Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2023 – 03:40 PM EDT

PDB ID	:	8FUM
Title	:	AibH1H2 metalated with Fe in the presence of Tris
Authors	:	Powell, M.M.; Rittle, J.
Deposited on	:	2023-01-17
Resolution	:	1.48 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:

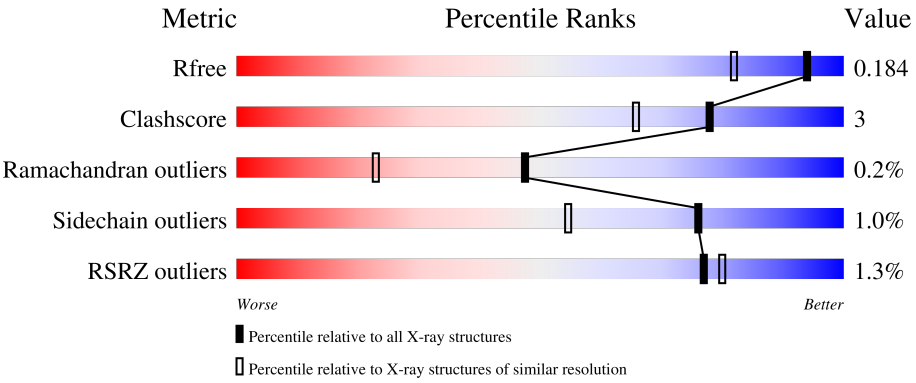
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	392	86% 11%
1	C	392	86% 11%
1	E	392	83% 6% 10%
1	G	392	84% 5% 10%
2	B	378	88% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	378	2% 89% 7%
2	H	378	4% 91% 5%
3	D	378	% 90% 5%

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	PG4	B	501	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 47082 atoms, of which 21982 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 Amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	H	N	O	S	0	2	0
			5527	1795	2716	491	520	5			
1	C	350	Total	C	H	N	O	S	0	1	0
			5513	1791	2706	491	520	5			
1	E	351	Total	C	H	N	O	S	0	4	0
			5539	1803	2712	495	524	5			
1	G	351	Total	C	H	N	O	S	0	6	0
			5554	1804	2728	495	522	5			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP A0A402C2V4
A	-5	GLY	-	expression tag	UNP A0A402C2V4
A	-4	HIS	-	expression tag	UNP A0A402C2V4
A	-3	HIS	-	expression tag	UNP A0A402C2V4
A	-2	HIS	-	expression tag	UNP A0A402C2V4
A	-1	HIS	-	expression tag	UNP A0A402C2V4
A	0	HIS	-	expression tag	UNP A0A402C2V4
A	1	HIS	-	expression tag	UNP A0A402C2V4
A	2	SER	-	expression tag	UNP A0A402C2V4
A	3	GLY	-	expression tag	UNP A0A402C2V4
A	4	GLU	-	expression tag	UNP A0A402C2V4
A	5	ASN	-	expression tag	UNP A0A402C2V4
A	6	LEU	-	expression tag	UNP A0A402C2V4
A	7	TYR	-	expression tag	UNP A0A402C2V4
A	8	PHE	-	expression tag	UNP A0A402C2V4
A	9	GLN	-	expression tag	UNP A0A402C2V4
A	10	SER	-	expression tag	UNP A0A402C2V4
A	11	GLY	-	expression tag	UNP A0A402C2V4
A	12	GLY	-	expression tag	UNP A0A402C2V4
C	-6	MET	-	expression tag	UNP A0A402C2V4
C	-5	GLY	-	expression tag	UNP A0A402C2V4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP A0A402C2V4
C	-3	HIS	-	expression tag	UNP A0A402C2V4
C	-2	HIS	-	expression tag	UNP A0A402C2V4
C	-1	HIS	-	expression tag	UNP A0A402C2V4
C	0	HIS	-	expression tag	UNP A0A402C2V4
C	1	HIS	-	expression tag	UNP A0A402C2V4
C	2	SER	-	expression tag	UNP A0A402C2V4
C	3	GLY	-	expression tag	UNP A0A402C2V4
C	4	GLU	-	expression tag	UNP A0A402C2V4
C	5	ASN	-	expression tag	UNP A0A402C2V4
C	6	LEU	-	expression tag	UNP A0A402C2V4
C	7	TYR	-	expression tag	UNP A0A402C2V4
C	8	PHE	-	expression tag	UNP A0A402C2V4
C	9	GLN	-	expression tag	UNP A0A402C2V4
C	10	SER	-	expression tag	UNP A0A402C2V4
C	11	GLY	-	expression tag	UNP A0A402C2V4
C	12	GLY	-	expression tag	UNP A0A402C2V4
E	-6	MET	-	expression tag	UNP A0A402C2V4
E	-5	GLY	-	expression tag	UNP A0A402C2V4
E	-4	HIS	-	expression tag	UNP A0A402C2V4
E	-3	HIS	-	expression tag	UNP A0A402C2V4
E	-2	HIS	-	expression tag	UNP A0A402C2V4
E	-1	HIS	-	expression tag	UNP A0A402C2V4
E	0	HIS	-	expression tag	UNP A0A402C2V4
E	1	HIS	-	expression tag	UNP A0A402C2V4
E	2	SER	-	expression tag	UNP A0A402C2V4
E	3	GLY	-	expression tag	UNP A0A402C2V4
E	4	GLU	-	expression tag	UNP A0A402C2V4
E	5	ASN	-	expression tag	UNP A0A402C2V4
E	6	LEU	-	expression tag	UNP A0A402C2V4
E	7	TYR	-	expression tag	UNP A0A402C2V4
E	8	PHE	-	expression tag	UNP A0A402C2V4
E	9	GLN	-	expression tag	UNP A0A402C2V4
E	10	SER	-	expression tag	UNP A0A402C2V4
E	11	GLY	-	expression tag	UNP A0A402C2V4
E	12	GLY	-	expression tag	UNP A0A402C2V4
G	-6	MET	-	expression tag	UNP A0A402C2V4
G	-5	GLY	-	expression tag	UNP A0A402C2V4
G	-4	HIS	-	expression tag	UNP A0A402C2V4
G	-3	HIS	-	expression tag	UNP A0A402C2V4
G	-2	HIS	-	expression tag	UNP A0A402C2V4
G	-1	HIS	-	expression tag	UNP A0A402C2V4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A402C2V4
G	1	HIS	-	expression tag	UNP A0A402C2V4
G	2	SER	-	expression tag	UNP A0A402C2V4
G	3	GLY	-	expression tag	UNP A0A402C2V4
G	4	GLU	-	expression tag	UNP A0A402C2V4
G	5	ASN	-	expression tag	UNP A0A402C2V4
G	6	LEU	-	expression tag	UNP A0A402C2V4
G	7	TYR	-	expression tag	UNP A0A402C2V4
G	8	PHE	-	expression tag	UNP A0A402C2V4
G	9	GLN	-	expression tag	UNP A0A402C2V4
G	10	SER	-	expression tag	UNP A0A402C2V4
G	11	GLY	-	expression tag	UNP A0A402C2V4
G	12	GLY	-	expression tag	UNP A0A402C2V4

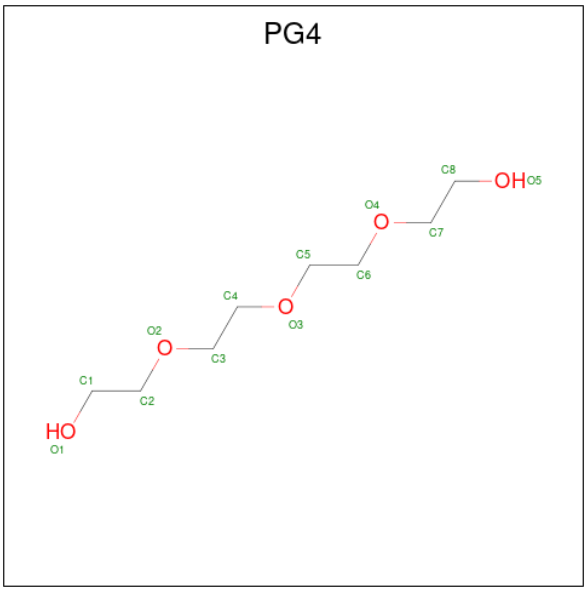
- Molecule 2 is a protein called Amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	363	Total	C	H	N	O	S	0	4	0
			5611	1839	2730	487	546	9			
2	F	362	Total	C	H	N	O	S	0	4	0
			5625	1834	2748	493	541	9			
2	H	364	Total	C	H	N	O	S	0	4	0
			5617	1834	2745	490	539	9			

- Molecule 3 is a protein called Amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	363	Total	C	H	N	O	S	0	3	0
			5644	1840	2761	493	541	9			

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 31 8 18 5	0	0
4	A	1	Total C H O 31 8 18 5	0	0
4	B	1	Total C H O 31 8 18 5	0	0
4	C	1	Total C H O 31 8 18 5	0	0
4	E	1	Total C H O 31 8 18 5	0	0
4	G	1	Total C H O 31 8 18 5	0	0
4	G	1	Total C H O 31 8 18 5	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe 1 1	0	0
5	B	2	Total Fe 2 2	0	0
5	C	1	Total Fe 1 1	0	0
5	D	2	Total Fe 2 2	0	0
5	E	1	Total Fe 1 1	0	0

Continued on next page...

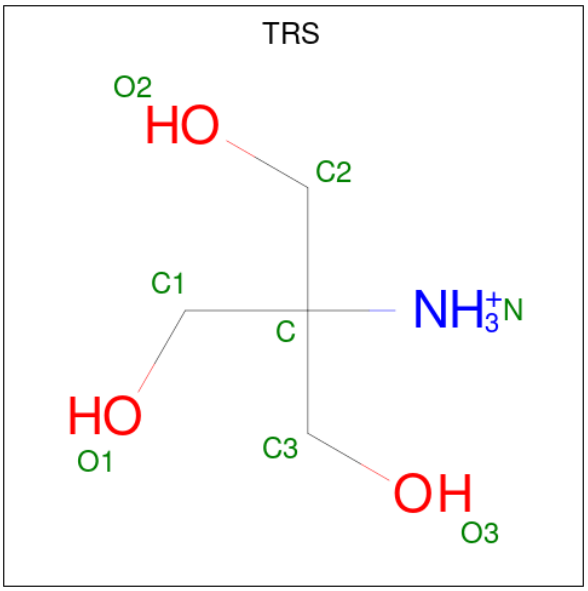
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	2	Total Fe 2 2	0	0
5	G	1	Total Fe 1 1	0	0
5	H	2	Total Fe 2 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

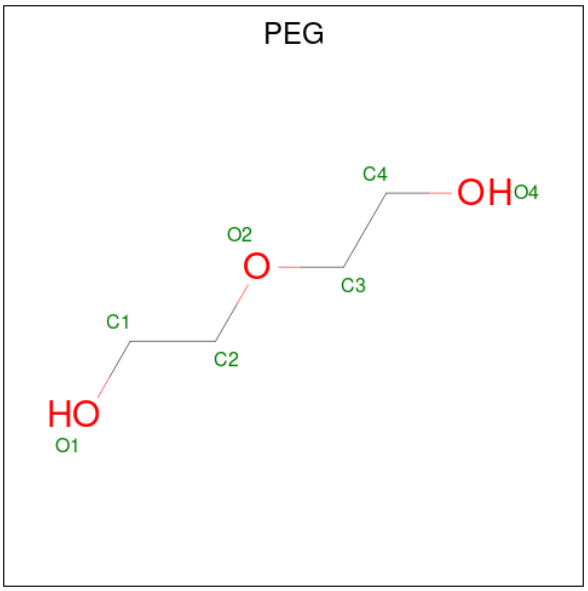
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	E	3	Total Mg 3 3	0	0
6	F	1	Total Mg 1 1	0	0
6	G	3	Total Mg 3 3	0	0
6	H	2	Total Mg 2 2	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 8 4 1 3	0	0
7	D	1	Total C N O 8 4 1 3	0	0
7	D	1	Total C N O 8 4 1 3	0	0
7	F	1	Total C N O 8 4 1 3	0	0
7	F	1	Total C N O 8 4 1 3	0	0
7	F	1	Total C N O 8 4 1 3	0	0
7	H	1	Total C N O 8 4 1 3	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C H O 17 4 10 3	0	0

- Molecule 9 is water.

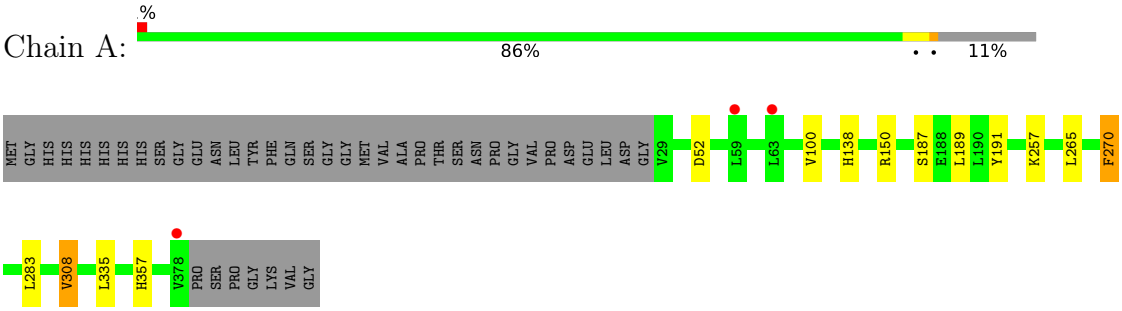
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	272	Total O 272 272	0	0
9	B	277	Total O 277 277	0	0
9	C	243	Total O 243 243	0	0
9	D	288	Total O 288 288	0	0
9	E	292	Total O 292 292	0	0
9	F	260	Total O 260 260	0	0
9	G	268	Total O 268 268	0	0
9	H	236	Total O 236 236	0	0

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.

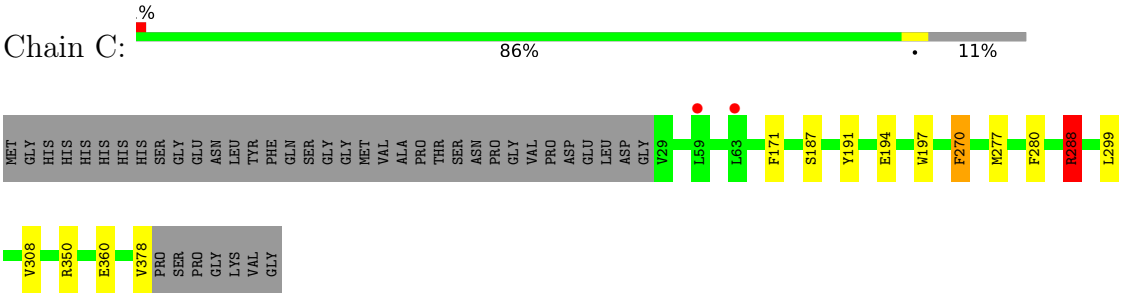
• Molecule 1: Amidohydrolase

Chain A:



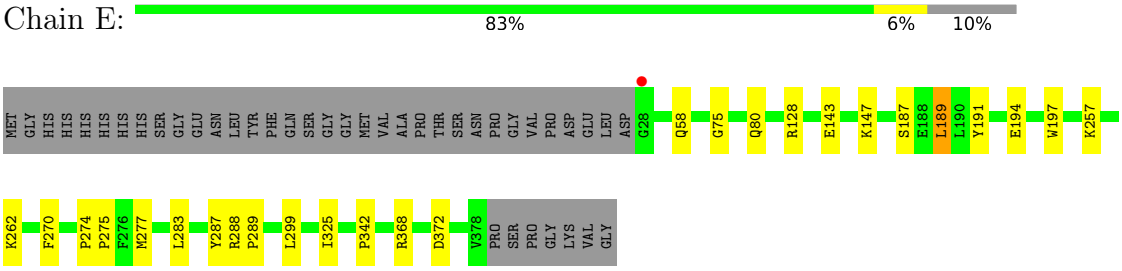
• Molecule 1: Amidohydrolase

Chain C:



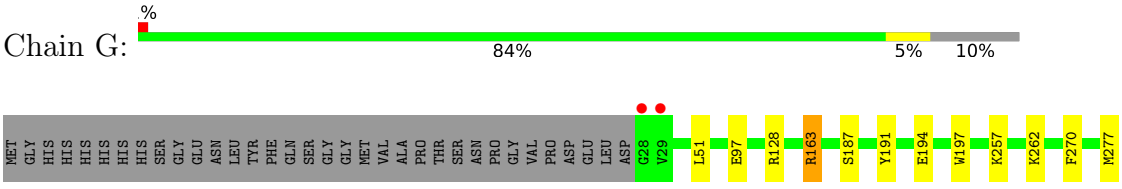
• Molecule 1: Amidohydrolase

Chain E:



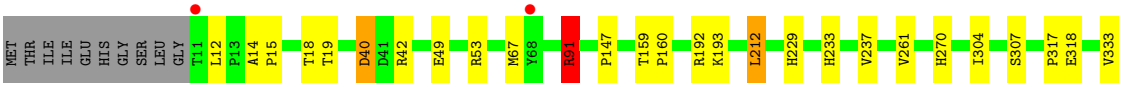
• Molecule 1: Amidohydrolase

Chain G:



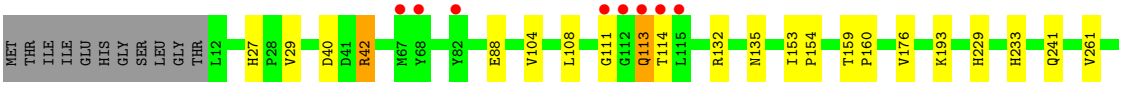
• Molecule 2: Amidohydrolase

Chain B:



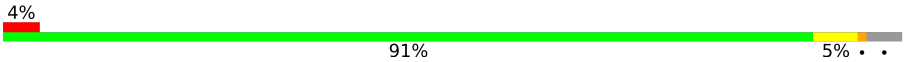
• Molecule 2: Amidohydrolase

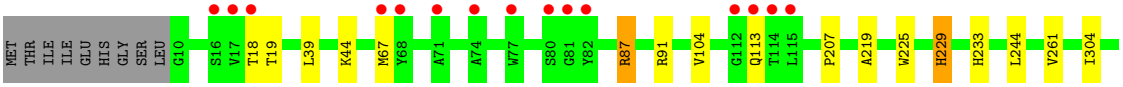
Chain F:



• Molecule 2: Amidohydrolase

Chain H:





• Molecule 3: Amidohydrolase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	82.59Å 232.64Å 147.64Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	45.58 – 1.48 77.75 – 1.48	Depositor EDS
% Data completeness (in resolution range)	93.7 (45.58-1.48) 88.7 (77.75-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.159 , 0.184 0.159 , 0.184	Depositor DCC
R_{free} test set	1414 reflections (0.33%)	wwPDB-VP
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	47082	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PEG, FE, PG4, CSO, TRS, MG

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	0.45	1/2901 (0.0%)	0.62	0/3965
1	C	0.43	0/2894	0.69	3/3955 (0.1%)
1	E	0.44	0/2924	0.64	0/3996
1	G	0.45	0/2929	0.61	0/4004
2	B	0.47	0/2971	0.68	4/4058 (0.1%)
2	F	0.43	0/2976	0.62	0/4064
2	H	0.45	0/2961	0.64	1/4044 (0.0%)
3	D	0.49	1/2978 (0.0%)	0.66	0/4067
All	All	0.45	2/23534 (0.0%)	0.64	8/32153 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	291	ASP	CG-OD2	-5.90	1.11	1.25
1	A	52	ASP	CB-CG	-5.17	1.40	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	350	ARG	NE-CZ-NH2	13.81	127.20	120.30
1	C	350	ARG	NE-CZ-NH1	-13.12	113.74	120.30
2	B	91	ARG	NE-CZ-NH1	10.89	125.74	120.30
2	H	87	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	288	ARG	NE-CZ-NH2	5.57	123.08	120.30
2	B	91	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	212	LEU	CA-CB-CG	5.27	127.42	115.30
2	B	91	ARG	CD-NE-CZ	5.05	130.66	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2811	2716	2714	10	0
1	C	2807	2706	2705	9	0
1	E	2827	2712	2716	21	0
1	G	2826	2728	2720	13	0
2	B	2881	2730	2749	25	0
2	F	2877	2748	2744	28	0
2	H	2872	2745	2749	13	0
3	D	2883	2761	2764	16	0
4	A	26	36	36	2	0
4	B	13	18	17	18	0
4	C	13	18	18	1	0
4	E	13	18	18	3	0
4	G	26	36	36	1	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
6	H	2	0	0	0	0
7	B	8	0	10	0	0
7	D	16	0	22	0	0
7	F	24	0	34	3	0
7	H	8	0	11	1	0
8	E	7	10	10	2	0
9	A	272	0	0	0	0
9	B	277	0	0	5	0
9	C	243	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	288	0	0	1	0
9	E	292	0	0	0	0
9	F	260	0	0	5	1
9	G	268	0	0	1	1
9	H	236	0	0	2	0
All	All	25100	21982	22073	130	2

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 (130) 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:308[B]:VAL:HG23	1:A:335:LEU:HD23	1.54	0.88
2:H:18:THR:HG23	2:H:19:THR:H	1.43	0.84
2:B:91:ARG:HG3	2:B:91:ARG:HH11	1.54	0.73
3:D:42[B]:ARG:HH21	3:D:42[B]:ARG:HG2	1.54	0.71
2:F:40:ASP:HA	7:F:403:TRS:H12	1.73	0.69
1:E:58:GLN:HE22	1:E:128:ARG:HE	1.41	0.69
4:B:501:PG4:H32	2:F:160:PRO:HD2	1.74	0.69
1:C:270:PHE:HB3	1:C:308:VAL:HG11	1.76	0.68
2:B:160:PRO:HD2	4:B:501:PG4:H81	1.82	0.62
4:B:501:PG4:H31	2:F:193:LYS:HE3	1.82	0.61
1:A:308[B]:VAL:CG2	1:A:335:LEU:HD23	2.29	0.60
4:B:501:PG4:H51	2:F:193:LYS:HA	1.82	0.60
7:H:401:TRS:H31	9:H:665:HOH:O	2.02	0.60
1:E:197:TRP:CH2	1:E:257:LYS:HE3	2.35	0.60
2:B:160:PRO:HD2	4:B:501:PG4:C8	2.31	0.59
2:B:159:THR:HA	4:B:501:PG4:H82	1.85	0.58
1:G:363:ASP:OD2	1:G:368:ARG:NE	2.36	0.58
1:E:143:GLU:HG2	4:E:401:PG4:H51	1.83	0.58
4:B:501:PG4:H22	2:F:159:THR:HA	1.83	0.58
1:E:197:TRP:CZ3	1:E:257:LYS:HE3	2.39	0.58
2:B:192:ARG:HD3	4:B:501:PG4:H12	1.85	0.58
2:B:53[A]:ARG:NH1	9:B:603:HOH:O	2.26	0.56
2:B:318:GLU:OE2	9:B:601:HOH:O	2.18	0.56
1:E:257:LYS:NZ	8:E:402:PEG:H41	2.20	0.56
1:A:270:PHE:HB3	1:A:308[A]:VAL:HG11	1.87	0.56
1:C:194:GLU:OE2	1:G:163:ARG:NE	2.39	0.55
2:B:193:LYS:HG3	4:B:501:PG4:H41	1.90	0.54
2:F:29:VAL:HG13	2:F:111:GLY:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97[A]:GLU:HG3	9:G:711:HOH:O	2.08	0.54
2:B:193:LYS:CG	4:B:501:PG4:H41	2.38	0.53
1:E:277:MET:HB3	1:E:299:LEU:HD23	1.91	0.53
1:G:262:LYS:HE2	1:G:372:ASP:OD2	2.09	0.53
2:H:104:VAL:HG21	2:H:371:PHE:CZ	2.44	0.53
4:B:501:PG4:H11	9:B:764:HOH:O	2.09	0.52
2:B:237:VAL:HG13	2:B:270:HIS:CE1	2.44	0.52
4:B:501:PG4:C5	9:F:573:HOH:O	2.57	0.52
2:B:53[A]:ARG:NH2	9:B:603:HOH:O	2.38	0.52
1:E:287:TYR:CZ	2:F:229:HIS:HD2	2.28	0.52
2:F:88:GLU:HA	2:F:88:GLU:OE1	2.10	0.51
2:H:261[A]:VAL:CG2	2:H:304:ILE:HD13	2.40	0.51
2:B:261:VAL:CG2	2:B:304:ILE:HD13	2.40	0.51
2:B:15:PRO:HG2	2:B:373:VAL:HG22	1.93	0.51
1:G:277:MET:HB3	1:G:299:LEU:HD23	1.93	0.50
2:B:14:ALA:O	9:B:602:HOH:O	2.20	0.50
3:D:67:MET:HE1	1:G:128:ARG:NH1	2.26	0.50
1:C:187:SER:HB3	1:C:191:TYR:CZ	2.47	0.50
3:D:42[B]:ARG:HG2	3:D:42[B]:ARG:NH2	2.25	0.50
2:B:336:THR:HB	2:B:343:PHE:CE1	2.47	0.49
3:D:15:PRO:HG2	3:D:373:VAL:HG22	1.94	0.49
1:A:265:LEU:HB2	1:A:308[B]:VAL:HG12	1.95	0.48
1:A:100:VAL:HG13	1:A:150:ARG:NH2	2.29	0.48
2:F:241:GLN:OE1	9:F:501:HOH:O	2.20	0.47
2:H:67:MET:HG2	2:H:229:HIS:CD2	2.49	0.47
1:E:147:LYS:CE	4:E:401:PG4:H52	2.45	0.47
1:C:360:GLU:H	1:C:360:GLU:CD	2.19	0.46
2:B:193:LYS:CB	4:B:501:PG4:H41	2.45	0.46
2:F:261[A]:VAL:CG2	2:F:304:ILE:HD13	2.46	0.46
2:H:67:MET:HG3	2:H:229:HIS:CG	2.51	0.46
2:H:91:ARG:HG3	9:H:517:HOH:O	2.15	0.46
2:B:18:THR:OG1	2:B:19:THR:N	2.47	0.46
1:G:364:ARG:HA	1:G:368:ARG:HB2	1.98	0.46
2:H:18:THR:HG23	2:H:19:THR:N	2.20	0.46
2:B:307:SER:HA	2:B:333:VAL:O	2.16	0.46
2:B:12:LEU:HD11	2:B:147:PRO:HB3	1.98	0.45
2:F:42[B]:ARG:HH11	2:F:42[B]:ARG:HG2	1.81	0.45
2:F:42[A]:ARG:HG2	9:F:580:HOH:O	2.16	0.45
2:F:307:SER:HA	2:F:333:VAL:O	2.17	0.45
1:A:187:SER:HB3	1:A:191:TYR:CZ	2.52	0.45
4:B:501:PG4:H22	2:F:160:PRO:HD2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:HIS:CE1	2:F:108:LEU:HD11	2.51	0.45
1:E:187:SER:HB3	1:E:191:TYR:CZ	2.51	0.45
1:G:51:LEU:O	4:G:402:PG4:H61	2.17	0.45
3:D:199:GLU:OE1	9:D:601:HOH:O	2.20	0.45
2:B:49:GLU:HA	1:E:75:GLY:HA3	1.97	0.44
2:B:317:PRO:HB3	2:B:351:PRO:HB3	1.98	0.44
1:E:262:LYS:HE2	1:E:372:ASP:OD2	2.18	0.44
2:F:369:ARG:NH2	9:F:511:HOH:O	2.50	0.44
1:A:265:LEU:HB2	1:A:308[A]:VAL:HG13	1.99	0.44
1:G:300:GLU:O	1:G:304:GLU:HG3	2.17	0.44
1:A:138:HIS:HE1	4:A:402:PG4:C6	2.30	0.44
3:D:29:VAL:HG13	3:D:111:GLY:O	2.18	0.44
1:C:194:GLU:HA	1:C:197:TRP:CE2	2.53	0.44
2:B:160:PRO:HD2	4:B:501:PG4:H61	1.98	0.44
3:D:307:SER:HA	3:D:333:VAL:O	2.17	0.44
1:C:277:MET:HB3	1:C:299:LEU:HD23	2.00	0.43
1:E:194:GLU:HA	1:E:197:TRP:CD2	2.53	0.43
1:E:325:ILE:HD12	1:E:325:ILE:HA	1.92	0.43
2:B:40:ASP:C	2:B:40:ASP:OD1	2.56	0.43
4:B:501:PG4:H51	9:F:573:HOH:O	2.16	0.43
3:D:121:ALA:HB3	3:D:127:ALA:HB2	2.00	0.43
3:D:302:ASP:CG	2:F:132:ARG:HH12	2.21	0.43
2:F:40:ASP:CA	7:F:403:TRS:H12	2.47	0.43
3:D:261:VAL:CG2	3:D:304:ILE:HD13	2.48	0.43
1:E:283:LEU:HD13	2:F:233:HIS:HB3	2.01	0.43
1:E:194:GLU:HA	1:E:197:TRP:CE2	2.54	0.42
1:G:194:GLU:HA	1:G:197:TRP:CE2	2.54	0.42
3:D:91:ARG:HG2	3:D:91:ARG:NH2	2.34	0.42
1:G:197:TRP:CH2	1:G:257:LYS:HE3	2.54	0.42
2:B:91:ARG:HH11	2:B:91:ARG:CG	2.27	0.42
1:E:80:GLN:HA	1:E:342:PRO:O	2.20	0.42
2:F:176:VAL:O	7:F:402:TRS:H31	2.19	0.42
1:A:283:LEU:HD13	2:B:233:HIS:HB3	2.02	0.42
2:H:207:PRO:HB2	2:H:370:PHE:CZ	2.54	0.42
2:F:104:VAL:HG21	2:F:371:PHE:CZ	2.55	0.42
1:G:187:SER:HB3	1:G:191:TYR:CZ	2.54	0.42
1:G:283:LEU:HD13	2:H:233:HIS:HB3	2.02	0.42
1:E:257:LYS:CE	8:E:402:PEG:H41	2.50	0.42
2:H:39:LEU:O	2:H:44:LYS:HE3	2.19	0.42
4:B:501:PG4:C3	2:F:193:LYS:HE3	2.48	0.41
1:A:189:LEU:HD11	1:E:189:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ARG:HG2	1:C:288:ARG:HH21	1.85	0.41
4:B:501:PG4:H32	2:F:160:PRO:CD	2.48	0.41
1:E:147:LYS:NZ	4:E:401:PG4:H72	2.36	0.41
1:C:194:GLU:HA	1:C:197:TRP:CD2	2.56	0.41
3:D:42[B]:ARG:NH1	3:D:46:HIS:ND1	2.69	0.41
3:D:302:ASP:OD1	2:F:132:ARG:NH1	2.50	0.41
1:E:288:ARG:N	1:E:289:PRO:HD2	2.36	0.41
2:H:219:ALA:HA	2:H:225:TRP:CZ2	2.56	0.41
1:C:171:PHE:CZ	4:C:401:PG4:H42	2.56	0.41
3:D:91:ARG:HG2	3:D:91:ARG:HH21	1.86	0.41
3:D:219:ALA:HA	3:D:225:TRP:CZ2	2.56	0.41
1:E:274:PRO:HB2	1:E:275:PRO:HD3	2.03	0.41
2:F:153:ILE:O	2:F:153:ILE:HG13	2.20	0.41
2:F:113:GLN:HG3	2:F:114:THR:N	2.36	0.41
3:D:327:PHE:O	3:D:328:CYS:HB2	2.20	0.40
2:F:113:GLN:HG3	2:F:114:THR:H	1.85	0.40
2:H:244:LEU:HD23	2:H:244:LEU:C	2.42	0.40
2:H:307:SER:HA	2:H:333:VAL:O	2.22	0.40
4:A:401:PG4:C1	4:A:401:PG4:H42	2.52	0.40
2:F:135:ASN:OD1	2:F:154:PRO:HD2	2.22	0.40

All (2) 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)
9:F:630:HOH:O	9:F:630:HOH:O[2_556]	2.10	0.10
9:G:666:HOH:O	9:G:763:HOH:O[2_556]	2.12	0.08

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	350/392 (89%)	345 (99%)	4 (1%)	1 (0%)	41 18
1	C	349/392 (89%)	345 (99%)	3 (1%)	1 (0%)	41 18
1	E	353/392 (90%)	349 (99%)	3 (1%)	1 (0%)	41 18
1	G	355/392 (91%)	349 (98%)	5 (1%)	1 (0%)	41 18
2	B	364/378 (96%)	347 (95%)	16 (4%)	1 (0%)	41 18
2	F	363/378 (96%)	345 (95%)	18 (5%)	0	100 100
2	H	365/378 (97%)	346 (95%)	19 (5%)	0	100 100
3	D	364/378 (96%)	347 (95%)	15 (4%)	2 (0%)	29 9
All	All	2863/3080 (93%)	2773 (97%)	83 (3%)	7 (0%)	47 23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	328	CYS
1	E	270	PHE
1	A	270	PHE
1	C	270	PHE
3	D	67	MET
1	G	270	PHE
2	B	67	MET

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	301/332 (91%)	297 (99%)	4 (1%)	69 42
1	C	300/332 (90%)	297 (99%)	3 (1%)	76 54
1	E	303/332 (91%)	301 (99%)	2 (1%)	84 68
1	G	303/332 (91%)	301 (99%)	2 (1%)	84 68
2	B	305/317 (96%)	299 (98%)	6 (2%)	55 24
2	F	305/317 (96%)	302 (99%)	3 (1%)	76 54
2	H	302/317 (95%)	299 (99%)	3 (1%)	76 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	306/318 (96%)	303 (99%)	3 (1%)	76 54
All	All	2425/2597 (93%)	2399 (99%)	26 (1%)	76 50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LYS
1	A	308[A]	VAL
1	A	308[B]	VAL
1	A	357	HIS
2	B	40	ASP
2	B	42	ARG
2	B	91	ARG
2	B	212	LEU
2	B	229	HIS
2	B	359	ARG
1	C	280	PHE
1	C	288	ARG
1	C	378	VAL
3	D	42[A]	ARG
3	D	42[B]	ARG
3	D	229	HIS
1	E	189	LEU
1	E	368	ARG
2	F	42[A]	ARG
2	F	42[B]	ARG
2	F	113	GLN
1	G	163	ARG
1	G	280	PHE
2	H	87	ARG
2	H	113	GLN
2	H	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	229	HIS
1	G	354	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSO	H	328	2	3,6,7	0.30	0	0,6,8	-	-
2	CSO	B	328	2	3,6,7	0.40	0	0,6,8	-	-
2	CSO	F	328	2	3,6,7	0.55	0	0,6,8	-	-

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
2	CSO	H	328	2	-	0/1/5/7	-
2	CSO	B	328	2	-	0/1/5/7	-
2	CSO	F	328	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 26 are monoatomic - leaving 15 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	PG4	A	402	-	12,12,12	0.44	0	11,11,11	0.86	0
7	TRS	H	401	5	7,7,7	0.35	0	9,9,9	0.86	0
4	PG4	E	401	-	12,12,12	0.50	0	11,11,11	0.37	0
8	PEG	E	402	-	6,6,6	0.52	0	5,5,5	0.67	0
4	PG4	G	402	6	12,12,12	0.39	0	11,11,11	0.56	0
7	TRS	B	502	5	7,7,7	0.29	0	9,9,9	0.56	0
4	PG4	C	401	-	12,12,12	0.38	0	11,11,11	0.44	0
4	PG4	B	501	-	12,12,12	0.64	0	11,11,11	1.02	1 (9%)
7	TRS	F	403	-	7,7,7	0.46	0	9,9,9	1.19	1 (11%)
4	PG4	G	401	-	12,12,12	0.49	0	11,11,11	0.58	0
7	TRS	F	402	-	7,7,7	0.26	0	9,9,9	0.81	0
7	TRS	D	501	-	7,7,7	0.18	0	9,9,9	0.65	0
7	TRS	D	502	5	7,7,7	0.19	0	9,9,9	0.39	0
7	TRS	F	401	5	7,7,7	0.20	0	9,9,9	0.53	0
4	PG4	A	401	-	12,12,12	0.46	0	11,11,11	0.61	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	PG4	A	402	-	-	6/10/10/10	-
7	TRS	H	401	5	-	0/9/9/9	-
4	PG4	E	401	-	-	2/10/10/10	-
8	PEG	E	402	-	-	2/4/4/4	-
4	PG4	G	402	6	-	7/10/10/10	-
7	TRS	B	502	5	-	2/9/9/9	-
4	PG4	C	401	-	-	7/10/10/10	-
4	PG4	B	501	-	-	7/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TRS	F	403	-	-	6/9/9/9	-
4	PG4	G	401	-	-	5/10/10/10	-
7	TRS	F	402	-	-	3/9/9/9	-
7	TRS	D	501	-	-	6/9/9/9	-
7	TRS	D	502	5	-	3/9/9/9	-
7	TRS	F	401	5	-	3/9/9/9	-
4	PG4	A	401	-	-	7/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	403	TRS	C2-C-N	2.69	116.00	107.98
4	B	501	PG4	C7-O4-C6	2.34	123.44	113.29

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	501	TRS	C2-C-C1-O1
7	D	501	TRS	C3-C-C1-O1
7	D	501	TRS	N-C-C1-O1
7	F	402	TRS	C1-C-C3-O3
7	F	402	TRS	C2-C-C3-O3
7	F	402	TRS	N-C-C3-O3
7	F	403	TRS	N-C-C1-O1
4	G	401	PG4	O4-C7-C8-O5
4	B	501	PG4	C5-C6-O4-C7
4	A	401	PG4	O2-C3-C4-O3
4	C	401	PG4	O3-C5-C6-O4
4	G	401	PG4	O3-C5-C6-O4
4	B	501	PG4	C6-C5-O3-C4
4	A	401	PG4	O4-C7-C8-O5
4	C	401	PG4	O1-C1-C2-O2
4	G	402	PG4	O1-C1-C2-O2
4	A	402	PG4	O3-C5-C6-O4
4	G	401	PG4	O2-C3-C4-O3
7	D	501	TRS	C1-C-C2-O2
7	F	403	TRS	C2-C-C1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	401	PG4	O1-C1-C2-O2
4	C	401	PG4	O4-C7-C8-O5
4	A	401	PG4	C8-C7-O4-C6
4	A	402	PG4	O2-C3-C4-O3
4	G	401	PG4	O1-C1-C2-O2
8	E	402	PEG	O2-C3-C4-O4
8	E	402	PEG	O1-C1-C2-O2
4	E	401	PG4	O2-C3-C4-O3
4	G	401	PG4	C4-C3-O2-C2
4	G	402	PG4	C4-C3-O2-C2
4	A	402	PG4	C6-C5-O3-C4
4	C	401	PG4	C6-C5-O3-C4
4	A	401	PG4	C3-C4-O3-C5
4	B	501	PG4	C1-C2-O2-C3
4	B	501	PG4	C8-C7-O4-C6
7	D	501	TRS	N-C-C2-O2
7	D	502	TRS	N-C-C1-O1
7	F	401	TRS	N-C-C1-O1
7	F	403	TRS	C2-C-C3-O3
4	G	402	PG4	O3-C5-C6-O4
4	E	401	PG4	C6-C5-O3-C4
4	G	402	PG4	C8-C7-O4-C6
4	A	402	PG4	O1-C1-C2-O2
4	G	402	PG4	C5-C6-O4-C7
4	B	501	PG4	C3-C4-O3-C5
4	A	402	PG4	C1-C2-O2-C3
7	D	501	TRS	C3-C-C2-O2
7	D	502	TRS	C3-C-C1-O1
7	F	401	TRS	C2-C-C1-O1
7	F	401	TRS	C3-C-C1-O1
7	F	403	TRS	C3-C-C1-O1
7	F	403	TRS	C1-C-C3-O3
4	A	402	PG4	C8-C7-O4-C6
4	C	401	PG4	C4-C3-O2-C2
4	C	401	PG4	C3-C4-O3-C5
4	G	402	PG4	C1-C2-O2-C3
4	G	402	PG4	C3-C4-O3-C5
4	A	401	PG4	O3-C5-C6-O4
4	B	501	PG4	O4-C7-C8-O5
7	B	502	TRS	C2-C-C1-O1
7	B	502	TRS	C3-C-C1-O1
7	D	502	TRS	C2-C-C1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	F	403	TRS	N-C-C3-O3
4	B	501	PG4	O3-C5-C6-O4
4	C	401	PG4	O2-C3-C4-O3
4	A	401	PG4	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	PG4	1	0
7	H	401	TRS	1	0
4	E	401	PG4	3	0
8	E	402	PEG	2	0
4	G	402	PG4	1	0
4	C	401	PG4	1	0
4	B	501	PG4	18	0
7	F	403	TRS	2	0
7	F	402	TRS	1	0
4	A	401	PG4	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	350/392 (89%)	-0.49	3 (0%)	84	86	8, 13, 31, 45	0
1	C	350/392 (89%)	-0.37	2 (0%)	89	91	8, 16, 37, 55	0
1	E	351/392 (89%)	-0.53	1 (0%)	94	95	8, 13, 27, 66	0
1	G	351/392 (89%)	-0.48	2 (0%)	89	91	8, 14, 29, 66	0
2	B	362/378 (95%)	-0.45	2 (0%)	89	91	8, 13, 32, 69	0
2	F	361/378 (95%)	-0.29	8 (2%)	62	66	8, 14, 39, 64	0
2	H	363/378 (96%)	-0.14	15 (4%)	37	40	8, 16, 44, 75	0
3	D	363/378 (96%)	-0.46	3 (0%)	86	88	8, 14, 31, 66	0
All	All	2851/3080 (92%)	-0.40	36 (1%)	77	80	8, 14, 35, 75	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	114	THR	7.7
1	G	28	GLY	5.1
2	F	112	GLY	5.0
2	F	68	TYR	4.8
2	B	11	THR	4.8
2	H	115	LEU	4.7
2	H	113	GLN	4.0
2	F	67	MET	3.5
2	F	115	LEU	3.4
1	E	28	GLY	3.4
2	H	82	TYR	3.2
2	H	18	THR	3.2
2	H	112	GLY	3.1
1	A	63	LEU	3.0
2	F	114	THR	2.8
3	D	11	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	68	TYR	2.7
2	H	17	VAL	2.7
2	H	71	ALA	2.6
1	A	59	LEU	2.6
1	C	63	LEU	2.6
1	A	378	VAL	2.6
2	H	81	GLY	2.6
2	B	68[A]	TYR	2.6
2	F	113	GLN	2.5
2	H	16	SER	2.5
2	H	77	TRP	2.4
3	D	373	VAL	2.4
2	H	67	MET	2.4
2	H	74	ALA	2.4
1	C	59	LEU	2.4
3	D	68[A]	TYR	2.3
1	G	29	VAL	2.3
2	F	82	TYR	2.2
2	H	80	SER	2.1
2	F	111	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	CSO	H	328	7/8	0.93	0.09	16,18,26,26	0
2	CSO	B	328	7/8	0.97	0.06	12,13,17,25	0
2	CSO	F	328	7/8	0.98	0.06	12,16,21,25	0

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
6	MG	G	406	1/1	0.59	0.13	54,54,54,54	0
7	TRS	F	403	8/8	0.66	0.26	28,36,50,52	0
6	MG	A	405	1/1	0.69	0.10	48,48,48,48	0
7	TRS	F	402	8/8	0.79	0.15	22,32,49,54	0
7	TRS	D	501	8/8	0.79	0.23	19,41,56,59	0
6	MG	C	403	1/1	0.81	0.17	53,53,53,53	0
6	MG	G	404	1/1	0.85	0.14	33,33,33,33	0
4	PG4	G	402	13/13	0.86	0.15	30,41,70,73	0
7	TRS	H	401	8/8	0.86	0.17	20,33,56,60	0
4	PG4	A	402	13/13	0.87	0.15	27,38,77,91	0
6	MG	E	405	1/1	0.87	0.16	37,37,37,37	0
4	PG4	E	401	13/13	0.88	0.15	29,52,69,70	0
8	PEG	E	402	7/7	0.89	0.08	22,32,43,52	0
4	PG4	G	401	13/13	0.90	0.11	25,42,66,67	0
4	PG4	C	401	13/13	0.90	0.15	30,45,81,88	0
4	PG4	A	401	13/13	0.91	0.12	27,38,73,75	0
6	MG	E	404	1/1	0.93	0.08	25,25,25,25	1
7	TRS	F	401	8/8	0.93	0.12	15,26,35,40	0
6	MG	H	404	1/1	0.94	0.06	32,32,32,32	0
4	PG4	B	501	13/13	0.95	0.18	8,24,74,78	0
6	MG	G	405	1/1	0.95	0.25	47,47,47,47	0
7	TRS	D	502	8/8	0.96	0.07	11,16,21,22	0
7	TRS	B	502	8/8	0.96	0.09	12,15,19,22	0
6	MG	H	405	1/1	0.97	0.18	26,26,26,26	0
6	MG	A	404	1/1	0.97	0.11	25,25,25,25	0
6	MG	D	505	1/1	0.97	0.14	30,30,30,30	0
6	MG	B	505	1/1	0.98	0.08	18,18,18,18	0
6	MG	F	406	1/1	0.99	0.18	19,19,19,19	0
6	MG	E	406	1/1	0.99	0.09	15,15,15,15	0
5	FE	H	402	1/1	1.00	0.06	15,15,15,15	0
5	FE	H	403	1/1	1.00	0.04	20,20,20,20	1
5	FE	A	403	1/1	1.00	0.06	9,9,9,9	0
5	FE	B	503	1/1	1.00	0.03	12,12,12,12	0
5	FE	B	504	1/1	1.00	0.06	11,11,11,11	0
5	FE	C	402	1/1	1.00	0.07	11,11,11,11	0
5	FE	D	503	1/1	1.00	0.03	12,12,12,12	0
5	FE	D	504	1/1	1.00	0.06	11,11,11,11	0
5	FE	E	403	1/1	1.00	0.07	9,9,9,9	0
5	FE	F	404	1/1	1.00	0.07	13,13,13,13	0
5	FE	F	405	1/1	1.00	0.05	16,16,16,16	1
5	FE	G	403	1/1	1.00	0.06	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.