



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 6XIX / pdb_00006xix
Title : Triuret Hydrolase (TrtA) from Herbaspirillum sp. BH-1
Authors : Tassoulas, L.T.; Elias, M.H.; Wackett, L.P.
Deposited on : 2020-06-22
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

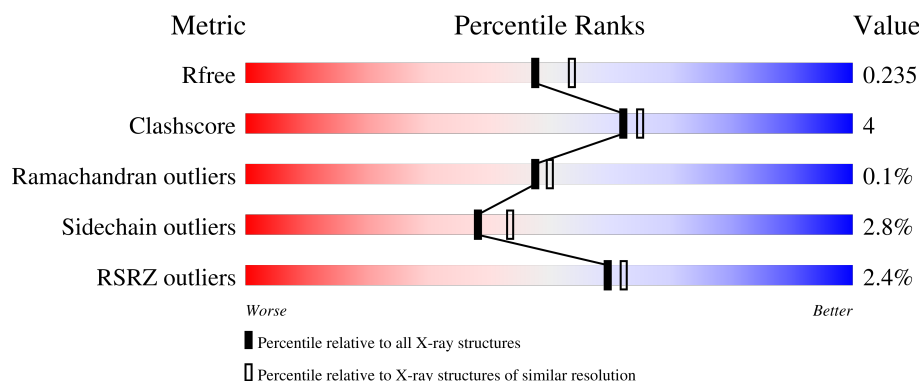
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	4% 83% 14% ..
1	B	223	87% 10% ..
1	C	223	3% 89% 9% .
1	D	223	4% 84% 14% .
1	E	223	3% 87% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	223	2% 88% 10%
1	G	223	87% 10%
1	H	223	4% 88% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14266 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 Cysteine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	1	0
			1681	1058	301	312	10			
1	B	219	Total	C	N	O	S	0	0	0
			1672	1053	299	310	10			
1	C	221	Total	C	N	O	S	0	1	0
			1698	1068	307	313	10			
1	D	220	Total	C	N	O	S	0	0	0
			1677	1056	300	311	10			
1	E	220	Total	C	N	O	S	0	1	0
			1686	1061	302	313	10			
1	F	220	Total	C	N	O	S	0	1	0
			1688	1062	304	312	10			
1	G	219	Total	C	N	O	S	0	0	0
			1672	1053	299	310	10			
1	H	220	Total	C	N	O	S	0	0	0
			1677	1056	300	311	10			

There are 24 discrepancies between the modelled and reference sequences:

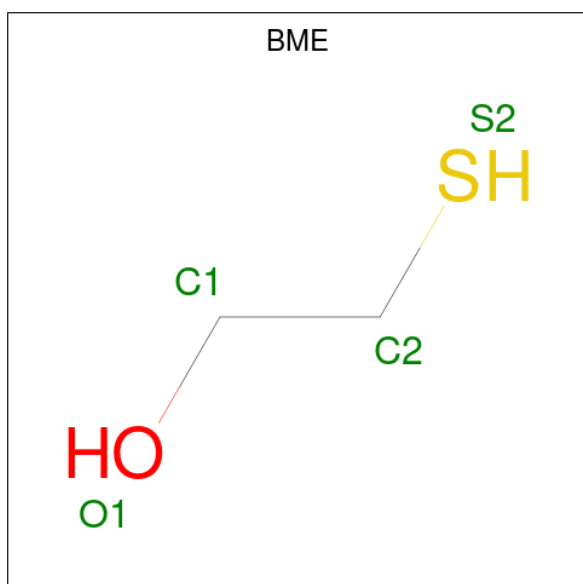
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A2N6JFX7
A	-1	SER	-	expression tag	UNP A0A2N6JFX7
A	0	HIS	-	expression tag	UNP A0A2N6JFX7
B	-2	GLY	-	expression tag	UNP A0A2N6JFX7
B	-1	SER	-	expression tag	UNP A0A2N6JFX7
B	0	HIS	-	expression tag	UNP A0A2N6JFX7
C	-2	GLY	-	expression tag	UNP A0A2N6JFX7
C	-1	SER	-	expression tag	UNP A0A2N6JFX7
C	0	HIS	-	expression tag	UNP A0A2N6JFX7
D	-2	GLY	-	expression tag	UNP A0A2N6JFX7
D	-1	SER	-	expression tag	UNP A0A2N6JFX7
D	0	HIS	-	expression tag	UNP A0A2N6JFX7
E	-2	GLY	-	expression tag	UNP A0A2N6JFX7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A0A2N6JFX7
E	0	HIS	-	expression tag	UNP A0A2N6JFX7
F	-2	GLY	-	expression tag	UNP A0A2N6JFX7
F	-1	SER	-	expression tag	UNP A0A2N6JFX7
F	0	HIS	-	expression tag	UNP A0A2N6JFX7
G	-2	GLY	-	expression tag	UNP A0A2N6JFX7
G	-1	SER	-	expression tag	UNP A0A2N6JFX7
G	0	HIS	-	expression tag	UNP A0A2N6JFX7
H	-2	GLY	-	expression tag	UNP A0A2N6JFX7
H	-1	SER	-	expression tag	UNP A0A2N6JFX7
H	0	HIS	-	expression tag	UNP A0A2N6JFX7

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	E	1	Total	C	O	S	0	0
			4	2	1	1		
2	F	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	S	0	0
			4	2	1	1		
2	H	1	Total	C	O	S	0	0
			4	2	1	1		

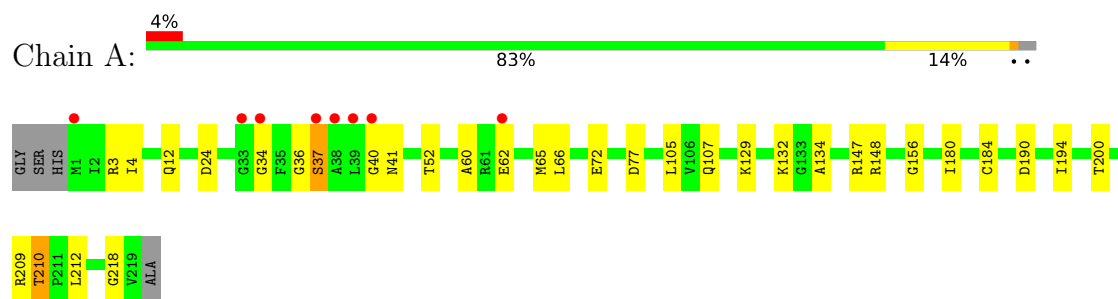
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	103	Total	O	0	0
			103	103		
3	C	86	Total	O	0	0
			86	86		
3	D	97	Total	O	0	0
			97	97		
3	E	103	Total	O	0	0
			103	103		
3	F	99	Total	O	0	0
			99	99		
3	G	103	Total	O	0	0
			103	103		
3	H	90	Total	O	0	0
			90	90		

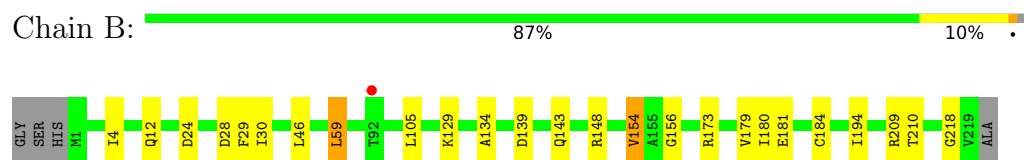
3 Residue-property plots [i](#)

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.

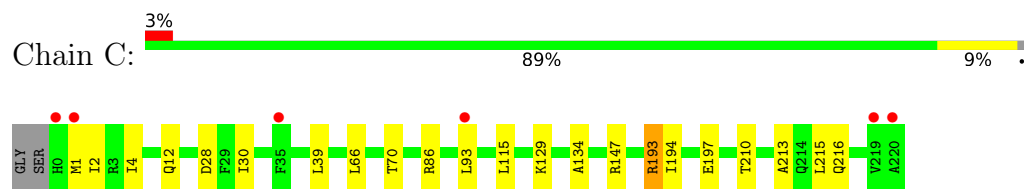
- Molecule 1: Cysteine hydrolase



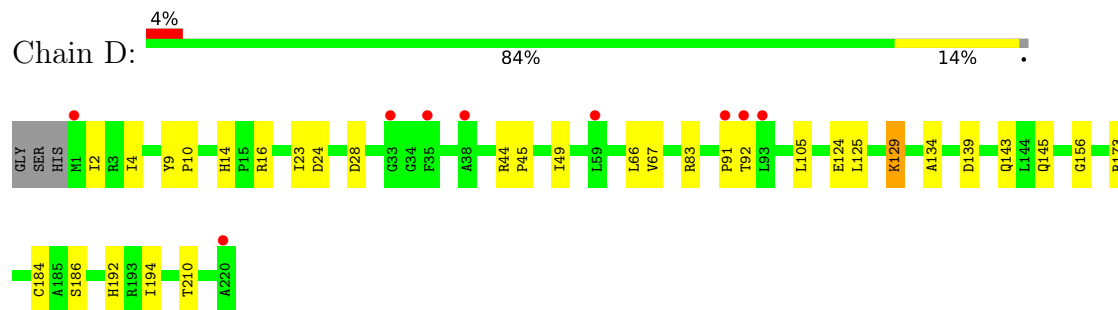
- Molecule 1: Cysteine hydrolase



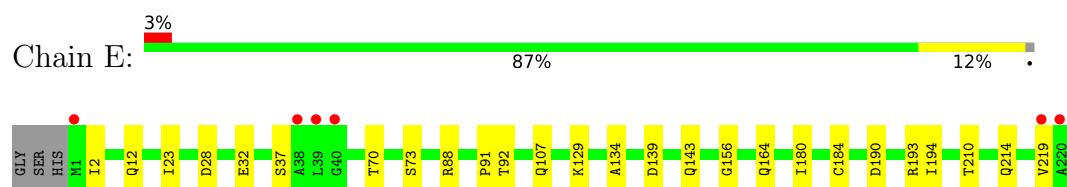
- Molecule 1: Cysteine hydrolase



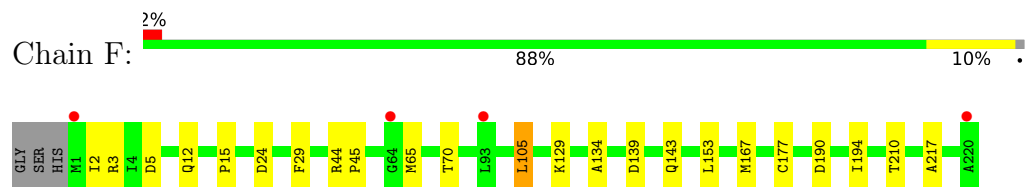
- Molecule 1: Cysteine hydrolase



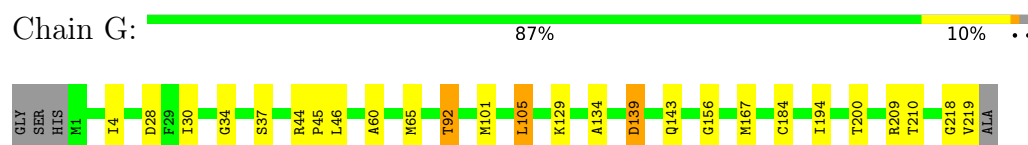
- Molecule 1: Cysteine hydrolase



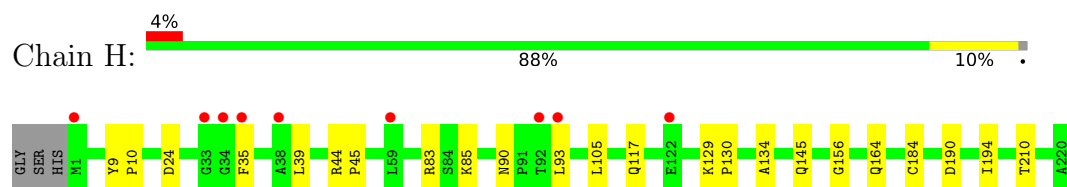
- Molecule 1: Cysteine hydrolase



- Molecule 1: Cysteine hydrolase



- Molecule 1: Cysteine hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.95Å 76.55Å 93.59Å 118.40° 89.61° 103.06°	Depositor
Resolution (Å)	70.57 – 2.10 70.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.7 (70.57-2.10) 90.7 (70.57-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.228 0.188 , 0.235	Depositor DCC
R_{free} test set	4561 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BME

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	1.10	0/1714	1.35	4/2331 (0.2%)
1	B	1.09	0/1705	1.36	3/2319 (0.1%)
1	C	1.11	0/1732	1.41	0/2355
1	D	1.09	1/1710 (0.1%)	1.38	6/2326 (0.3%)
1	E	1.09	0/1719	1.38	2/2338 (0.1%)
1	F	1.11	0/1721	1.40	2/2340 (0.1%)
1	G	1.09	0/1705	1.37	2/2319 (0.1%)
1	H	1.07	1/1710 (0.1%)	1.43	3/2326 (0.1%)
All	All	1.09	2/13716 (0.0%)	1.39	22/18654 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	ILE	C-O	5.22	1.29	1.24
1	H	90	ASN	N-CA	5.20	1.50	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	92	THR	CB-CA-C	7.83	123.94	110.79
1	A	77	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	180	ILE	CA-C-N	5.82	128.40	120.54
1	B	180	ILE	C-N-CA	5.82	128.40	120.54
1	F	217	ALA	CA-C-N	5.77	126.38	119.98
1	F	217	ALA	C-N-CA	5.77	126.38	119.98
1	D	91	PRO	CA-C-N	5.63	128.29	120.63
1	D	91	PRO	C-N-CA	5.63	128.29	120.63
1	H	145	GLN	CA-C-N	5.59	128.33	120.28
1	H	145	GLN	C-N-CA	5.59	128.33	120.28
1	E	180	ILE	CA-C-N	5.58	128.02	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	ILE	C-N-CA	5.58	128.02	120.38
1	D	49	ILE	CA-C-N	5.25	123.55	120.24
1	D	49	ILE	C-N-CA	5.25	123.55	120.24
1	G	139	ASP	N-CA-C	-5.08	106.92	112.72
1	H	90	ASN	CB-CA-C	-5.08	106.58	111.00
1	D	145	GLN	CA-C-N	5.08	127.59	120.28
1	D	145	GLN	C-N-CA	5.08	127.59	120.28
1	A	180	ILE	CA-C-N	5.05	127.04	120.28
1	A	180	ILE	C-N-CA	5.05	127.04	120.28
1	A	210	THR	CB-CA-C	5.04	116.77	109.92
1	B	59	LEU	CA-C-O	-5.02	115.55	120.82

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	1681	0	1689	18	0
1	B	1672	0	1682	15	0
1	C	1698	0	1706	11	0
1	D	1677	0	1687	17	0
1	E	1686	0	1694	12	0
1	F	1688	0	1699	13	0
1	G	1672	0	1682	20	0
1	H	1677	0	1687	14	0
2	A	4	0	5	0	0
2	B	4	0	5	1	0
2	C	4	0	5	0	0
2	D	4	0	5	0	0
2	E	4	0	5	0	0
2	F	4	0	5	1	0
2	G	4	0	5	0	0
2	H	4	0	5	0	0
3	A	102	0	0	2	0
3	B	103	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	86	0	0	1	0
3	D	97	0	0	2	0
3	E	103	0	0	1	0
3	F	99	0	0	0	0
3	G	103	0	0	0	0
3	H	90	0	0	1	0
All	All	14266	0	13566	112	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 4.

All (112) 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:G:28:ASP:OD1	1:G:101:MET:HE3	1.71	0.90
1:G:28:ASP:HA	1:G:101:MET:CE	2.05	0.87
1:G:34:GLY:HA2	1:G:101:MET:HE2	1.57	0.85
1:H:129:LYS:HD2	1:H:134:ALA:HA	1.64	0.79
1:A:129:LYS:HD2	1:A:134:ALA:HA	1.66	0.76
1:G:28:ASP:HA	1:G:101:MET:HE1	1.67	0.75
1:C:194:ILE:HG21	1:D:194:ILE:HG21	1.73	0.70
1:G:34:GLY:CA	1:G:101:MET:HE2	2.20	0.69
1:B:194:ILE:HG21	1:E:194:ILE:HG21	1.74	0.69
1:B:173:ARG:NH2	3:B:401:HOH:O	2.26	0.68
1:A:194:ILE:HG21	1:G:194:ILE:HG21	1.73	0.68
1:F:194:ILE:HG21	1:H:194:ILE:HG21	1.75	0.67
1:E:190:ASP:OD1	1:E:193:ARG:NH2	2.31	0.64
1:G:200:THR:HG21	1:G:209:ARG:HG2	1.81	0.63
1:B:129:LYS:HD2	1:B:134:ALA:HA	1.80	0.62
1:G:129:LYS:HD2	1:G:134:ALA:HA	1.83	0.60
1:C:213:ALA:HA	1:C:216:GLN:HE21	1.68	0.59
1:E:32:GLU:HG2	3:E:408:HOH:O	2.03	0.58
1:B:154:VAL:HG13	1:B:179:VAL:HA	1.85	0.58
1:G:28:ASP:HA	1:G:101:MET:HE3	1.82	0.58
1:G:28:ASP:OD1	1:G:101:MET:CE	2.50	0.57
1:D:92:THR:N	3:D:401:HOH:O	2.24	0.56
1:C:30:ILE:HG21	1:C:115:LEU:HD11	1.87	0.55
1:F:24:ASP:OD2	1:F:129:LYS:NZ	2.38	0.54
1:F:129:LYS:HD2	1:F:134:ALA:HA	1.90	0.54
1:F:190:ASP:O	1:F:194:ILE:HG13	2.07	0.54
1:E:129:LYS:HD2	1:E:134:ALA:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:HD2	1:D:134:ALA:HA	1.91	0.53
1:G:30:ILE:HG12	1:G:46:LEU:HB3	1.91	0.53
1:A:52:THR:HG23	1:A:212:LEU:HD22	1.92	0.52
1:F:2:ILE:HD13	1:F:15:PRO:HD3	1.91	0.52
1:C:70:THR:HB	1:C:129:LYS:HD3	1.92	0.52
1:D:24:ASP:OD2	1:D:129:LYS:NZ	2.42	0.52
1:B:59:LEU:HD23	1:B:59:LEU:C	2.34	0.51
1:A:4:ILE:CD1	1:A:218:GLY:HA3	2.40	0.51
1:A:66:LEU:HD22	1:A:147:ARG:HD3	1.93	0.51
1:F:29:PHE:CE2	2:F:301:BME:H11	2.46	0.50
1:H:24:ASP:OD1	1:H:129:LYS:NZ	2.45	0.50
1:F:65:MET:HE1	1:F:153:LEU:HD12	1.93	0.50
1:A:60:ALA:HA	1:A:65:MET:HE3	1.92	0.49
1:H:35:PHE:CE1	1:H:39:LEU:HD21	2.48	0.49
1:G:60:ALA:HA	1:G:65:MET:HE3	1.95	0.49
1:F:139:ASP:O	1:F:143:GLN:HG3	2.13	0.49
1:D:156:GLY:O	1:D:184:CYS:HA	2.12	0.49
1:H:117:GLN:HB2	3:H:407:HOH:O	2.13	0.48
1:F:3:ARG:NH1	1:F:12:GLN:OE1	2.44	0.48
1:G:28:ASP:CG	1:G:101:MET:HE3	2.36	0.48
1:A:190:ASP:HB2	3:A:483:HOH:O	2.13	0.48
1:C:66:LEU:HD22	1:C:147:ARG:HD3	1.95	0.48
1:C:194:ILE:HG21	1:D:194:ILE:CG2	2.40	0.48
1:D:186:SER:HB3	1:D:192:HIS:HB2	1.94	0.48
1:B:139:ASP:O	1:B:143:GLN:HG2	2.14	0.47
1:E:73:SER:HB2	1:E:107:GLN:HG3	1.96	0.47
1:E:2:ILE:HD13	1:E:219:VAL:HG12	1.97	0.47
1:F:167:MET:HE3	1:F:177:CYS:HB2	1.96	0.47
1:C:86[B]:ARG:HG2	3:C:435:HOH:O	2.14	0.47
1:H:24:ASP:OD2	1:H:129:LYS:NZ	2.48	0.47
1:B:156:GLY:O	1:B:184:CYS:HA	2.15	0.46
1:B:24:ASP:OD2	1:B:129:LYS:NZ	2.48	0.46
1:C:129:LYS:HD2	1:C:134:ALA:HA	1.97	0.46
1:G:139:ASP:O	1:G:143:GLN:HG3	2.16	0.46
1:G:44:ARG:N	1:G:45:PRO:CD	2.80	0.45
1:B:194:ILE:CG2	1:E:194:ILE:HG21	2.46	0.45
1:F:70:THR:HB	1:F:129:LYS:HD3	1.97	0.45
1:D:67:VAL:HB	1:D:124:GLU:HG2	1.98	0.45
1:G:156:GLY:O	1:G:184:CYS:HA	2.16	0.45
1:B:181:GLU:OE2	1:B:209:ARG:HD2	2.17	0.44
1:E:214:GLN:HA	1:E:214:GLN:OE1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:O	1:A:40:GLY:N	2.46	0.44
1:B:30:ILE:HD13	1:B:46:LEU:HD23	1.98	0.44
1:B:4:ILE:CD1	1:B:218:GLY:HA3	2.47	0.44
1:H:44:ARG:N	1:H:45:PRO:CD	2.81	0.44
1:A:194:ILE:HD13	1:G:194:ILE:CD1	2.47	0.44
1:A:4:ILE:HD13	1:A:218:GLY:HA3	1.98	0.44
1:A:107:GLN:HG2	3:A:422:HOH:O	2.18	0.44
1:A:194:ILE:HG21	1:G:194:ILE:CG2	2.46	0.44
1:D:44:ARG:N	1:D:45:PRO:CD	2.81	0.43
1:H:85:LYS:NZ	1:H:130:PRO:O	2.52	0.43
1:E:88:ARG:O	1:E:91:PRO:HD3	2.18	0.43
1:D:2:ILE:HG22	1:D:4:ILE:HD11	2.01	0.43
1:F:105:LEU:HD23	1:F:105:LEU:HA	1.89	0.43
1:D:66:LEU:HD11	1:D:125:LEU:CD2	2.49	0.43
1:G:4:ILE:CD1	1:G:218:GLY:HA3	2.49	0.43
1:D:14:HIS:ND1	1:D:16:ARG:HG2	2.33	0.43
1:D:173:ARG:NH2	3:D:402:HOH:O	2.28	0.43
1:G:105:LEU:HD23	1:G:105:LEU:HA	1.89	0.42
1:A:156:GLY:O	1:A:184:CYS:HA	2.19	0.42
1:A:200:THR:HG21	1:A:209:ARG:HG2	2.01	0.42
1:F:44:ARG:N	1:F:45:PRO:CD	2.82	0.42
1:E:156:GLY:O	1:E:184:CYS:HA	2.18	0.42
1:B:30:ILE:CD1	1:B:46:LEU:HB3	2.49	0.42
1:A:24:ASP:OD2	1:A:129:LYS:NZ	2.53	0.41
1:E:23:ILE:HA	1:E:70:THR:OG1	2.20	0.41
1:B:29:PHE:CE2	2:B:301:BME:H12	2.55	0.41
1:D:2:ILE:CG2	1:D:4:ILE:HD11	2.50	0.41
1:C:1:MET:HB3	1:C:12:GLN:HG2	2.02	0.41
1:A:72:GLU:OE2	1:A:132:LYS:NZ	2.51	0.41
1:H:24:ASP:CG	1:H:129:LYS:NZ	2.79	0.41
1:C:193:ARG:HD2	1:C:197:GLU:OE2	2.20	0.41
1:D:105:LEU:HD23	1:D:105:LEU:HA	1.86	0.41
1:C:4:ILE:HD12	1:C:215:LEU:HA	2.03	0.41
1:D:9:TYR:HB2	1:D:10:PRO:CD	2.51	0.41
1:E:139:ASP:O	1:E:143:GLN:HG3	2.21	0.41
1:H:9:TYR:HB2	1:H:10:PRO:CD	2.51	0.41
1:H:156:GLY:O	1:H:184:CYS:HA	2.21	0.41
1:H:105:LEU:HD23	1:H:105:LEU:HA	1.88	0.41
1:H:9:TYR:HB2	1:H:10:PRO:HD2	2.02	0.40
1:A:3:ARG:NH2	1:A:12:GLN:OE1	2.54	0.40
1:H:190:ASP:O	1:H:194:ILE:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:O	1:A:41:ASN:ND2	2.44	0.40
1:B:30:ILE:HD13	1:B:46:LEU:HB3	2.02	0.40
1:D:139:ASP:OD1	1:D:143:GLN:NE2	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	218/223 (98%)	214 (98%)	3 (1%)	1 (0%)	24	22
1	B	217/223 (97%)	215 (99%)	2 (1%)	0	100	100
1	C	220/223 (99%)	219 (100%)	1 (0%)	0	100	100
1	D	218/223 (98%)	216 (99%)	2 (1%)	0	100	100
1	E	219/223 (98%)	218 (100%)	1 (0%)	0	100	100
1	F	219/223 (98%)	217 (99%)	2 (1%)	0	100	100
1	G	217/223 (97%)	215 (99%)	2 (1%)	0	100	100
1	H	218/223 (98%)	215 (99%)	3 (1%)	0	100	100
All	All	1746/1784 (98%)	1729 (99%)	16 (1%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLY

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	179/180 (99%)	174 (97%)	5 (3%)	38	43
1	B	178/180 (99%)	172 (97%)	6 (3%)	32	35
1	C	180/180 (100%)	174 (97%)	6 (3%)	33	37
1	D	178/180 (99%)	174 (98%)	4 (2%)	45	53
1	E	179/180 (99%)	173 (97%)	6 (3%)	32	35
1	F	179/180 (99%)	176 (98%)	3 (2%)	53	62
1	G	178/180 (99%)	172 (97%)	6 (3%)	32	35
1	H	178/180 (99%)	174 (98%)	4 (2%)	45	53
All	All	1429/1440 (99%)	1389 (97%)	40 (3%)	38	43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	62	GLU
1	A	105	LEU
1	A	148	ARG
1	A	210	THR
1	B	12	GLN
1	B	28	ASP
1	B	105	LEU
1	B	148	ARG
1	B	154	VAL
1	B	210	THR
1	C	2	ILE
1	C	28	ASP
1	C	39	LEU
1	C	93	LEU
1	C	193	ARG
1	C	210	THR
1	D	28	ASP
1	D	83	ARG
1	D	129	LYS
1	D	210	THR
1	E	12	GLN
1	E	28	ASP
1	E	37	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	92	THR
1	E	164	GLN
1	E	210	THR
1	F	5	ASP
1	F	105	LEU
1	F	210	THR
1	G	37	SER
1	G	92	THR
1	G	105	LEU
1	G	167	MET
1	G	210	THR
1	G	219	VAL
1	H	83	ARG
1	H	93	LEU
1	H	164	GLN
1	H	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	202	GLN
1	A	216	GLN
1	B	58	GLN
1	B	202	GLN
1	C	216	GLN
1	D	214	GLN
1	E	145	GLN
1	F	145	GLN
1	F	202	GLN
1	G	12	GLN
1	G	58	GLN
1	G	107	GLN
1	G	202	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands 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	BME	A	301	1	3,3,3	0.24	0	2,2,2	0.81	0
2	BME	G	301	1	3,3,3	0.25	0	2,2,2	0.44	0
2	BME	C	301	1	3,3,3	0.26	0	2,2,2	0.27	0
2	BME	E	301	1	3,3,3	0.28	0	2,2,2	0.41	0
2	BME	F	301	1	3,3,3	0.23	0	2,2,2	0.59	0
2	BME	D	301	1	3,3,3	0.28	0	2,2,2	0.08	0
2	BME	H	301	1	3,3,3	0.32	0	2,2,2	0.48	0
2	BME	B	301	1	3,3,3	0.25	0	2,2,2	0.30	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
2	BME	A	301	1	-	1/1/1/1	-
2	BME	G	301	1	-	0/1/1/1	-
2	BME	C	301	1	-	0/1/1/1	-
2	BME	E	301	1	-	0/1/1/1	-
2	BME	F	301	1	-	0/1/1/1	-
2	BME	D	301	1	-	0/1/1/1	-
2	BME	H	301	1	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	B	301	1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	BME	O1-C1-C2-S2
2	A	301	BME	O1-C1-C2-S2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	BME	1	0
2	B	301	BME	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/223 (98%)	0.12	8 (3%) 45 47	9, 19, 37, 60	1 (0%)
1	B	219/223 (98%)	-0.09	1 (0%) 87 88	10, 16, 31, 41	0
1	C	221/223 (99%)	0.21	6 (2%) 56 59	11, 21, 34, 63	1 (0%)
1	D	220/223 (98%)	0.24	9 (4%) 41 43	11, 21, 41, 49	0
1	E	220/223 (98%)	0.17	6 (2%) 56 59	11, 20, 37, 52	1 (0%)
1	F	220/223 (98%)	0.27	4 (1%) 67 70	8, 22, 35, 47	1 (0%)
1	G	219/223 (98%)	-0.05	0 100 100	10, 17, 30, 46	0
1	H	220/223 (98%)	0.26	9 (4%) 41 43	13, 22, 44, 54	0
All	All	1758/1784 (98%)	0.14	43 (2%) 59 62	8, 20, 36, 63	4 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	LEU	6.1
1	A	40	GLY	5.5
1	E	39	LEU	4.8
1	C	220	ALA	3.7
1	C	0	HIS	3.4
1	A	38	ALA	3.4
1	H	33	GLY	3.4
1	H	35	PHE	3.3
1	D	220	ALA	3.3
1	D	92	THR	3.0
1	E	38	ALA	3.0
1	H	93	LEU	3.0
1	A	1	MET	2.7
1	F	1	MET	2.6
1	H	1	MET	2.6
1	A	34	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.5
1	E	1	MET	2.4
1	F	220	ALA	2.4
1	C	35	PHE	2.4
1	C	1	MET	2.4
1	F	93	LEU	2.4
1	A	62	GLU	2.4
1	H	92	THR	2.3
1	B	92	THR	2.2
1	D	33	GLY	2.2
1	C	93	LEU	2.2
1	A	37	SER	2.2
1	D	93	LEU	2.2
1	H	122	GLU	2.1
1	D	59	LEU	2.1
1	E	40	GLY	2.1
1	F	64	GLY	2.1
1	D	38	ALA	2.1
1	D	91	PRO	2.1
1	E	219	VAL	2.1
1	H	38	ALA	2.1
1	H	59	LEU	2.1
1	D	35	PHE	2.1
1	E	220	ALA	2.1
1	A	33	GLY	2.0
1	H	34	GLY	2.0
1	C	219	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BME	H	301	4/4	0.92	0.12	29,34,35,42	0
2	BME	C	301	4/4	0.93	0.15	26,26,27,28	0
2	BME	D	301	4/4	0.93	0.10	23,24,24,25	0
2	BME	A	301	4/4	0.93	0.11	29,31,31,34	0
2	BME	B	301	4/4	0.94	0.10	22,25,26,28	0
2	BME	F	301	4/4	0.95	0.14	27,33,36,37	0
2	BME	E	301	4/4	0.96	0.10	24,24,26,27	0
2	BME	G	301	4/4	0.97	0.07	25,26,26,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.