Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2022 – 03:37 pm GMT

PDB ID	:	7PO7
Title	:	Phosphoglycolate phosphatase from Mus musculus
Authors	:	Schloetzer, J.; Schindelin, H.; Fratz, S.
Deposited on	:	2021-09-08
Resolution	:	2.31 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:

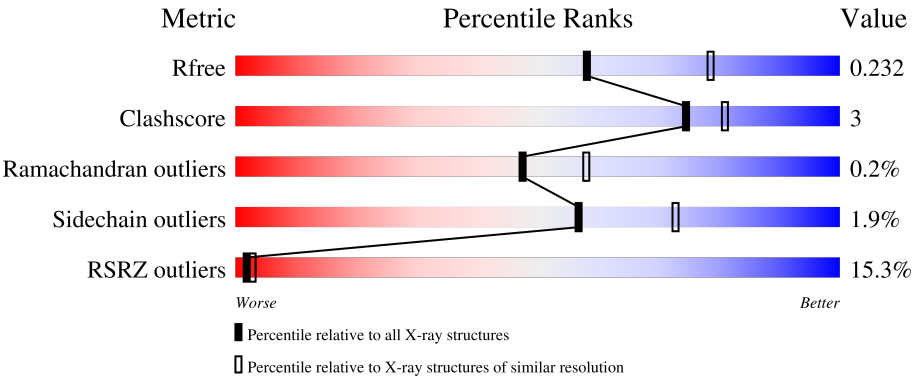
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	321	21% 84% 10% 6%
1	B	321	26% 86% 11%
1	C	321	6% 88% 7%
1	D	321	6% 89% 7%
1	E	321	10% 86% 10%

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Mol	Chain	Length	Quality of chain
1	F	321	12% 89% 7%
1	G	321	13% 62% 36%
1	H	321	17% 86% 9%

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
3	SO4	H	407	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36998 atoms, of which 18482 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 Glycerol-3-phosphate phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	H	N	O	S	0	2	0
			4653	1460	2346	402	430	15			
1	B	310	Total	C	H	N	O	S	0	0	0
			4738	1486	2387	411	441	13			
1	C	310	Total	C	H	N	O	S	0	0	0
			4738	1486	2387	411	441	13			
1	D	310	Total	C	H	N	O	S	0	3	0
			4767	1498	2402	411	441	15			
1	E	310	Total	C	H	N	O	S	0	2	0
			4769	1498	2405	411	441	14			
1	F	311	Total	C	H	N	O	S	0	1	0
			4774	1496	2406	415	444	13			
1	G	207	Total	C	H	N	O	S	0	1	0
			3216	1021	1616	274	296	9			
1	H	311	Total	C	H	N	O	S	0	0	0
			4746	1488	2390	412	443	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ASN	ASP	engineered mutation	UNP Q8CHP8
A	297	SER	CYS	engineered mutation	UNP Q8CHP8
B	34	ASN	ASP	engineered mutation	UNP Q8CHP8
B	297	SER	CYS	engineered mutation	UNP Q8CHP8
C	34	ASN	ASP	engineered mutation	UNP Q8CHP8
C	297	SER	CYS	engineered mutation	UNP Q8CHP8
D	34	ASN	ASP	engineered mutation	UNP Q8CHP8
D	297	SER	CYS	engineered mutation	UNP Q8CHP8
E	34	ASN	ASP	engineered mutation	UNP Q8CHP8
E	297	SER	CYS	engineered mutation	UNP Q8CHP8
F	34	ASN	ASP	engineered mutation	UNP Q8CHP8
F	297	SER	CYS	engineered mutation	UNP Q8CHP8
G	34	ASN	ASP	engineered mutation	UNP Q8CHP8

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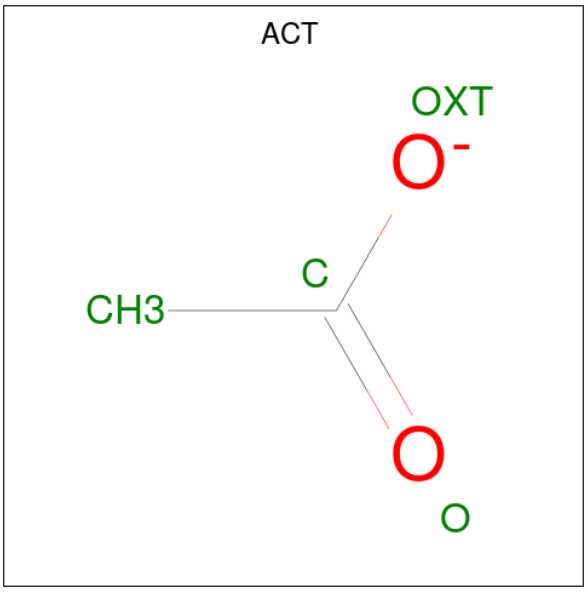
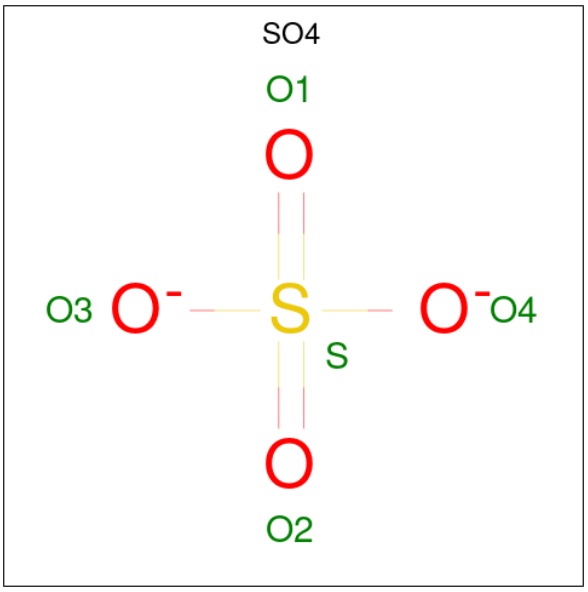
Chain	Residue	Modelled	Actual	Comment	Reference
G	297	SER	CYS	engineered mutation	UNP Q8CHP8
H	34	ASN	ASP	engineered mutation	UNP Q8CHP8
H	297	SER	CYS	engineered mutation	UNP Q8CHP8

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



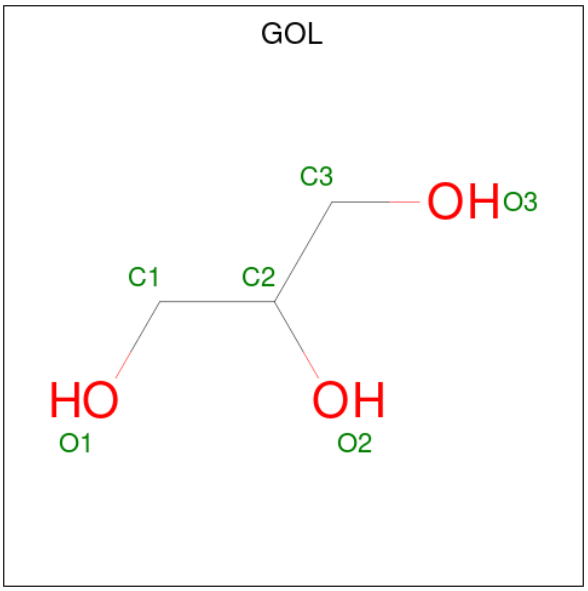
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	H	O	0	0
			7	2	3	2		
2	D	1	Total	C	H	O	0	0
			7	2	3	2		
2	E	1	Total	C	H	O	0	0
			7	2	3	2		
2	F	1	Total	C	H	O	0	0
			7	2	3	2		
2	G	1	Total	C	H	O	0	0
			7	2	3	2		
2	H	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			13	3	7	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Ca 1 1	0	0

- Molecule 6 is water.

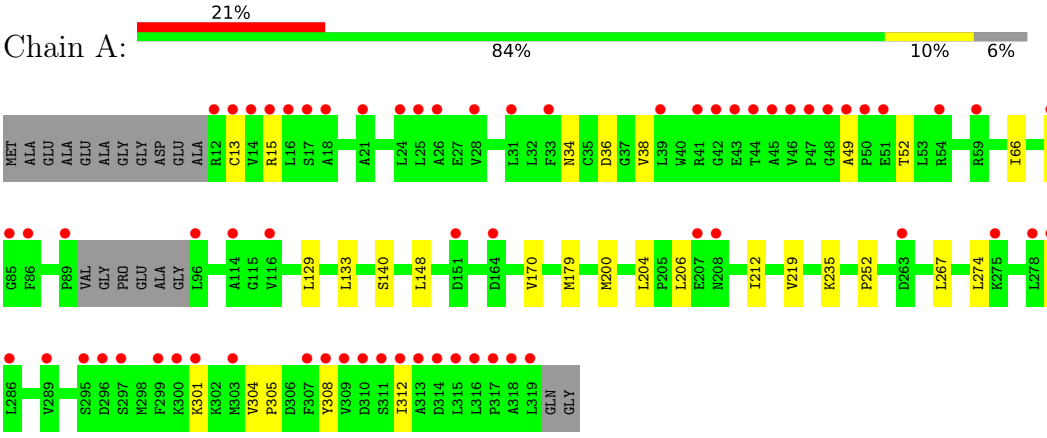
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	15	Total O 16 16	0	1
6	B	34	Total O 35 35	0	1
6	C	86	Total O 86 86	0	0
6	D	37	Total O 37 37	0	0
6	E	27	Total O 28 28	0	1
6	F	52	Total O 53 53	0	1
6	G	5	Total O 5 5	0	0
6	H	31	Total O 31 31	0	0

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.

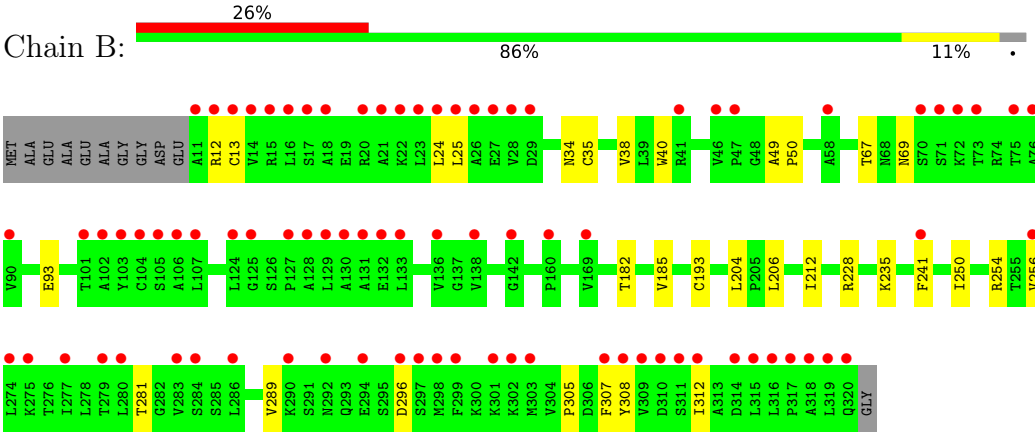
• Molecule 1: Glycerol-3-phosphate phosphatase

Chain A:



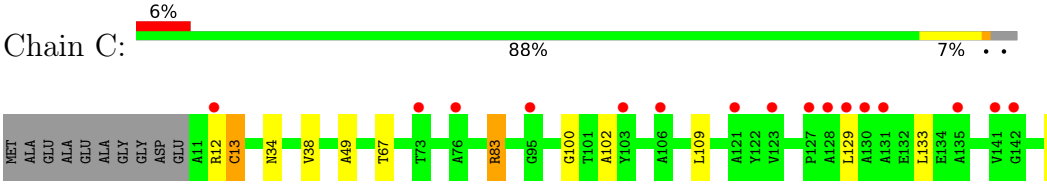
• Molecule 1: Glycerol-3-phosphate phosphatase

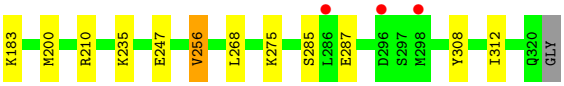
Chain B:



• Molecule 1: Glycerol-3-phosphate phosphatase

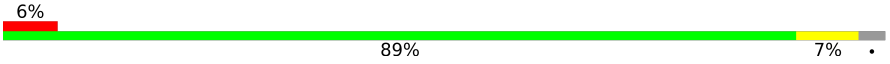
Chain C:

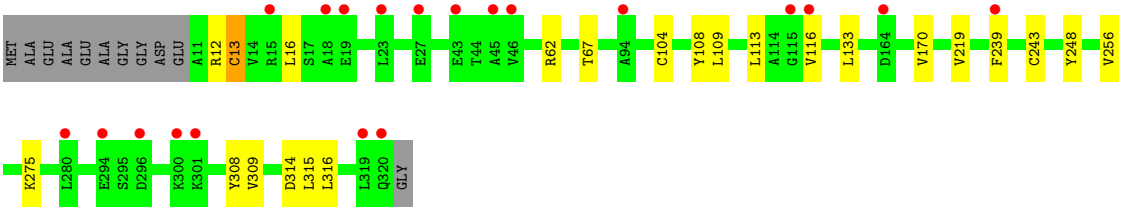




• Molecule 1: Glycerol-3-phosphate phosphatase

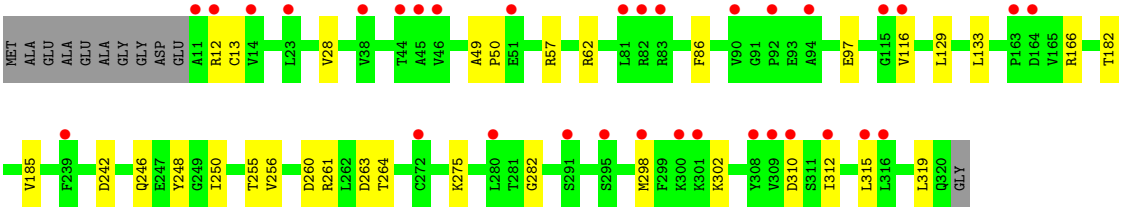
Chain D:





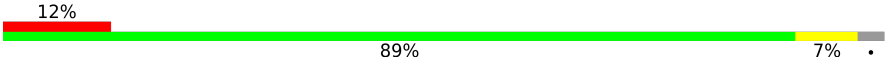
• Molecule 1: Glycerol-3-phosphate phosphatase

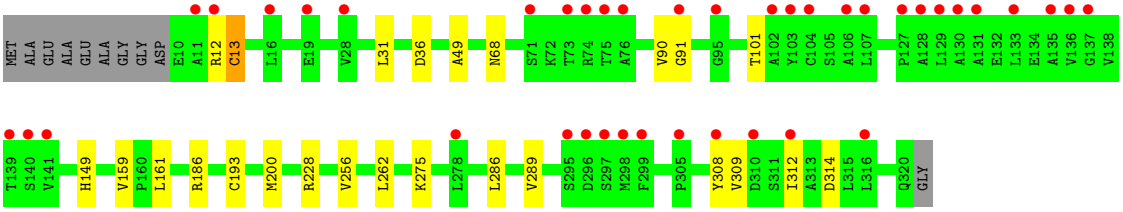
Chain E:



• Molecule 1: Glycerol-3-phosphate phosphatase

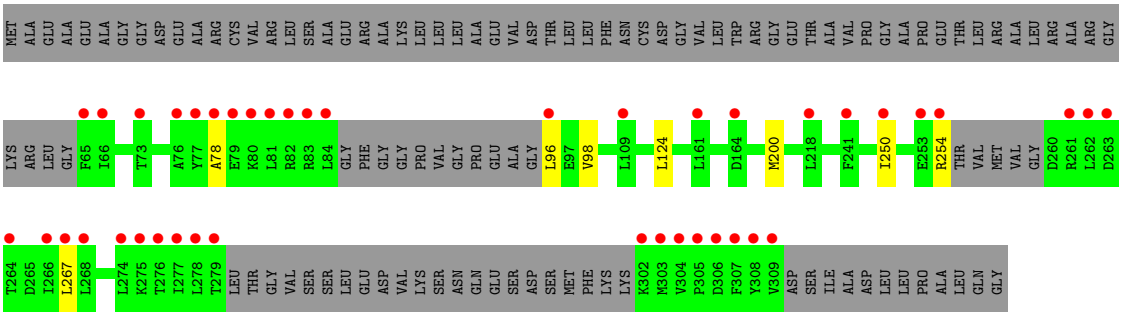
Chain F:





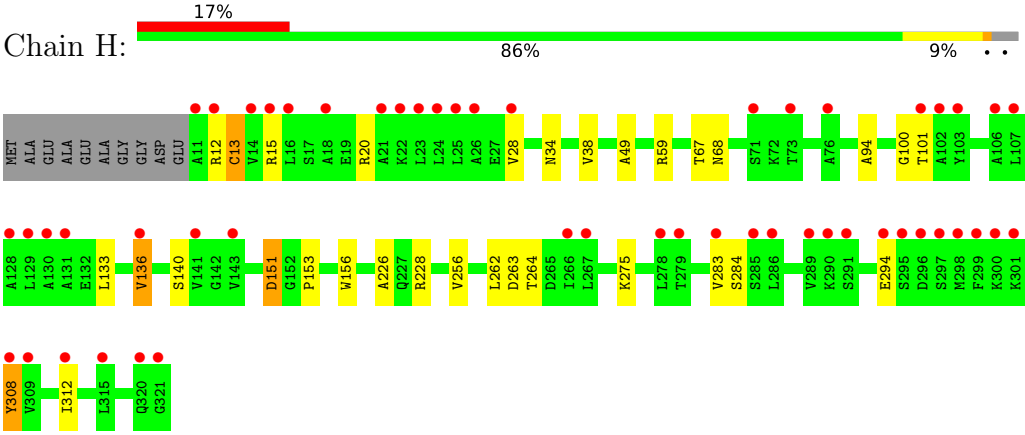
• Molecule 1: Glycerol-3-phosphate phosphatase

Chain G:



• Molecule 1: Glycerol-3-phosphate phosphatase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.26Å 91.20Å 101.32Å 103.46° 89.98° 104.63°	Depositor
Resolution (Å)	19.97 – 2.31 49.17 – 2.31	Depositor EDS
% Data completeness (in resolution range)	71.3 (19.97-2.31) 71.3 (49.17-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.208 , 0.230 0.211 , 0.232	Depositor DCC
R_{free} test set	2233 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36998	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CA, SO4, ACT, GOL

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	0.28	0/2353	0.53	0/3190
1	B	0.28	0/2393	0.51	0/3247
1	C	0.28	0/2393	0.51	0/3247
1	D	0.29	0/2417	0.52	0/3279
1	E	0.28	0/2413	0.52	0/3273
1	F	0.28	0/2413	0.53	0/3273
1	G	0.26	0/1633	0.45	0/2215
1	H	0.28	0/2398	0.51	0/3252
All	All	0.28	0/18413	0.51	0/24976

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	2307	2346	2350	20	0
1	B	2351	2387	2387	17	2
1	C	2351	2387	2387	12	1
1	D	2365	2402	2406	13	0
1	E	2364	2405	2405	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2368	2406	2406	16	1
1	G	1600	1616	1612	4	1
1	H	2356	2390	2390	17	1
2	A	4	3	3	0	0
2	B	4	3	3	0	0
2	C	4	3	3	0	0
2	D	4	3	3	0	0
2	E	4	3	3	0	0
2	F	4	3	3	0	0
2	G	4	3	3	0	0
2	H	4	3	3	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
3	H	5	0	0	0	0
4	B	12	16	16	0	0
4	C	18	24	24	0	0
4	D	12	16	16	1	0
4	E	6	8	8	0	0
4	F	12	15	16	1	0
4	G	6	8	8	0	0
4	H	24	32	32	0	0
5	H	1	0	0	0	0
6	A	16	0	0	0	0
6	B	35	0	0	1	0
6	C	86	0	0	0	0
6	D	37	0	0	0	0
6	E	28	0	0	0	0
6	F	53	0	0	0	0
6	G	5	0	0	0	0
6	H	31	0	0	0	0
All	All	18516	18482	18487	118	3

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 (118) 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:A:38:VAL:HG12	1:A:312:ILE:HD11	1.47	0.96
1:A:38:VAL:CG1	1:A:312:ILE:HD11	2.00	0.92
1:H:28:VAL:HG11	1:H:256:VAL:HG23	1.60	0.84
1:H:151:ASP:N	1:H:151:ASP:OD1	2.17	0.76
1:B:67:THR:HG22	1:B:69:ASN:H	1.52	0.73
1:E:263:ASP:OD1	1:E:264:THR:HG23	1.87	0.73
1:B:49:ALA:HB1	1:B:312:ILE:HD11	1.71	0.71
1:F:49:ALA:HB1	1:F:312:ILE:HD11	1.71	0.71
1:E:49:ALA:HB1	1:E:312:ILE:HD11	1.72	0.70
1:H:263:ASP:OD1	1:H:264:THR:HG23	1.91	0.70
1:H:28:VAL:HG11	1:H:256:VAL:CG2	2.21	0.69
1:B:289:VAL:HG21	1:B:305:PRO:HD2	1.78	0.66
1:F:49:ALA:CB	1:F:312:ILE:HD11	2.24	0.66
1:A:38:VAL:HG22	1:A:279:THR:CG2	2.26	0.65
1:D:109:LEU:HD12	1:D:133:LEU:HD21	1.78	0.65
1:C:49:ALA:HB1	1:C:312:ILE:HD11	1.77	0.65
1:A:38:VAL:HG12	1:A:312:ILE:CD1	2.25	0.63
1:F:90:VAL:HG23	1:F:91:GLY:N	2.15	0.62
1:E:28:VAL:HG11	1:E:256:VAL:HG23	1.82	0.61
1:A:38:VAL:HG22	1:A:279:THR:HG21	1.83	0.60
1:A:52:THR:HG21	1:A:312:ILE:HG22	1.84	0.59
1:C:148:LEU:HD12	1:C:179:MET:CE	2.33	0.59
1:B:241:PHE:HZ	1:B:250:ILE:HD11	1.67	0.58
1:A:38:VAL:HG13	1:A:312:ILE:HD11	1.83	0.57
1:E:256:VAL:HG22	1:E:275:LYS:HB2	1.86	0.57
1:F:12:ARG:O	1:F:12:ARG:HG3	2.05	0.57
1:G:250:ILE:HD12	1:G:250:ILE:O	2.07	0.55
1:D:239[B]:PHE:CE2	1:D:243[B]:CYS:SG	3.00	0.55
1:C:49:ALA:CB	1:C:312:ILE:HD11	2.39	0.53
1:E:116:VAL:HG11	1:E:166:ARG:HG3	1.91	0.53
1:B:34:ASN:O	1:B:38:VAL:HB	2.09	0.52
1:E:49:ALA:CB	1:E:312:ILE:HD11	2.40	0.52
1:D:108:TYR:HB2	1:D:239[B]:PHE:CE2	2.45	0.52
1:E:57:ARG:NH2	1:E:97:GLU:OE1	2.43	0.52
1:F:90:VAL:HG23	1:F:91:GLY:H	1.75	0.52
1:A:204:LEU:HD23	1:A:212:ILE:HD11	1.91	0.52
1:B:49:ALA:CB	1:B:312:ILE:HD11	2.39	0.51
1:D:12:ARG:O	1:D:13:CYS:C	2.48	0.50
1:F:256:VAL:HG22	1:F:275:LYS:HB2	1.91	0.50
1:E:242:ASP:O	1:E:246:GLN:HG2	2.12	0.49
1:C:67:THR:HG22	1:C:100:GLY:HA2	1.93	0.49
1:B:281:THR:O	1:B:281:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:THR:OG1	4:D:401:GOL:H31	2.12	0.49
1:H:136:VAL:O	1:H:136:VAL:HG13	2.12	0.49
1:C:235:LYS:HG2	1:C:268:LEU:HD22	1.95	0.49
1:D:62:ARG:HD3	1:D:248:TYR:CD2	2.48	0.48
1:H:12:ARG:O	1:H:13:CYS:C	2.52	0.48
1:D:104[B]:CYS:HB3	1:D:243[B]:CYS:SG	2.54	0.48
1:H:226:ALA:HB1	1:H:228:ARG:HD2	1.95	0.48
1:A:206:LEU:HD11	1:A:212:ILE:HG23	1.95	0.48
1:A:129:LEU:O	1:A:133:LEU:HD13	2.14	0.48
1:F:309:VAL:CG2	1:F:314:ASP:HB2	2.44	0.48
1:B:235:LYS:O	6:B:501:HOH:O	2.20	0.47
1:F:12:ARG:O	1:F:13:CYS:C	2.51	0.47
1:F:149:HIS:CE1	1:F:159:VAL:HG11	2.50	0.47
1:B:204:LEU:HD23	1:B:212:ILE:HD11	1.97	0.47
1:D:309:VAL:CG2	1:D:314:ASP:HB2	2.45	0.47
1:H:34:ASN:O	1:H:38:VAL:HB	2.15	0.47
1:B:241:PHE:CZ	1:B:250:ILE:HD11	2.49	0.47
1:C:256:VAL:HG23	1:C:275:LYS:HB2	1.97	0.47
1:H:67:THR:HG22	1:H:100:GLY:HA2	1.97	0.47
1:C:12:ARG:O	1:C:13:CYS:C	2.54	0.46
1:A:34:ASN:O	1:A:38:VAL:HB	2.16	0.46
1:H:109:LEU:HD12	1:H:133:LEU:HD21	1.96	0.46
1:H:256:VAL:HG22	1:H:275:LYS:HB2	1.96	0.46
1:H:15:ARG:O	1:H:20:ARG:NH1	2.49	0.46
1:C:285:SER:OG	1:C:287:GLU:HG2	2.16	0.45
1:G:124:LEU:HD12	1:G:124:LEU:N	2.32	0.44
1:E:62:ARG:NH2	1:E:248:TYR:O	2.49	0.44
1:F:68:ASN:HA	1:F:101:THR:HG23	1.98	0.44
1:A:49:ALA:HA	1:A:52:THR:HG22	2.00	0.44
1:C:148:LEU:HD12	1:C:179:MET:HE3	1.98	0.44
1:A:301:LYS:O	1:A:304:VAL:HG22	2.16	0.43
1:E:261:ARG:HG2	1:E:263:ASP:OD1	2.17	0.43
1:B:24:LEU:HD11	1:B:307:PHE:CZ	2.53	0.43
1:G:96:LEU:HG	1:G:98:VAL:HG12	2.00	0.43
1:F:36:ASP:HB2	4:F:401:GOL:C1	2.48	0.43
1:D:16:LEU:HD23	1:D:315:LEU:HD21	2.01	0.43
1:E:315:LEU:HD13	1:E:319:LEU:HD11	2.00	0.43
1:F:193:CYS:O	1:F:228:ARG:NH1	2.49	0.43
1:B:206:LEU:HD11	1:B:212:ILE:HG23	2.01	0.43
1:E:57:ARG:NH1	1:E:86:PHE:O	2.51	0.43
1:F:31:LEU:CD2	1:F:256:VAL:HB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:ALA:HB2	1:G:96:LEU:HD21	2.01	0.43
1:B:182:THR:O	1:B:185:VAL:HG22	2.19	0.42
1:D:256:VAL:HG22	1:D:275:LYS:HB2	2.00	0.42
1:H:13:CYS:SG	1:H:308:TYR:HB3	2.58	0.42
1:E:12:ARG:O	1:E:13:CYS:C	2.57	0.42
1:B:24:LEU:HD11	1:B:307:PHE:CE1	2.54	0.42
1:F:161:LEU:HD11	1:F:186:ARG:HB3	2.01	0.42
1:H:49:ALA:HB1	1:H:312:ILE:HD11	2.02	0.42
1:F:90:VAL:CG2	1:F:91:GLY:N	2.81	0.42
1:C:109:LEU:HD12	1:C:133:LEU:HD21	2.01	0.42
1:A:66:ILE:HG22	1:A:235:LYS:HE3	2.01	0.41
1:E:182:THR:O	1:E:185:VAL:HG22	2.20	0.41
1:H:153:PRO:HA	1:H:156:TRP:CE3	2.54	0.41
1:H:283:VAL:HG23	1:H:284:SER:N	2.35	0.41
1:E:129:LEU:O	1:E:133:LEU:HD13	2.19	0.41
1:A:252:PRO:HA	1:A:274:LEU:HD23	2.01	0.41
1:E:250:ILE:HG23	1:E:255:THR:OG1	2.20	0.41
1:C:34:ASN:O	1:C:38:VAL:HB	2.20	0.41
1:A:267:LEU:O	1:A:267:LEU:HD23	2.21	0.41
1:A:13:CYS:SG	1:A:305:PRO:HG2	2.61	0.41
1:C:102:ALA:HA	1:C:129:LEU:HD13	2.03	0.41
1:A:148:LEU:HA	1:A:179:MET:HG3	2.02	0.41
1:A:170:VAL:HB	1:A:219:VAL:HG22	2.03	0.40
1:B:35:CYS:HB3	1:B:40:TRP:CZ2	2.56	0.40
1:B:193:CYS:O	1:B:228:ARG:NH1	2.53	0.40
1:A:267:LEU:HD23	1:A:267:LEU:C	2.42	0.40
1:D:113:LEU:HD22	1:D:116:VAL:HG21	2.03	0.40
1:D:170:VAL:HB	1:D:219:VAL:HG22	2.03	0.40
1:E:49:ALA:N	1:E:50:PRO:CD	2.85	0.40
1:D:239[B]:PHE:CD2	1:D:243[B]:CYS:SG	3.15	0.40
1:F:262:LEU:HD21	1:F:289:VAL:HG22	2.03	0.40
1:B:49:ALA:N	1:B:50:PRO:CD	2.85	0.40
1:E:260:ASP:HB2	1:E:282:GLY:HA3	2.03	0.40
1:E:298:MET:O	1:E:302:LYS:HG2	2.22	0.40
1:H:68:ASN:HA	1:H:101:THR:HG23	2.02	0.40

All (3) 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:B:93:GLU:OE2	1:G:254:ARG:NH1[1_455]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:NH1	1:H:94:ALA:O[1_556]	2.04	0.16
1:B:82:ARG:NH1	1:F:91:GLY:O[1_455]	2.10	0.10

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	300/321 (94%)	297 (99%)	3 (1%)	0	100	100
1	B	308/321 (96%)	305 (99%)	2 (1%)	1 (0%)	41	50
1	C	308/321 (96%)	303 (98%)	4 (1%)	1 (0%)	41	50
1	D	311/321 (97%)	307 (99%)	3 (1%)	1 (0%)	41	50
1	E	310/321 (97%)	306 (99%)	4 (1%)	0	100	100
1	F	310/321 (97%)	304 (98%)	5 (2%)	1 (0%)	41	50
1	G	200/321 (62%)	198 (99%)	2 (1%)	0	100	100
1	H	309/321 (96%)	305 (99%)	3 (1%)	1 (0%)	41	50
All	All	2356/2568 (92%)	2325 (99%)	26 (1%)	5 (0%)	47	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	13	CYS
1	F	13	CYS
1	H	13	CYS
1	B	13	CYS
1	C	13	CYS

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	251/258 (97%)	244 (97%)	7 (3%)	43	59
1	B	253/258 (98%)	246 (97%)	7 (3%)	43	59
1	C	253/258 (98%)	246 (97%)	7 (3%)	43	59
1	D	256/258 (99%)	254 (99%)	2 (1%)	81	90
1	E	255/258 (99%)	254 (100%)	1 (0%)	91	96
1	F	255/258 (99%)	252 (99%)	3 (1%)	71	83
1	G	174/258 (67%)	172 (99%)	2 (1%)	73	85
1	H	253/258 (98%)	245 (97%)	8 (3%)	39	53
All	All	1950/2064 (94%)	1913 (98%)	37 (2%)	57	73

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	36	ASP
1	A	72	LYS
1	A	140	SER
1	A	200	MET
1	A	281	THR
1	A	308	TYR
1	B	12	ARG
1	B	25	LEU
1	B	83	ARG
1	B	254	ARG
1	B	256	VAL
1	B	296	ASP
1	B	308	TYR
1	C	83	ARG
1	C	183	LYS
1	C	200	MET
1	C	210	ARG
1	C	247	GLU
1	C	256	VAL
1	C	308	TYR
1	D	308	TYR
1	D	316	LEU

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Mol	Chain	Res	Type
1	E	310	ASP
1	F	200	MET
1	F	286	LEU
1	F	308	TYR
1	G	200	MET
1	G	267	LEU
1	H	59	ARG
1	H	110	ARG
1	H	136	VAL
1	H	140	SER
1	H	151	ASP
1	H	262	LEU
1	H	294	GLU
1	H	308	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	246	GLN

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 32 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
2	ACT	B	402	-	3,3,3	1.19	0	3,3,3	1.61	0
4	GOL	H	405	-	5,5,5	0.88	0	5,5,5	0.99	0
4	GOL	H	402	-	5,5,5	0.85	0	5,5,5	0.97	0
4	GOL	C	404	-	5,5,5	0.88	0	5,5,5	0.80	0
4	GOL	D	401	-	5,5,5	0.94	0	5,5,5	0.97	0
2	ACT	F	402	-	3,3,3	1.22	0	3,3,3	1.62	1 (33%)
2	ACT	G	401	-	3,3,3	1.18	0	3,3,3	1.46	0
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	H	403	-	5,5,5	0.86	0	5,5,5	0.89	0
4	GOL	D	403	-	5,5,5	0.87	0	5,5,5	0.98	0
2	ACT	A	401	-	3,3,3	1.24	0	3,3,3	1.45	0
4	GOL	B	401	-	5,5,5	0.87	0	5,5,5	0.94	0
2	ACT	H	401	-	3,3,3	1.21	0	3,3,3	1.48	0
3	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.06	0
4	GOL	B	403	-	5,5,5	0.87	0	5,5,5	0.97	0
3	SO4	F	405	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	405	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.06	0
4	GOL	F	401	-	5,5,5	0.85	0	5,5,5	1.04	0
4	GOL	F	403	-	5,5,5	0.88	0	5,5,5	0.99	0
3	SO4	F	404	-	4,4,4	0.14	0	6,6,6	0.05	0
2	ACT	D	402	-	3,3,3	1.08	0	3,3,3	1.47	0
4	GOL	C	403	-	5,5,5	0.88	0	5,5,5	1.01	0
4	GOL	E	402	-	5,5,5	0.90	0	5,5,5	0.98	0
3	SO4	H	407	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	E	403	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GOL	H	404	-	5,5,5	0.89	0	5,5,5	1.01	0
4	GOL	C	401	-	5,5,5	0.88	0	5,5,5	1.03	0
2	ACT	C	402	-	3,3,3	1.21	0	3,3,3	1.52	0
2	ACT	E	401	-	3,3,3	1.19	0	3,3,3	1.59	0
4	GOL	G	402	-	5,5,5	0.84	0	5,5,5	0.82	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	GOL	C	401	-	-	0/4/4/4	-
4	GOL	F	401	-	-	0/4/4/4	-
4	GOL	F	403	-	-	0/4/4/4	-
4	GOL	H	403	-	-	0/4/4/4	-
4	GOL	H	405	-	-	0/4/4/4	-
4	GOL	D	403	-	-	1/4/4/4	-
4	GOL	H	402	-	-	0/4/4/4	-
4	GOL	C	404	-	-	2/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
4	GOL	B	401	-	-	0/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	E	402	-	-	0/4/4/4	-
4	GOL	H	404	-	-	0/4/4/4	-
4	GOL	D	401	-	-	2/4/4/4	-
4	GOL	G	402	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	402	ACT	O-C-CH3	-2.00	114.54	122.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	GOL	O1-C1-C2-C3
4	C	404	GOL	O2-C2-C3-O3
4	C	404	GOL	C1-C2-C3-O3
4	D	401	GOL	O1-C1-C2-O2
4	D	403	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	GOL	1	0
4	F	401	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	302/321 (94%)	1.24	68 (22%)	0	1	40, 82, 131, 145	0
1	B	310/321 (96%)	1.49	85 (27%)	0	0	38, 73, 133, 157	0
1	C	310/321 (96%)	0.63	19 (6%)	21	27	28, 48, 82, 136	0
1	D	310/321 (96%)	0.55	20 (6%)	18	24	35, 57, 97, 131	0
1	E	310/321 (96%)	0.76	33 (10%)	6	9	37, 68, 124, 158	0
1	F	311/321 (96%)	0.96	40 (12%)	3	5	30, 54, 97, 160	0
1	G	207/321 (64%)	1.38	42 (20%)	1	1	46, 74, 136, 165	0
1	H	311/321 (96%)	1.16	56 (18%)	1	1	35, 67, 114, 176	0
All	All	2371/2568 (92%)	1.00	363 (15%)	2	3	28, 64, 124, 176	0

All (363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	308	TYR	11.0
1	G	307	PHE	10.4
1	G	278	LEU	10.1
1	G	309	VAL	9.5
1	G	79	GLU	8.5
1	B	319	LEU	8.4
1	A	316	LEU	8.3
1	B	16	LEU	8.3
1	A	315	LEU	8.0
1	H	295	SER	7.9
1	B	296	ASP	7.3
1	B	316	LEU	7.2
1	G	83	ARG	7.0
1	G	78	ALA	6.8
1	G	277	ILE	6.8
1	H	296	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	297	SER	6.4
1	A	312	ILE	6.3
1	H	299	PHE	6.2
1	A	16	LEU	6.2
1	B	312	ILE	6.1
1	H	11	ALA	6.0
1	E	90	VAL	6.0
1	H	16	LEU	5.8
1	A	14	VAL	5.8
1	G	82	ARG	5.7
1	A	15	ARG	5.6
1	H	309	VAL	5.6
1	A	319	LEU	5.6
1	G	81	LEU	5.5
1	B	280	LEU	5.4
1	B	315	LEU	5.4
1	A	49	ALA	5.3
1	B	24	LEU	5.3
1	B	286	LEU	5.3
1	H	25	LEU	5.2
1	E	92	PRO	5.2
1	A	24	LEU	5.2
1	A	39	LEU	5.2
1	G	263	ASP	5.2
1	G	250	ILE	5.1
1	H	14	VAL	5.1
1	A	44	THR	5.1
1	B	299	PHE	5.1
1	B	15	ARG	5.1
1	A	317	PRO	5.1
1	E	298	MET	5.1
1	G	80	LYS	5.1
1	A	286	LEU	5.1
1	F	312	ILE	5.0
1	H	286	LEU	4.9
1	G	77	TYR	4.9
1	A	114	ALA	4.9
1	B	317	PRO	4.9
1	A	307	PHE	4.8
1	B	12	ARG	4.8
1	G	303	MET	4.8
1	H	321	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	23	LEU	4.8
1	A	21	ALA	4.7
1	G	279	THR	4.7
1	A	54	ARG	4.7
1	A	308	TYR	4.7
1	B	17	SER	4.7
1	E	94	ALA	4.7
1	E	312	ILE	4.6
1	F	131	ALA	4.5
1	G	266	ILE	4.5
1	G	275	LYS	4.5
1	B	311	SER	4.5
1	A	279	THR	4.5
1	B	131	ALA	4.5
1	H	289	VAL	4.5
1	A	313	ALA	4.5
1	A	47	PRO	4.5
1	B	318	ALA	4.4
1	E	51	GLU	4.4
1	E	23	LEU	4.4
1	G	304	VAL	4.4
1	F	130	ALA	4.4
1	B	128	ALA	4.3
1	B	28	VAL	4.3
1	A	13	CYS	4.3
1	B	320	GLN	4.3
1	B	130	ALA	4.2
1	B	23	LEU	4.2
1	F	128	ALA	4.2
1	A	318	ALA	4.2
1	G	73	THR	4.2
1	F	299	PHE	4.2
1	F	127	PRO	4.2
1	D	164	ASP	4.1
1	A	300	LYS	4.1
1	E	316	LEU	4.1
1	B	11	ALA	4.1
1	H	102	ALA	4.0
1	F	296	ASP	4.0
1	H	15	ARG	4.0
1	B	127	PRO	3.9
1	G	161	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	22	LYS	3.9
1	E	315	LEU	3.9
1	F	16	LEU	3.9
1	G	84	LEU	3.9
1	A	164	ASP	3.9
1	H	24	LEU	3.9
1	H	300	LYS	3.9
1	B	25	LEU	3.9
1	B	284	SER	3.8
1	G	65	PHE	3.8
1	A	82	ARG	3.8
1	A	296	ASP	3.8
1	E	44	THR	3.8
1	A	51	GLU	3.7
1	F	129	LEU	3.7
1	G	305	PRO	3.7
1	B	14	VAL	3.7
1	B	301	LYS	3.7
1	B	129	LEU	3.7
1	B	294	GLU	3.7
1	E	83	ARG	3.7
1	B	102	ALA	3.7
1	B	13	CYS	3.7
1	A	96	LEU	3.7
1	E	12	ARG	3.7
1	A	25	LEU	3.6
1	H	308	TYR	3.6
1	G	262	LEU	3.6
1	G	276	THR	3.6
1	F	11	ALA	3.6
1	E	11	ALA	3.6
1	H	28	VAL	3.6
1	E	82	ARG	3.6
1	A	59	ARG	3.5
1	H	302	LYS	3.5
1	E	81	LEU	3.5
1	A	48	GLY	3.5
1	B	18	ALA	3.5
1	E	295	SER	3.5
1	H	12	ARG	3.5
1	B	314	ASP	3.5
1	G	76	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	294	GLU	3.5
1	B	58	ALA	3.4
1	A	309	VAL	3.4
1	A	314	ASP	3.4
1	A	33	PHE	3.4
1	B	310	ASP	3.4
1	B	275	LYS	3.4
1	B	307	PHE	3.4
1	D	27	GLU	3.4
1	H	283	VAL	3.3
1	A	295	SER	3.3
1	H	297	SER	3.3
1	B	308	TYR	3.3
1	B	273	SER	3.3
1	H	18	ALA	3.3
1	F	103	TYR	3.3
1	B	47	PRO	3.3
1	G	274	LEU	3.3
1	B	76	ALA	3.2
1	H	285	SER	3.2
1	C	130	ALA	3.2
1	A	278	LEU	3.2
1	H	320	GLN	3.2
1	A	275	LYS	3.2
1	C	127	PRO	3.1
1	F	295	SER	3.1
1	A	28	VAL	3.1
1	B	90	VAL	3.1
1	A	310	ASP	3.1
1	B	277	ILE	3.1
1	E	45	ALA	3.1
1	H	312	ILE	3.1
1	A	263	ASP	3.1
1	A	42	GLY	3.1
1	A	86	PHE	3.1
1	B	46	VAL	3.0
1	B	290	LYS	3.0
1	C	131	ALA	3.0
1	F	297	SER	3.0
1	F	102	ALA	3.0
1	F	19	GLU	3.0
1	H	21	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	301	LYS	3.0
1	H	278	LEU	3.0
1	A	43	GLU	3.0
1	D	115	GLY	3.0
1	H	71	SER	3.0
1	A	289	VAL	3.0
1	B	279	THR	3.0
1	A	41	ARG	3.0
1	B	71	SER	2.9
1	E	239[A]	PHE	2.9
1	H	127	PRO	2.9
1	G	267	LEU	2.9
1	G	302	LYS	2.9
1	H	22	LYS	2.9
1	H	298	MET	2.9
1	B	104	CYS	2.9
1	F	73	THR	2.9
1	B	283	VAL	2.9
1	C	298	MET	2.9
1	H	129	LEU	2.9
1	B	106	ALA	2.9
1	B	20	ARG	2.9
1	A	303	MET	2.8
1	F	308	TYR	2.8
1	B	101	THR	2.8
1	E	14	VAL	2.8
1	F	133	LEU	2.8
1	H	305	PRO	2.8
1	G	261	ARG	2.8
1	D	300	LYS	2.8
1	A	297	SER	2.8
1	A	45	ALA	2.7
1	G	306	ASP	2.7
1	F	107	LEU	2.7
1	F	298	MET	2.7
1	B	75	THR	2.7
1	C	129	LEU	2.7
1	H	315	LEU	2.7
1	G	253	GLU	2.7
1	H	301	LYS	2.7
1	C	142	GLY	2.7
1	E	301	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	130	ALA	2.7
1	E	272	CYS	2.7
1	H	290	LYS	2.7
1	H	131	ALA	2.7
1	E	280	LEU	2.7
1	C	141	VAL	2.6
1	D	15	ARG	2.6
1	C	106	ALA	2.6
1	A	85	GLY	2.6
1	H	107	LEU	2.6
1	H	294	GLU	2.6
1	B	70	SER	2.6
1	A	46	VAL	2.6
1	F	278	LEU	2.6
1	B	73	THR	2.6
1	E	116	VAL	2.6
1	A	301	LYS	2.6
1	B	21	ALA	2.6
1	E	291	SER	2.6
1	B	256	VAL	2.6
1	B	107	LEU	2.5
1	B	309	VAL	2.5
1	F	135	ALA	2.5
1	B	41	ARG	2.5
1	E	310	ASP	2.5
1	A	17	SER	2.5
1	B	27	GLU	2.5
1	G	164	ASP	2.5
1	D	116	VAL	2.5
1	F	106	ALA	2.5
1	B	29	ASP	2.5
1	C	73	THR	2.5
1	F	28	VAL	2.5
1	H	26	ALA	2.5
1	C	296	ASP	2.5
1	C	12	ARG	2.5
1	B	262	LEU	2.5
1	D	23	LEU	2.5
1	G	241	PHE	2.4
1	B	302	LYS	2.4
1	A	207	GLU	2.4
1	B	133	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	115	GLY	2.4
1	B	124	LEU	2.4
1	B	298	MET	2.4
1	D	19	GLU	2.4
1	B	274	LEU	2.4
1	B	26	ALA	2.4
1	A	116	VAL	2.4
1	D	46	VAL	2.4
1	D	296	ASP	2.4
1	C	123	VAL	2.4
1	D	320	GLN	2.4
1	F	71	SER	2.4
1	D	280	LEU	2.3
1	A	72	LYS	2.3
1	F	139	THR	2.3
1	F	104	CYS	2.3
1	G	66	ILE	2.3
1	C	103	TYR	2.3
1	E	163	PRO	2.3
1	F	76	ALA	2.3
1	A	281	THR	2.3
1	E	46	VAL	2.3
1	B	142	GLY	2.3
1	A	12	ARG	2.3
1	A	31	LEU	2.3
1	E	309	VAL	2.3
1	H	136	VAL	2.3
1	F	12	ARG	2.3
1	B	103	TYR	2.3
1	G	264	THR	2.3
1	D	239[A]	PHE	2.3
1	A	208	ASN	2.3
1	F	310	ASP	2.3
1	A	311	SER	2.3
1	C	128	ALA	2.3
1	F	316	LEU	2.3
1	C	95	GLY	2.3
1	H	291	SER	2.3
1	D	319	LEU	2.2
1	G	96	LEU	2.2
1	H	143	VAL	2.2
1	F	75	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	103	TYR	2.2
1	B	160	PRO	2.2
1	A	299	PHE	2.2
1	F	140	SER	2.2
1	C	76	ALA	2.2
1	C	121	ALA	2.2
1	H	106	ALA	2.2
1	B	72	LYS	2.2
1	F	141	VAL	2.2
1	H	128	ALA	2.2
1	E	300	LYS	2.2
1	B	105	SER	2.2
1	F	136	VAL	2.2
1	D	94	ALA	2.2
1	H	76	ALA	2.2
1	H	101	THR	2.2
1	B	132	GLU	2.2
1	F	95	GLY	2.2
1	A	50	PRO	2.1
1	A	280	LEU	2.1
1	G	218	LEU	2.1
1	H	267	LEU	2.1
1	C	135	ALA	2.1
1	A	151	ASP	2.1
1	A	89	PRO	2.1
1	F	91	GLY	2.1
1	F	305	PRO	2.1
1	B	136	VAL	2.1
1	B	138	VAL	2.1
1	H	304	VAL	2.1
1	H	266	ILE	2.1
1	G	109	LEU	2.1
1	G	268	LEU	2.1
1	B	303	MET	2.1
1	D	45	ALA	2.1
1	B	125	GLY	2.1
1	B	292	ASN	2.1
1	H	279	THR	2.1
1	D	18	ALA	2.1
1	E	38	VAL	2.0
1	H	141	VAL	2.0
1	G	254	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	286	LEU	2.0
1	D	43	GLU	2.0
1	A	18	ALA	2.0
1	A	26	ALA	2.0
1	F	74	ARG	2.0
1	B	169	VAL	2.0
1	B	241	PHE	2.0
1	E	308	TYR	2.0
1	F	137	GLY	2.0
1	E	164	ASP	2.0
1	H	73	THR	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
4	GOL	G	402	6/6	0.52	0.26	102,123,128,128	0
4	GOL	H	405	6/6	0.60	0.21	107,129,135,137	0
3	SO4	H	407	5/5	0.63	0.48	132,133,134,137	0
4	GOL	C	404	6/6	0.67	0.33	78,94,111,112	0
4	GOL	C	403	6/6	0.77	0.35	87,105,110,111	0
3	SO4	B	404	5/5	0.78	0.34	137,139,139,140	0
4	GOL	E	402	6/6	0.78	0.23	91,110,114,114	0
4	GOL	H	404	6/6	0.80	0.28	81,98,111,111	0
4	GOL	H	403	6/6	0.84	0.30	76,92,95,99	0
4	GOL	B	401	6/6	0.84	0.31	76,93,102,110	0
4	GOL	B	403	6/6	0.84	0.33	75,91,93,100	0
4	GOL	D	403	6/6	0.85	0.13	78,95,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	F	403	6/6	0.85	0.16	89,108,117,119	0
3	SO4	A	402	5/5	0.87	0.40	151,152,152,152	0
2	ACT	F	402	4/4	0.87	0.14	45,55,55,57	0
3	SO4	F	404	5/5	0.87	0.17	136,137,138,138	0
3	SO4	E	403	5/5	0.89	0.20	125,125,126,127	0
4	GOL	D	401	6/6	0.89	0.13	62,75,80,88	0
2	ACT	A	401	4/4	0.89	0.15	70,72,87,87	0
4	GOL	H	402	6/6	0.90	0.22	79,95,101,102	0
2	ACT	G	401	4/4	0.90	0.09	75,78,92,92	0
3	SO4	F	405	5/5	0.92	0.16	105,106,107,109	0
2	ACT	E	401	4/4	0.92	0.15	58,62,71,71	0
3	SO4	C	405	5/5	0.92	0.17	99,100,104,104	0
4	GOL	F	401	6/6	0.93	0.25	49,69,84,87	0
3	SO4	D	404	5/5	0.94	0.23	106,107,108,108	0
4	GOL	C	401	6/6	0.94	0.28	43,61,78,79	0
2	ACT	B	402	4/4	0.95	0.14	59,66,80,80	0
2	ACT	D	402	4/4	0.95	0.23	63,65,79,79	0
5	CA	H	406	1/1	0.96	0.19	57,57,57,57	0
2	ACT	C	402	4/4	0.97	0.14	49,54,67,67	0
2	ACT	H	401	4/4	0.97	0.13	58,60,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.