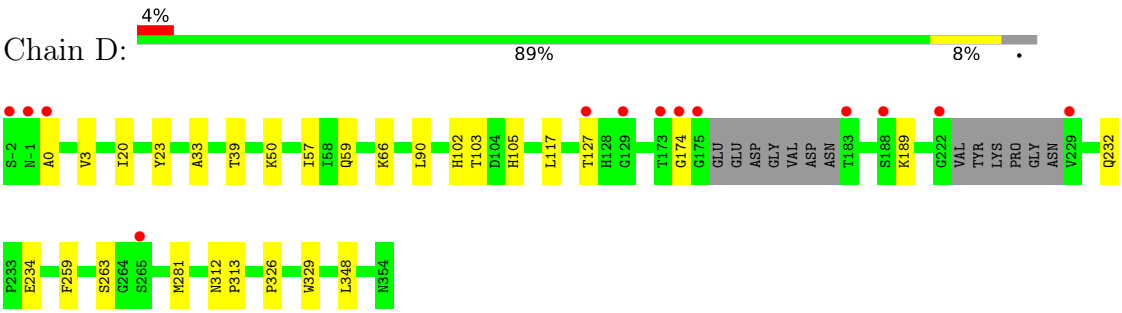
• Molecule 1: Fructose-bisphosphate aldolase

Chain C:



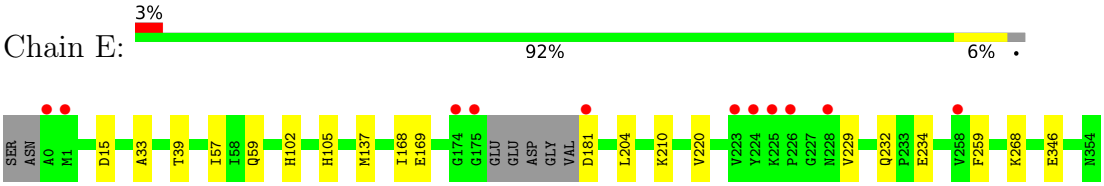
• Molecule 1: Fructose-bisphosphate aldolase

Chain D:



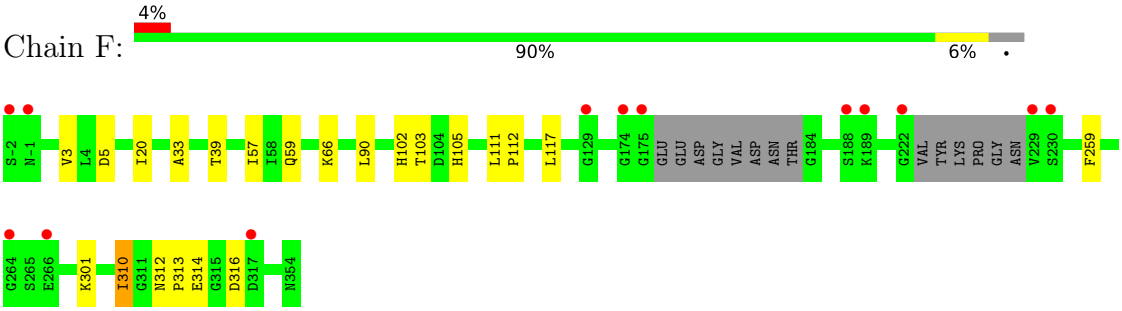
• Molecule 1: Fructose-bisphosphate aldolase

Chain E:



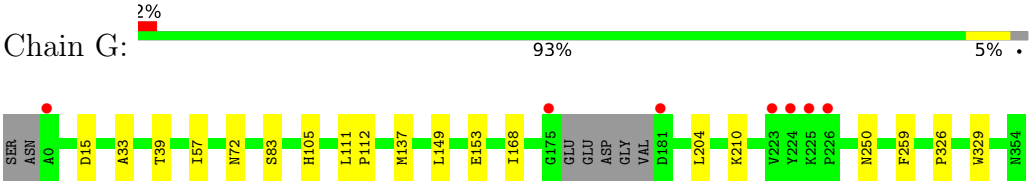
• Molecule 1: Fructose-bisphosphate aldolase

Chain F:



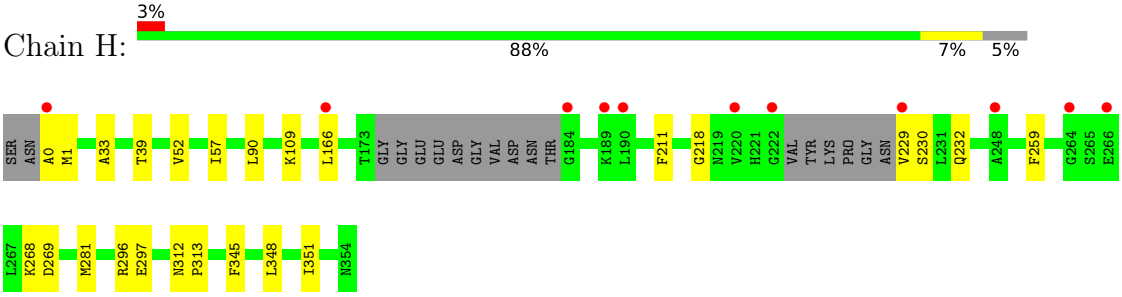
• Molecule 1: Fructose-bisphosphate aldolase

Chain G:



• Molecule 1: Fructose-bisphosphate aldolase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.00Å 101.97Å 105.66Å 113.27° 95.34° 95.75°	Depositor
Resolution (Å)	29.66 – 1.85 29.56 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.66-1.85) 97.6 (29.56-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.149 , 0.191 0.164 , 0.205	Depositor DCC
R_{free} test set	12186 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25480	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 53.20 % 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 4.3615e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CL, FMT, SO4, ZN

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	0.60	0/2803	0.66	0/3783
1	B	0.55	0/2744	0.64	0/3703
1	C	0.62	0/2734	0.67	0/3689
1	D	0.59	0/2743	0.63	0/3699
1	E	0.59	0/2802	0.64	0/3783
1	F	0.56	0/2751	0.63	0/3709
1	G	0.62	0/2768	0.67	0/3739
1	H	0.54	0/2742	0.64	0/3697
All	All	0.58	0/22087	0.65	0/29802

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	A	2748	0	2735	17	0
1	B	2695	0	2682	22	0
1	C	2685	0	2667	18	0
1	D	2694	0	2677	18	0
1	E	2750	0	2727	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2702	0	2698	16	0
1	G	2716	0	2688	11	0
1	H	2693	0	2685	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	3	0	1	0	0
3	D	6	0	2	0	0
3	F	3	0	1	0	0
3	H	3	0	1	0	0
4	A	10	0	0	0	0
4	B	15	0	0	1	0
4	C	15	0	0	1	0
4	D	10	0	0	0	0
4	E	20	0	0	0	0
4	F	5	0	0	0	0
4	G	20	0	0	0	0
4	H	10	0	0	0	0
5	B	12	0	16	4	0
5	C	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	8	1	0
6	D	1	0	0	1	0
7	A	561	0	0	5	0
7	B	362	0	0	3	0
7	C	524	0	0	8	0
7	D	400	0	0	3	0
7	E	506	0	0	3	0
7	F	347	0	0	6	0
7	G	560	0	0	4	0
7	H	378	0	0	2	0
All	All	25480	0	21604	124	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 3.

All (124) 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:E:220:VAL:HG13	7:E:3143:HOH:O	1.40	1.20
1:C:93:LYS:O	1:C:93:LYS:HD3	1.54	1.06
7:G:1291:HOH:O	1:H:90[A]:LEU:HD11	1.75	0.86
1:D:90:LEU:HD12	7:D:871:HOH:O	1.77	0.84
1:H:90[A]:LEU:HD12	7:H:720:HOH:O	1.77	0.82
1:C:93:LYS:HD3	1:C:93:LYS:C	2.00	0.81
1:G:15:ASP:OD1	1:G:210:LYS:HE2	1.91	0.71
1:D:232:GLN:NE2	1:D:234[B]:GLU:OE2	2.23	0.71
7:E:2221:HOH:O	1:F:90[A]:LEU:HD11	1.94	0.66
1:H:230:SER:O	1:H:232:GLN:HG2	1.96	0.65
1:F:310:ILE:HD13	7:F:1582:HOH:O	1.97	0.65
1:E:229:VAL:HG13	7:E:3143:HOH:O	1.98	0.64
1:D:3:VAL:HG13	1:D:20:ILE:HD12	1.82	0.61
1:A:237[B]:LYS:HB3	1:A:237[B]:LYS:NZ	2.15	0.61
1:B:3:VAL:HG13	1:B:20:ILE:HD12	1.83	0.61
1:E:168:ILE:HD13	1:E:204:LEU:HD11	1.83	0.61
1:B:71:LYS:NZ	4:B:360:SO4:O3	2.24	0.60
5:B:357:GOL:H31	7:B:2637:HOH:O	2.01	0.60
1:C:93:LYS:O	1:C:93:LYS:CD	2.43	0.60
1:A:39:THR:HG23	1:B:39:THR:HG23	1.84	0.60
1:G:72:ASN:ND2	7:G:2616:HOH:O	2.34	0.59
1:A:237[B]:LYS:HB3	1:A:237[B]:LYS:HZ3	1.66	0.58
1:A:220:VAL:HG11	7:A:2107:HOH:O	2.04	0.58
1:C:130:GLN:NE2	7:C:1576:HOH:O	2.39	0.56
1:B:157:GLN:OE1	1:B:207[A]:ILE:HD12	2.06	0.56
1:C:72:ASN:ND2	7:C:3174:HOH:O	2.39	0.55
1:C:9:ALA:HB3	1:C:93:LYS:HE2	1.89	0.54
1:E:33:ALA:HA	1:E:57:ILE:HB	1.89	0.54
1:C:19:LYS:HE2	7:C:1825:HOH:O	2.06	0.54
1:D:33:ALA:HA	1:D:57:ILE:HB	1.89	0.54
1:F:103:THR:HG21	1:F:117:LEU:HD13	1.90	0.53
1:H:90[A]:LEU:CD1	7:H:720:HOH:O	2.46	0.53
1:B:127:THR:O	1:B:127:THR:CG2	2.56	0.53
1:D:263:SER:HB3	6:D:356[B]:CL:CL	2.46	0.53
1:C:39:THR:HG23	1:D:39:THR:HG23	1.91	0.53
1:B:33:ALA:HA	1:B:57:ILE:HB	1.91	0.53
1:B:138:LEU:HD13	1:B:166:LEU:HD11	1.91	0.53
1:H:33:ALA:HA	1:H:57:ILE:HB	1.90	0.52
1:B:127:THR:O	1:B:127:THR:HG22	2.10	0.52
1:H:296:ARG:NH2	1:H:297:GLU:HG2	2.24	0.52
1:E:39:THR:HG23	1:F:39:THR:HG23	1.92	0.52
1:F:310:ILE:HD13	1:F:310:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:MET:CE	1:H:348:LEU:HD21	2.40	0.52
1:E:137:MET:CE	1:E:169:GLU:HB2	2.41	0.51
1:A:33:ALA:HA	1:A:57:ILE:HB	1.92	0.51
1:A:237[B]:LYS:NZ	1:A:237[B]:LYS:CB	2.73	0.51
1:A:125:LYS:NZ	7:A:3391[A]:HOH:O	2.43	0.51
1:C:33:ALA:HA	1:C:57:ILE:HB	1.91	0.51
1:E:15:ASP:OD1	1:E:210:LYS:HE2	2.11	0.51
1:D:174:GLY:HA2	1:D:189:LYS:HA	1.93	0.51
1:G:33:ALA:HA	1:G:57:ILE:HB	1.91	0.50
1:H:166:LEU:O	1:H:211:PHE:HA	2.11	0.50
1:G:39:THR:HG23	1:H:39:THR:HG23	1.94	0.49
1:F:3:VAL:HG13	1:F:20:ILE:HD12	1.94	0.49
1:D:127:THR:HG22	1:D:127:THR:O	2.12	0.49
1:C:130:GLN:NE2	7:C:1515:HOH:O	2.37	0.49
1:B:284:ASP:H	5:B:357:GOL:H32	1.78	0.48
1:A:108:ARG:NH1	7:A:2905:HOH:O	2.41	0.48
1:B:50:LYS:HE2	7:G:2461:HOH:O	2.12	0.48
1:H:218:GLY:HA2	1:H:229:VAL:HG13	1.94	0.48
1:D:103:THR:HG21	1:D:117:LEU:HD13	1.96	0.48
1:F:90[A]:LEU:HD12	7:F:1578:HOH:O	2.12	0.48
1:G:15:ASP:OD2	7:G:2934:HOH:O	2.20	0.48
1:D:90:LEU:CD1	7:D:871:HOH:O	2.50	0.48
1:C:93:LYS:HG2	7:C:3398:HOH:O	2.13	0.48
1:D:281:MET:CE	1:D:348:LEU:HD21	2.43	0.47
1:F:310:ILE:HD13	1:F:310:ILE:H	1.79	0.47
1:C:19:LYS:CE	7:C:1825:HOH:O	2.63	0.47
1:F:310:ILE:CD1	7:F:1582:HOH:O	2.58	0.47
1:B:93:LYS:HD3	7:B:912:HOH:O	2.15	0.47
1:B:89:HIS:ND1	5:B:356:GOL:H11	2.30	0.46
1:C:326:PRO:HA	1:C:329:TRP:CE2	2.49	0.46
1:A:83:SER:HB2	1:B:90:LEU:HD23	1.98	0.46
1:F:111:LEU:N	1:F:112:PRO:CD	2.79	0.46
5:F:357:GOL:H2	7:F:3596:HOH:O	2.15	0.45
1:F:59:GLN:HA	1:F:102:HIS:O	2.16	0.45
1:F:312:ASN:HB2	1:F:313:PRO:CD	2.47	0.45
1:D:50:LYS:HE3	1:E:346:GLU:OE1	2.17	0.45
1:D:66:LYS:NZ	7:D:748:HOH:O	2.48	0.44
1:F:66[A]:LYS:HG3	7:F:2364:HOH:O	2.16	0.44
1:H:52[B]:VAL:HG13	1:H:351:ILE:HD13	1.99	0.44
1:C:229:VAL:O	1:C:229:VAL:HG13	2.17	0.44
1:F:33:ALA:HA	1:F:57:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:MET:HE1	1:H:348:LEU:HD21	1.98	0.44
1:C:210:LYS:HE3	7:C:3328:HOH:O	2.17	0.43
1:A:241[B]:LYS:NZ	7:A:3502:HOH:O	2.50	0.43
1:B:262:GLY:N	7:B:2637:HOH:O	2.51	0.43
1:B:284:ASP:N	5:B:357:GOL:H32	2.33	0.43
1:B:312:ASN:HB2	1:B:313:PRO:CD	2.49	0.43
1:D:0:ALA:HB1	1:D:23:TYR:OH	2.19	0.43
1:G:83:SER:HB2	1:H:90[A]:LEU:HD23	2.00	0.43
1:A:312:ASN:HB2	1:A:313:PRO:HD2	2.01	0.43
1:B:57:ILE:HG12	1:B:100:ILE:HB	2.01	0.43
1:D:312:ASN:HB2	1:D:313:PRO:CD	2.48	0.43
1:G:149:LEU:O	1:G:153:GLU:HG3	2.19	0.43
1:G:111:LEU:N	1:G:112:PRO:CD	2.82	0.43
1:H:268:LYS:HG3	1:H:269:ASP:N	2.33	0.42
1:G:326:PRO:HA	1:G:329:TRP:CE2	2.54	0.42
1:C:93:LYS:NZ	7:C:3409:HOH:O	2.51	0.42
1:A:3:VAL:HG13	1:A:20:ILE:HD12	2.02	0.42
1:C:263:SER:OG	4:C:359:SO4:O1	2.26	0.42
1:D:59:GLN:HA	1:D:102:HIS:O	2.20	0.42
1:E:268[B]:LYS:HE3	1:E:268[B]:LYS:HB2	1.67	0.42
1:F:301[B]:LYS:HD3	7:F:1211:HOH:O	2.19	0.42
1:H:312:ASN:HB2	1:H:313:PRO:CD	2.49	0.42
1:A:93[A]:LYS:O	1:A:93[A]:LYS:HD3	2.19	0.42
1:A:326:PRO:HA	1:A:329:TRP:CE2	2.55	0.41
1:H:0:ALA:O	1:H:1[A]:MET:HB2	2.20	0.41
1:G:168:ILE:HD13	1:G:204:LEU:HD11	2.02	0.41
1:E:232:GLN:NE2	1:E:234:GLU:OE2	2.51	0.41
1:B:0:ALA:C	1:B:1[A]:MET:O	2.58	0.41
1:C:111:LEU:N	1:C:112:PRO:CD	2.84	0.41
1:H:52[B]:VAL:HG21	1:H:345:PHE:CD2	2.56	0.41
1:F:316:ASP:OD1	1:G:250:ASN:ND2	2.54	0.41
1:B:93:LYS:O	1:B:93:LYS:HD2	2.21	0.41
1:A:12:ILE:HD11	1:A:98:PRO:HB2	2.03	0.41
1:B:326:PRO:HA	1:B:329:TRP:CE2	2.56	0.41
1:B:111:LEU:N	1:B:112:PRO:CD	2.84	0.40
1:D:326:PRO:HA	1:D:329:TRP:CE2	2.55	0.40
1:E:59:GLN:HA	1:E:102:HIS:O	2.21	0.40
1:A:297:GLU:HG2	7:A:3583:HOH:O	2.20	0.40
1:A:312:ASN:HB2	1:A:313:PRO:CD	2.52	0.40
1:D:127:THR:O	1:D:127:THR:CG2	2.69	0.40
1:B:3:VAL:HG13	1:B:20:ILE:CD1	2.50	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	352/357 (99%)	345 (98%)	6 (2%)	1 (0%)	41	26
1	B	344/357 (96%)	337 (98%)	7 (2%)	0	100	100
1	C	342/357 (96%)	336 (98%)	5 (2%)	1 (0%)	41	26
1	D	343/357 (96%)	337 (98%)	5 (2%)	1 (0%)	41	26
1	E	352/357 (99%)	349 (99%)	2 (1%)	1 (0%)	41	26
1	F	344/357 (96%)	337 (98%)	6 (2%)	1 (0%)	41	26
1	G	348/357 (98%)	341 (98%)	6 (2%)	1 (0%)	41	26
1	H	342/357 (96%)	333 (97%)	9 (3%)	0	100	100
All	All	2767/2856 (97%)	2715 (98%)	46 (2%)	6 (0%)	47	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	105	HIS
1	C	105	HIS
1	G	105	HIS
1	A	105	HIS
1	D	105	HIS
1	F	105	HIS

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	293/293 (100%)	292 (100%)	1 (0%)	92	91
1	B	287/293 (98%)	286 (100%)	1 (0%)	92	91
1	C	286/293 (98%)	284 (99%)	2 (1%)	84	79
1	D	287/293 (98%)	286 (100%)	1 (0%)	92	91
1	E	293/293 (100%)	291 (99%)	2 (1%)	84	79
1	F	288/293 (98%)	284 (99%)	4 (1%)	67	55
1	G	289/293 (99%)	287 (99%)	2 (1%)	84	79
1	H	287/293 (98%)	285 (99%)	2 (1%)	84	79
All	All	2310/2344 (98%)	2295 (99%)	15 (1%)	84	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	PHE
1	B	259	PHE
1	C	93	LYS
1	C	259	PHE
1	D	259	PHE
1	E	181	ASP
1	E	259	PHE
1	F	5	ASP
1	F	259	PHE
1	F	310	ILE
1	F	314	GLU
1	G	137	MET
1	G	259	PHE
1	H	109	LYS
1	H	259	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	B	182	ASN
1	C	128	HIS

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 40 ligands modelled in this entry, 9 are monoatomic - leaving 31 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	SO4	B	358	-	4,4,4	0.27	0	6,6,6	0.30	0
4	SO4	A	357	-	4,4,4	0.17	0	6,6,6	0.15	0
4	SO4	D	360[A]	-	4,4,4	0.33	0	6,6,6	0.26	0
4	SO4	C	358	-	4,4,4	0.19	0	6,6,6	0.76	0
4	SO4	E	360	-	4,4,4	0.12	0	6,6,6	0.22	0
5	GOL	F	357	-	5,5,5	0.45	0	5,5,5	0.30	0
4	SO4	H	357	-	4,4,4	0.16	0	6,6,6	0.20	0
4	SO4	B	359	-	4,4,4	0.24	0	6,6,6	0.70	0
3	FMT	D	358	-	2,2,2	0.64	0	1,1,1	0.36	0
5	GOL	E	356	-	5,5,5	0.44	0	5,5,5	0.29	0
5	GOL	C	356	-	5,5,5	0.79	0	5,5,5	0.61	0
3	FMT	H	356	-	2,2,2	0.68	0	1,1,1	0.45	0
4	SO4	D	359	-	4,4,4	0.16	0	6,6,6	0.25	0
4	SO4	G	356	-	4,4,4	0.24	0	6,6,6	0.46	0
4	SO4	A	358	-	4,4,4	0.22	0	6,6,6	0.56	0
4	SO4	C	359	-	4,4,4	0.09	0	6,6,6	0.33	0
3	FMT	D	357	-	2,2,2	0.65	0	1,1,1	0.46	0
4	SO4	F	358	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	E	357	-	4,4,4	0.24	0	6,6,6	0.42	0
3	FMT	A	356	-	2,2,2	0.69	0	1,1,1	0.38	0
4	SO4	G	357	-	4,4,4	0.43	0	6,6,6	0.41	0
5	GOL	B	356	-	5,5,5	0.32	0	5,5,5	0.25	0
3	FMT	F	356	-	2,2,2	0.70	0	1,1,1	0.47	0
4	SO4	E	359	-	4,4,4	0.29	0	6,6,6	0.25	0
4	SO4	G	359	-	4,4,4	0.19	0	6,6,6	0.34	0
4	SO4	H	358[A]	-	4,4,4	0.07	0	6,6,6	0.19	0
4	SO4	G	358	-	4,4,4	0.13	0	6,6,6	0.24	0
4	SO4	E	358	-	4,4,4	0.59	0	6,6,6	0.52	0
5	GOL	B	357	-	5,5,5	0.84	0	5,5,5	0.63	0
4	SO4	B	360	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	C	357	-	4,4,4	0.15	0	6,6,6	0.34	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
5	GOL	E	356	-	-	2/4/4/4	-
5	GOL	B	357	-	-	1/4/4/4	-
5	GOL	C	356	-	-	2/4/4/4	-
5	GOL	F	357	-	-	0/4/4/4	-
5	GOL	B	356	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	356	GOL	O1-C1-C2-C3
5	E	356	GOL	O1-C1-C2-O2
5	B	356	GOL	C1-C2-C3-O3
5	B	357	GOL	C1-C2-C3-O3
5	C	356	GOL	O2-C2-C3-O3
5	C	356	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	357	GOL	1	0
4	C	359	SO4	1	0
5	B	356	GOL	1	0
5	B	357	GOL	3	0
4	B	360	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^{th} 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	350/357 (98%)	-0.37	5 (1%)	75	76	10, 16, 31, 45	0
1	B	344/357 (96%)	-0.08	12 (3%)	44	41	10, 21, 47, 74	0
1	C	344/357 (96%)	-0.45	4 (1%)	79	79	9, 15, 27, 46	0
1	D	344/357 (96%)	-0.22	13 (3%)	40	38	9, 19, 42, 62	0
1	E	350/357 (98%)	-0.30	11 (3%)	49	47	11, 18, 36, 64	0
1	F	343/357 (96%)	-0.06	13 (3%)	40	38	12, 23, 48, 64	0
1	G	350/357 (98%)	-0.37	7 (2%)	65	64	9, 16, 32, 51	0
1	H	339/357 (94%)	-0.11	11 (3%)	47	45	10, 22, 47, 64	0
All	All	2764/2856 (96%)	-0.25	76 (2%)	54	53	9, 18, 42, 74	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	224	TYR	10.1
1	B	183	THR	9.3
1	H	0	ALA	7.5
1	E	0	ALA	7.4
1	E	223	VAL	7.0
1	H	229	VAL	6.7
1	E	225	LYS	6.6
1	E	226	PRO	6.6
1	G	175	GLY	6.5
1	B	223	VAL	6.5
1	D	-2	SER	6.2
1	F	175	GLY	5.6
1	G	224	TYR	5.6
1	B	264	GLY	5.5
1	F	229	VAL	5.3
1	B	182	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	223	VAL	5.0
1	D	229	VAL	5.0
1	D	175	GLY	4.9
1	A	224	TYR	4.8
1	C	175	GLY	4.8
1	A	175	GLY	4.7
1	F	174	GLY	4.6
1	B	190	LEU	4.5
1	B	229	VAL	4.4
1	A	223	VAL	4.3
1	D	174	GLY	4.1
1	G	225	LYS	4.0
1	G	0	ALA	4.0
1	B	175	GLY	3.9
1	G	181	ASP	3.7
1	B	0	ALA	3.7
1	B	189	LYS	3.7
1	H	184	GLY	3.4
1	D	129	GLY	3.3
1	E	175	GLY	3.3
1	H	220	VAL	3.2
1	H	264	GLY	3.1
1	F	-2	SER	3.1
1	C	174	GLY	3.0
1	F	264	GLY	3.0
1	F	317	ASP	3.0
1	D	127	THR	2.9
1	G	226	PRO	2.9
1	C	222	GLY	2.9
1	H	190	LEU	2.8
1	H	248	ALA	2.8
1	B	174	GLY	2.8
1	F	222	GLY	2.7
1	A	181	ASP	2.7
1	F	189	LYS	2.6
1	D	183	THR	2.6
1	D	188	SER	2.5
1	F	188	SER	2.5
1	F	129	GLY	2.5
1	H	222	GLY	2.4
1	E	1	MET	2.4
1	E	174	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	-1	ASN	2.3
1	A	226	PRO	2.3
1	B	129	GLY	2.3
1	D	-1	ASN	2.3
1	H	266	GLU	2.3
1	E	181	ASP	2.3
1	F	230	SER	2.2
1	F	266	GLU	2.2
1	D	265	SER	2.2
1	D	173	THR	2.2
1	E	258	VAL	2.2
1	D	222	GLY	2.1
1	H	189	LYS	2.1
1	C	181	ASP	2.1
1	E	228	ASN	2.0
1	D	0	ALA	2.0
1	H	166	LEU	2.0
1	B	266	GLU	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, 95^{th} 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
5	GOL	B	356	6/6	0.83	0.20	45,49,53,54	0
3	FMT	D	358	3/3	0.84	0.11	45,45,47,47	0
5	GOL	C	356	6/6	0.86	0.17	27,34,40,45	0
5	GOL	E	356	6/6	0.87	0.14	33,40,41,45	0
4	SO4	H	358[A]	5/5	0.88	0.15	26,28,30,32	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	A	356	3/3	0.88	0.11	30,30,31,32	0
4	SO4	E	360	5/5	0.89	0.10	76,76,77,79	0
4	SO4	G	358	5/5	0.89	0.11	63,65,67,68	0
4	SO4	D	360[A]	5/5	0.89	0.13	8,24,31,32	5
3	FMT	F	356	3/3	0.90	0.08	34,34,35,35	0
5	GOL	B	357	6/6	0.91	0.13	22,30,39,45	0
4	SO4	C	358	5/5	0.91	0.12	35,39,42,43	0
4	SO4	B	360	5/5	0.91	0.15	45,48,50,51	5
5	GOL	F	357	6/6	0.91	0.12	25,34,38,43	0
4	SO4	F	358	5/5	0.92	0.12	37,38,39,40	5
3	FMT	D	357	3/3	0.92	0.09	32,32,33,34	0
4	SO4	G	359	5/5	0.92	0.16	38,42,48,48	0
4	SO4	A	358	5/5	0.93	0.12	20,25,38,39	0
3	FMT	H	356	3/3	0.94	0.07	34,34,35,35	0
4	SO4	G	357	5/5	0.94	0.11	21,27,40,40	0
4	SO4	B	359	5/5	0.95	0.09	39,42,45,45	0
4	SO4	D	359	5/5	0.95	0.18	46,49,52,53	0
4	SO4	E	358	5/5	0.96	0.11	24,29,32,37	0
4	SO4	C	359	5/5	0.96	0.08	19,26,29,29	0
4	SO4	H	357	5/5	0.96	0.09	33,37,38,42	0
4	SO4	B	358	5/5	0.97	0.07	28,28,31,34	0
4	SO4	E	359	5/5	0.97	0.08	21,22,32,32	0
4	SO4	C	357	5/5	0.97	0.07	24,27,31,32	0
4	SO4	E	357	5/5	0.97	0.06	30,30,32,36	0
4	SO4	G	356	5/5	0.97	0.07	29,29,33,37	0
4	SO4	A	357	5/5	0.98	0.07	56,56,58,59	0
6	CL	D	356[B]	1/1	0.98	0.15	16,16,16,16	1
2	ZN	C	355	1/1	0.99	0.04	18,18,18,18	0
2	ZN	D	355	1/1	0.99	0.04	23,23,23,23	0
2	ZN	F	355	1/1	0.99	0.03	28,28,28,28	0
2	ZN	H	355	1/1	0.99	0.04	27,27,27,27	0
2	ZN	E	355	1/1	1.00	0.04	16,16,16,16	0
2	ZN	A	355	1/1	1.00	0.05	16,16,16,16	0
2	ZN	G	355	1/1	1.00	0.04	17,17,17,17	0
2	ZN	B	355	1/1	1.00	0.03	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.