Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 04:50 AM EDT

PDB ID	:	4LIH
Title	:	The crystal structure of Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase from Burkholderia cenocepacia J2315
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2013-07-02
Resolution	:	1.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

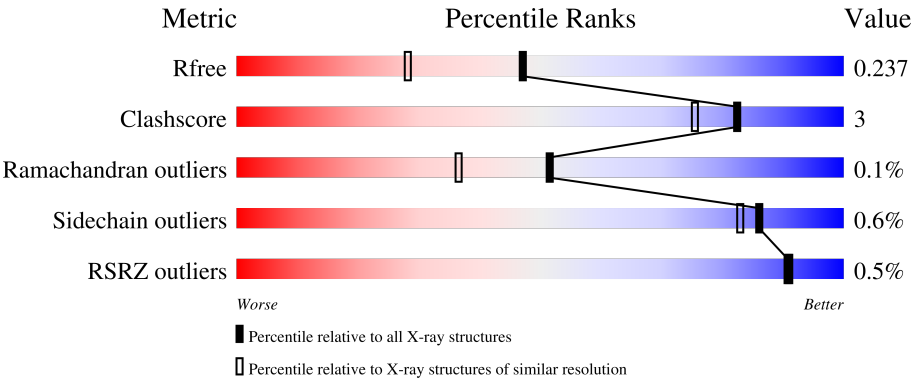
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	504	93% 5% •
1	B	504	91% 7% •
1	C	504	92% 6% •
1	D	504	92% 6% •
1	E	504	90% 8% •

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Mol	Chain	Length	Quality of chain
1	F	504	91% 7%
1	G	504	92% 6%
1	H	504	2% 92% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33175 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 Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	10	0
			3771	2385	662	709	15			
1	B	493	Total	C	N	O	S	0	6	0
			3713	2355	647	695	16			
1	C	493	Total	C	N	O	S	0	5	0
			3717	2353	652	697	15			
1	D	494	Total	C	N	O	S	0	2	0
			3670	2328	639	689	14			
1	E	493	Total	C	N	O	S	0	11	0
			3776	2386	666	708	16			
1	F	493	Total	C	N	O	S	0	3	0
			3694	2340	647	692	15			
1	G	493	Total	C	N	O	S	0	3	0
			3688	2338	645	690	15			
1	H	494	Total	C	N	O	S	0	3	0
			3681	2335	641	690	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP B4E926
A	-6	ALA	-	expression tag	UNP B4E926
A	-5	HIS	-	expression tag	UNP B4E926
A	-4	HIS	-	expression tag	UNP B4E926
A	-3	HIS	-	expression tag	UNP B4E926
A	-2	HIS	-	expression tag	UNP B4E926
A	-1	HIS	-	expression tag	UNP B4E926
A	0	HIS	-	expression tag	UNP B4E926
B	-7	MET	-	expression tag	UNP B4E926
B	-6	ALA	-	expression tag	UNP B4E926
B	-5	HIS	-	expression tag	UNP B4E926
B	-4	HIS	-	expression tag	UNP B4E926
B	-3	HIS	-	expression tag	UNP B4E926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B4E926
B	-1	HIS	-	expression tag	UNP B4E926
B	0	HIS	-	expression tag	UNP B4E926
C	-7	MET	-	expression tag	UNP B4E926
C	-6	ALA	-	expression tag	UNP B4E926
C	-5	HIS	-	expression tag	UNP B4E926
C	-4	HIS	-	expression tag	UNP B4E926
C	-3	HIS	-	expression tag	UNP B4E926
C	-2	HIS	-	expression tag	UNP B4E926
C	-1	HIS	-	expression tag	UNP B4E926
C	0	HIS	-	expression tag	UNP B4E926
D	-7	MET	-	expression tag	UNP B4E926
D	-6	ALA	-	expression tag	UNP B4E926
D	-5	HIS	-	expression tag	UNP B4E926
D	-4	HIS	-	expression tag	UNP B4E926
D	-3	HIS	-	expression tag	UNP B4E926
D	-2	HIS	-	expression tag	UNP B4E926
D	-1	HIS	-	expression tag	UNP B4E926
D	0	HIS	-	expression tag	UNP B4E926
E	-7	MET	-	expression tag	UNP B4E926
E	-6	ALA	-	expression tag	UNP B4E926
E	-5	HIS	-	expression tag	UNP B4E926
E	-4	HIS	-	expression tag	UNP B4E926
E	-3	HIS	-	expression tag	UNP B4E926
E	-2	HIS	-	expression tag	UNP B4E926
E	-1	HIS	-	expression tag	UNP B4E926
E	0	HIS	-	expression tag	UNP B4E926
F	-7	MET	-	expression tag	UNP B4E926
F	-6	ALA	-	expression tag	UNP B4E926
F	-5	HIS	-	expression tag	UNP B4E926
F	-4	HIS	-	expression tag	UNP B4E926
F	-3	HIS	-	expression tag	UNP B4E926
F	-2	HIS	-	expression tag	UNP B4E926
F	-1	HIS	-	expression tag	UNP B4E926
F	0	HIS	-	expression tag	UNP B4E926
G	-7	MET	-	expression tag	UNP B4E926
G	-6	ALA	-	expression tag	UNP B4E926
G	-5	HIS	-	expression tag	UNP B4E926
G	-4	HIS	-	expression tag	UNP B4E926
G	-3	HIS	-	expression tag	UNP B4E926
G	-2	HIS	-	expression tag	UNP B4E926
G	-1	HIS	-	expression tag	UNP B4E926

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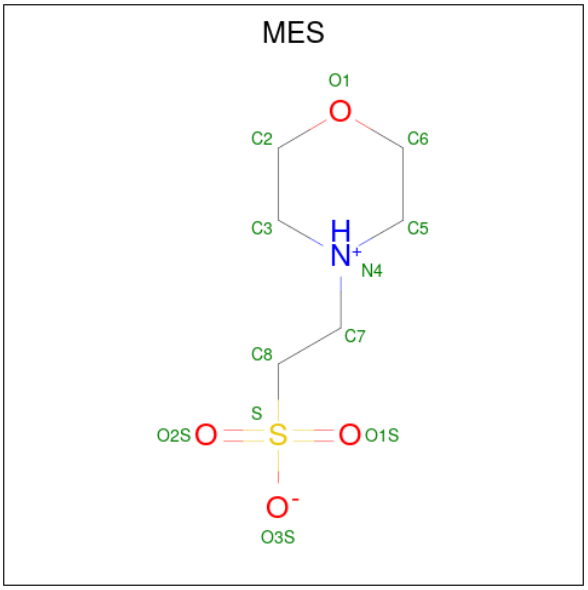
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP B4E926
H	-7	MET	-	expression tag	UNP B4E926
H	-6	ALA	-	expression tag	UNP B4E926
H	-5	HIS	-	expression tag	UNP B4E926
H	-4	HIS	-	expression tag	UNP B4E926
H	-3	HIS	-	expression tag	UNP B4E926
H	-2	HIS	-	expression tag	UNP B4E926
H	-1	HIS	-	expression tag	UNP B4E926
H	0	HIS	-	expression tag	UNP B4E926

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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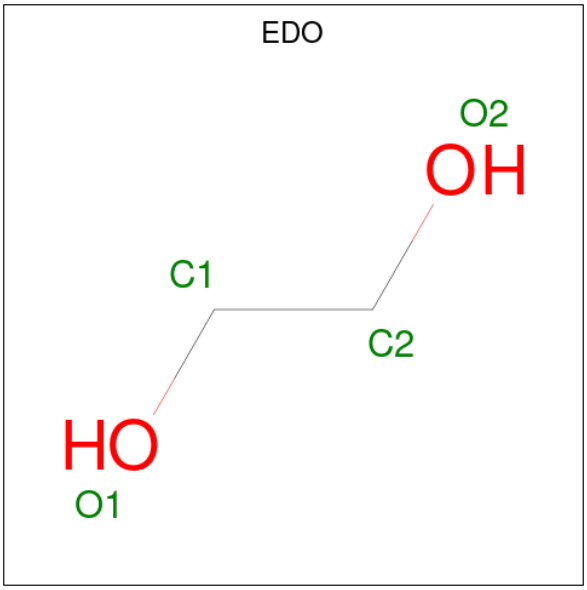
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O S 12 6 1 4 1	0	0
2	H	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

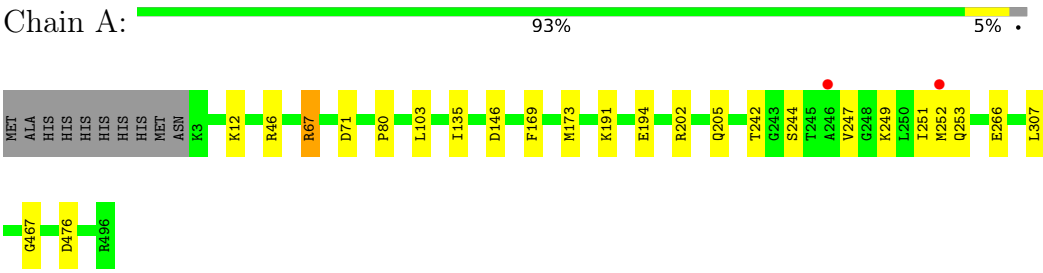
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	469	Total O 469 469	0	0
4	B	460	Total O 460 460	0	0
4	C	390	Total O 390 390	0	0
4	D	384	Total O 384 384	0	0
4	E	445	Total O 445 445	0	0
4	F	431	Total O 431 431	0	0
4	G	415	Total O 415 415	0	0
4	H	347	Total O 347 347	0	0

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.

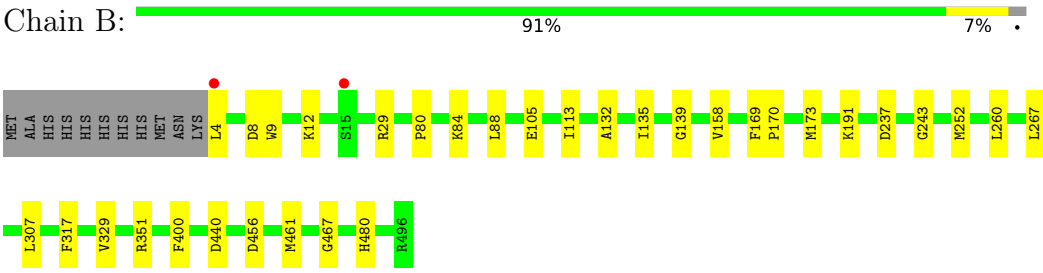
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain A:



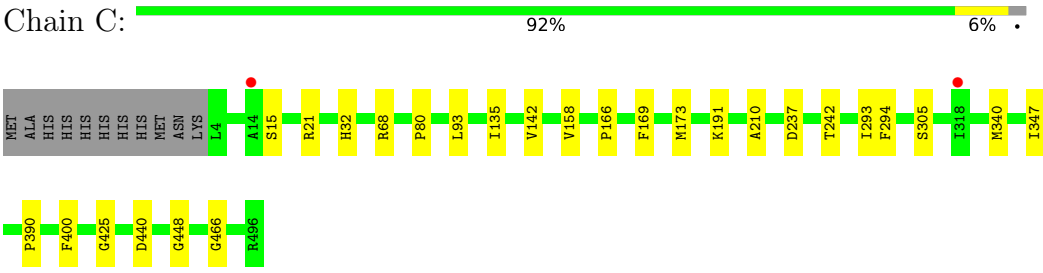
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain B:



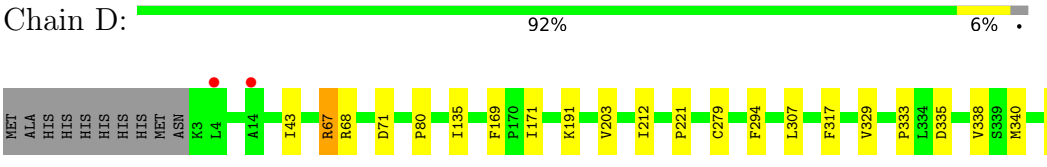
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain C:



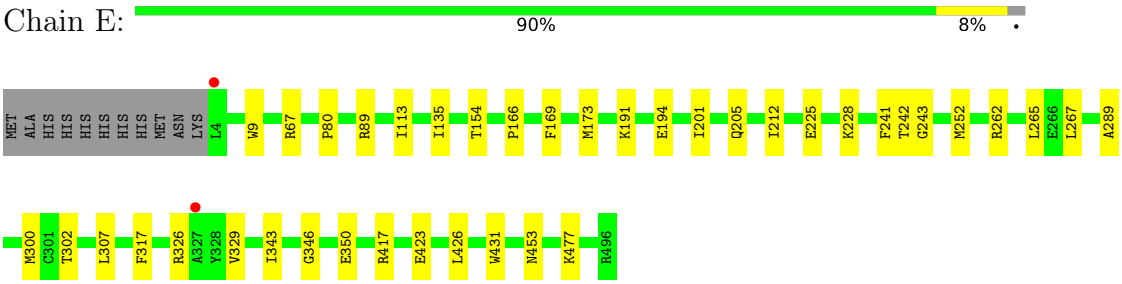
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain D:



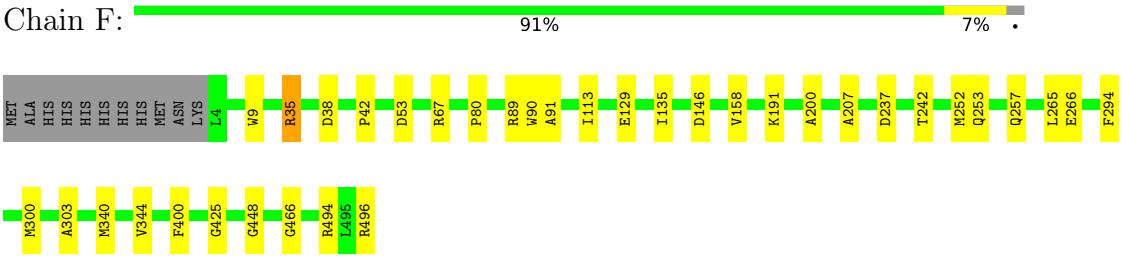
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain E:



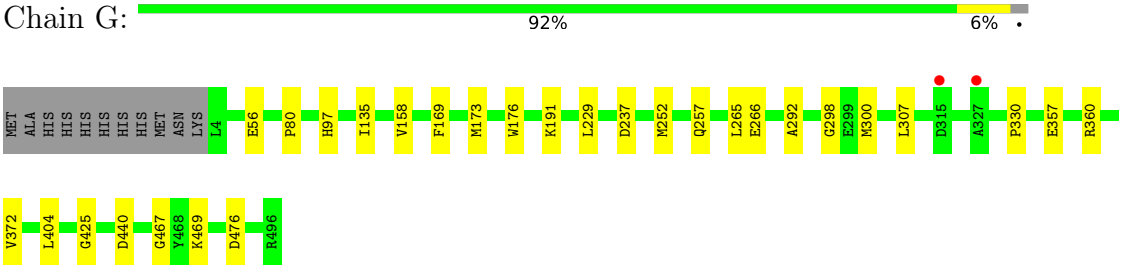
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain F:



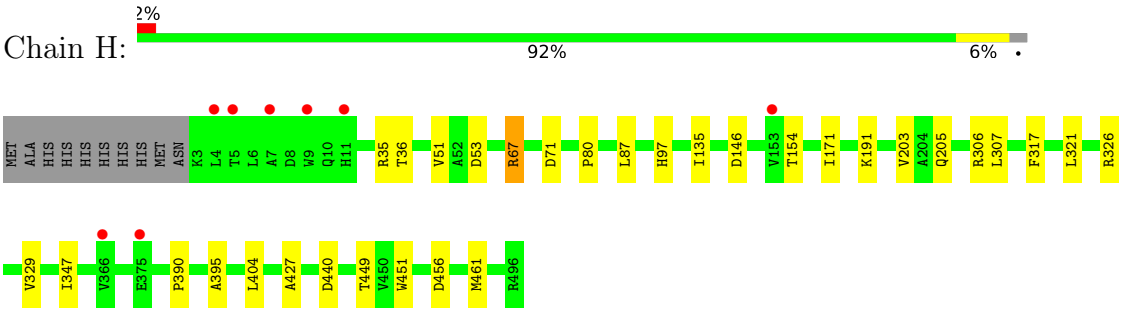
• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain G:



• Molecule 1: Gamma-glutamyl-gamma-aminobutyraldehyde dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.31Å 104.19Å 108.28Å 91.70° 99.04° 90.02°	Depositor
Resolution (Å)	48.19 – 1.85 48.14 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.19-1.85) 97.8 (48.14-1.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.232 0.198 , 0.237	Depositor DCC
R_{free} test set	16432 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.085 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33175	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: EDO, MES

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	0.70	1/3849 (0.0%)	0.83	5/5236 (0.1%)
1	B	0.66	0/3792	0.76	2/5158 (0.0%)
1	C	0.65	0/3793	0.78	1/5160 (0.0%)
1	D	0.62	0/3746	0.78	5/5103 (0.1%)
1	E	0.68	1/3858 (0.0%)	0.79	2/5242 (0.0%)
1	F	0.66	0/3771	0.79	6/5134 (0.1%)
1	G	0.65	1/3764 (0.0%)	0.77	2/5122 (0.0%)
1	H	0.58	0/3757	0.75	3/5117 (0.1%)
All	All	0.65	3/30330 (0.0%)	0.78	26/41272 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	G	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	176	TRP	CB-CG	-5.79	1.39	1.50
1	E	194	GLU	CD-OE1	5.59	1.31	1.25
1	A	194	GLU	CD-OE1	5.51	1.31	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	67	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	67	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	D	67	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	67	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	H	67	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	440	ASP	CB-CG-OD1	6.43	124.08	118.30
1	F	494	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	476	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	29	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	68	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	E	67	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	461	MET	CG-SD-CE	5.51	109.02	100.20
1	A	202	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	146	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	G	476	ASP	CB-CG-OD1	5.44	123.19	118.30
1	F	35	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	38	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	D	461	MET	CG-SD-CE	5.37	108.79	100.20
1	C	21	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	H	461	MET	CG-SD-CE	5.30	108.67	100.20
1	D	329	VAL	CB-CA-C	-5.28	101.37	111.40
1	H	146	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	262	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	146	ASP	CB-CG-OD1	5.09	122.88	118.30
1	F	67	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	38	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	GLY	Peptide
1	B	467	GLY	Peptide
1	G	467	GLY	Peptide

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	3771	0	3712	20	0
1	B	3713	0	3675	25	0
1	C	3717	0	3675	15	0
1	D	3670	0	3618	15	0
1	E	3776	0	3740	24	0
1	F	3694	0	3650	18	0
1	G	3688	0	3644	14	0
1	H	3681	0	3629	18	0
2	A	12	0	13	1	0
2	B	12	0	13	4	0
2	C	12	0	13	1	0
2	D	12	0	13	2	0
2	E	12	0	13	1	0
2	F	12	0	13	0	0
2	G	12	0	13	0	0
2	H	12	0	13	1	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
3	F	4	0	6	0	0
3	G	4	0	6	0	0
3	H	8	0	12	1	0
4	A	469	0	0	9	0
4	B	460	0	0	7	0
4	C	390	0	0	5	0
4	D	384	0	0	3	0
4	E	445	0	0	4	0
4	F	431	0	0	2	0
4	G	415	0	0	4	0
4	H	347	0	0	7	0
All	All	33175	0	29489	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (149) 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:B:351:ARG:HD3	4:B:1057:HOH:O	1.63	0.96
1:E:154[B]:THR:HG21	4:E:727:HOH:O	1.72	0.88
4:A:784:HOH:O	1:B:252[A]:MET:SD	2.37	0.82
1:E:300[A]:MET:HE3	2:E:501:MES:O1S	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ARG:HD2	1:D:71:ASP:OD2	1.87	0.74
1:B:84:LYS:O	1:B:88[B]:LEU:HD13	1.88	0.73
1:D:440[A]:ASP:OD1	4:D:859:HOH:O	2.07	0.72
1:D:171:ILE:HD11	1:D:203:VAL:HG11	1.74	0.69
1:E:346:GLY:O	1:E:350:GLU:HG2	1.93	0.69
1:A:46[B]:ARG:NH2	4:A:706:HOH:O	2.28	0.66
1:C:32:HIS:HA	4:C:835:HOH:O	1.98	0.63
1:H:347:ILE:HG12	4:H:867:HOH:O	1.98	0.62
1:A:67:ARG:HD2	1:A:71:ASP:OD2	2.00	0.61
1:D:67:ARG:CD	1:D:71:ASP:OD2	2.47	0.61
1:D:169:PHE:CE2	2:D:502:MES:H81	2.36	0.60
1:G:257:GLN:NE2	4:G:922:HOH:O	2.34	0.60
1:C:294:PHE:HB3	1:C:340:MET:HE3	1.85	0.59
1:G:80:PRO:HB3	1:G:135:ILE:HG22	1.85	0.59
1:G:252:MET:HG2	1:G:265:LEU:HD11	1.83	0.59
1:A:80:PRO:HB3	1:A:135:ILE:HG22	1.85	0.59
1:F:35:ARG:NH2	1:F:53:ASP:OD2	2.36	0.57
1:B:8:ASP:O	1:B:12:LYS:HG2	2.04	0.57
1:E:154[B]:THR:HG22	4:E:666:HOH:O	2.06	0.56
1:D:307:LEU:HD21	1:D:317:PHE:CE2	2.41	0.56
1:E:423[A]:GLU:HA	1:E:423[A]:GLU:OE1	2.07	0.55
1:B:80:PRO:HB3	1:B:135:ILE:HG22	1.89	0.55
1:C:294:PHE:HB3	1:C:340:MET:CE	2.38	0.54
1:A:205[B]:GLN:OE1	4:A:813:HOH:O	2.18	0.54
1:B:329:VAL:HG22	4:B:944:HOH:O	2.07	0.53
1:E:417[B]:ARG:HG2	1:E:417[B]:ARG:NH1	2.24	0.53
1:B:307:LEU:HD21	1:B:317:PHE:HE2	1.74	0.53
1:A:244:SER:HB2	4:A:1004:HOH:O	2.09	0.52
2:B:502:MES:H21	4:B:874:HOH:O	2.10	0.51
1:H:205:GLN:HG3	4:H:946:HOH:O	2.09	0.51
1:H:326:ARG:O	1:H:329:VAL:HG23	2.11	0.51
1:H:440[A]:ASP:OD1	4:H:891:HOH:O	2.19	0.51
1:A:252[A]:MET:CE	4:B:865:HOH:O	2.58	0.51
1:C:93:LEU:HD12	1:C:210:ALA:HB2	1.93	0.51
1:D:409:PHE:CD2	1:D:415:ALA:HB2	2.45	0.51
2:H:503:MES:H22	4:H:727:HOH:O	2.10	0.51
1:H:307:LEU:HD21	1:H:317:PHE:CE2	2.46	0.50
1:D:294:PHE:HB3	1:D:340:MET:HE2	1.94	0.50
1:C:370:ALA:O	1:C:382:GLU:HG3	2.12	0.50
2:C:502:MES:H62	4:C:662:HOH:O	2.12	0.50
1:B:300[B]:MET:HB2	1:B:303:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:CD	1:A:71:ASP:OD2	2.59	0.49
1:H:80:PRO:HB3	1:H:135:ILE:HG22	1.94	0.49
1:B:4:LEU:HD11	4:B:870:HOH:O	2.11	0.49
1:E:417[B]:ARG:HG2	1:E:417[B]:ARG:HH11	1.78	0.48
1:G:158:VAL:HG22	1:G:237:ASP:HB3	1.95	0.48
1:G:357:GLU:OE1	1:G:360:ARG:NH1	2.46	0.48
1:H:97:HIS:NE2	4:H:845:HOH:O	2.24	0.48
1:B:307:LEU:HD21	1:B:317:PHE:CE2	2.48	0.48
1:D:279:CYS:SG	4:D:840:HOH:O	2.49	0.48
1:C:440[A]:ASP:OD1	4:C:925:HOH:O	2.19	0.48
1:E:343:ILE:HD12	4:E:950:HOH:O	2.12	0.48
1:H:154:THR:HG22	3:H:502:EDO:H21	1.96	0.48
1:F:253:GLN:O	1:F:257:GLN:HG3	2.14	0.48
1:E:80:PRO:HB3	1:E:135:ILE:HG22	1.96	0.48
1:E:225:GLU:O	1:E:228:LYS:HB2	2.14	0.48
1:A:12:LYS:HD2	1:A:103:LEU:HD22	1.96	0.47
1:D:43:ILE:HG12	1:D:333:PRO:HG2	1.96	0.47
1:F:158:VAL:HG22	1:F:237:ASP:HB3	1.96	0.47
1:F:496:ARG:HD3	4:F:923:HOH:O	2.13	0.47
1:E:241:PHE:CZ	1:E:243:GLY:HA3	2.50	0.47
1:E:302:THR:HG22	1:E:426:LEU:HG	1.97	0.47
1:F:80:PRO:HB3	1:F:135:ILE:HG22	1.96	0.47
1:B:88[B]:LEU:CD1	1:B:132:ALA:HB1	2.44	0.47
4:A:784:HOH:O	1:B:252[A]:MET:HE1	2.15	0.47
1:A:252[A]:MET:HE3	4:B:865:HOH:O	2.14	0.46
1:D:371:ARG:NH2	4:D:813:HOH:O	2.47	0.46
1:C:166:PRO:HD3	1:C:242:THR:HB	1.97	0.46
1:E:289:ALA:HB1	1:E:307:LEU:HD13	1.98	0.46
1:A:247:VAL:O	1:A:251:ILE:HG12	2.16	0.46
1:A:252[A]:MET:HE1	1:B:260:LEU:HD23	1.98	0.46
1:C:293:ILE:HD13	1:C:305:SER:HA	1.97	0.46
4:A:959:HOH:O	1:B:480:HIS:HE1	1.99	0.45
1:D:456:ASP:OD2	2:D:502:MES:H61	2.16	0.45
1:F:294:PHE:HB3	1:F:340:MET:HE3	1.98	0.45
1:B:105:GLU:OE2	1:B:170:PRO:HD2	2.17	0.45
1:B:440[A]:ASP:OD1	4:B:966:HOH:O	2.21	0.45
1:E:201:ILE:HG22	1:E:205[B]:GLN:HE22	1.81	0.45
1:G:169:PHE:HB2	1:G:173:MET:HG2	1.97	0.45
1:G:298:GLY:HA2	1:G:300[B]:MET:HE2	1.98	0.45
1:H:171:ILE:HD11	1:H:203:VAL:HG11	1.98	0.45
1:F:89[A]:ARG:O	1:F:89[A]:ARG:HD2	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483[B]:GLU:HG3	1:D:484:LYS:N	2.31	0.44
1:F:200:ALA:HA	4:F:927:HOH:O	2.18	0.44
1:A:252[A]:MET:CE	1:B:260:LEU:HD23	2.47	0.44
1:F:9:TRP:CE2	1:F:113:ILE:HG12	2.52	0.44
1:E:252[A]:MET:HG2	1:E:265:LEU:HD11	1.99	0.44
1:F:300[B]:MET:HB2	1:F:303:ALA:HB2	2.00	0.44
1:A:249:LYS:O	1:A:253:GLN:HG3	2.17	0.44
1:A:348[A]:GLN:HG2	4:A:963:HOH:O	2.16	0.44
1:E:166:PRO:HD3	1:E:242:THR:HB	1.99	0.43
1:G:330:PRO:HG2	1:G:372:VAL:HG21	2.00	0.43
1:H:67:ARG:HD2	1:H:71:ASP:OD2	2.18	0.43
1:C:158:VAL:HG22	1:C:237:ASP:HB3	2.00	0.43
1:E:89[B]:ARG:HD3	4:E:881:HOH:O	2.19	0.43
1:H:307:LEU:HD21	1:H:317:PHE:HE2	1.83	0.43
1:B:169:PHE:CE2	2:B:502:MES:H82	2.53	0.43
1:A:12:LYS:NZ	4:A:912:HOH:O	2.36	0.43
1:E:9:TRP:CE2	1:E:113:ILE:HG12	2.54	0.43
1:E:265:LEU:HB3	1:E:267:LEU:HD21	1.99	0.43
1:G:266:GLU:HB3	4:G:945:HOH:O	2.18	0.43
1:A:242:THR:HA	1:A:266:GLU:O	2.19	0.43
1:A:307:LEU:HD21	1:A:317:PHE:CE2	2.54	0.43
1:H:87:LEU:HD22	4:H:709:HOH:O	2.18	0.43
1:E:431:TRP:CE3	1:E:453:ASN:HA	2.54	0.43
1:H:427:ALA:HA	1:H:449:THR:O	2.19	0.42
1:B:158:VAL:HG22	1:B:237:ASP:HB3	2.00	0.42
1:B:300[A]:MET:HE1	2:B:502:MES:H51	2.00	0.42
1:A:46[B]:ARG:HD2	4:A:947:HOH:O	2.19	0.42
1:E:307:LEU:HD21	1:E:317:PHE:CE2	2.54	0.42
1:F:252:MET:CE	4:H:889:HOH:O	2.66	0.42
1:F:252:MET:HG3	1:F:265:LEU:HD11	2.00	0.42
1:D:335:ASP:HB3	1:D:338:VAL:HG23	2.02	0.42
1:F:90:TRP:CE2	1:F:207:ALA:HB2	2.55	0.42
1:F:448:GLY:HA3	1:F:466:GLY:O	2.20	0.42
1:A:169:PHE:CE2	2:A:501:MES:H82	2.55	0.42
1:H:36:THR:HA	1:H:51:VAL:O	2.20	0.42
1:C:169:PHE:HB2	1:C:173:MET:HG2	2.01	0.41
1:D:80:PRO:HB3	1:D:135:ILE:HG22	2.01	0.41
1:B:169:PHE:HB2	1:B:173:MET:HG2	2.02	0.41
1:B:456:ASP:OD2	2:B:502:MES:H62	2.19	0.41
1:G:97:HIS:ND1	4:G:783:HOH:O	2.36	0.41
1:B:9:TRP:CE2	1:B:113:ILE:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLY:HA3	1:C:142:VAL:O	2.20	0.41
1:F:91:ALA:CB	1:F:129:GLU:HG3	2.51	0.41
1:G:307:LEU:HB2	1:G:404:LEU:HD11	2.02	0.41
1:C:347:ILE:HG12	4:C:879:HOH:O	2.20	0.41
1:E:243:GLY:O	1:E:267:LEU:HA	2.20	0.41
1:H:35:ARG:HB3	1:H:53:ASP:HB3	2.01	0.41
1:F:42:PRO:HB3	1:F:344:VAL:O	2.21	0.41
1:H:306:ARG:HD3	1:H:395:ALA:O	2.21	0.41
1:H:451:TRP:CZ2	1:H:456:ASP:HA	2.56	0.41
1:F:242:THR:HA	1:F:266:GLU:O	2.20	0.41
1:C:448:GLY:HA3	1:C:466:GLY:O	2.21	0.41
1:F:294:PHE:HB3	1:F:340:MET:CE	2.51	0.41
1:C:68:ARG:NH1	4:C:844:HOH:O	2.53	0.40
1:B:243:GLY:O	1:B:267:LEU:HA	2.21	0.40
1:G:469:LYS:HD3	4:G:951:HOH:O	2.20	0.40
1:C:80:PRO:HB3	1:C:135:ILE:HG22	2.03	0.40
1:E:169:PHE:HB2	1:E:173:MET:HG2	2.03	0.40
1:E:326:ARG:O	1:E:329:VAL:HG23	2.21	0.40
1:G:56:GLU:HA	1:G:229:LEU:HD13	2.03	0.40
1:G:292:ALA:O	1:G:300[B]:MET:HE3	2.21	0.40
1:A:169:PHE:HB2	1:A:173:MET:HG2	2.04	0.40
1:H:321:LEU:HD21	1:H:404:LEU:HD23	2.04	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	502/504 (100%)	487 (97%)	15 (3%)	0	100	100
1	B	496/504 (98%)	482 (97%)	14 (3%)	0	100	100
1	C	495/504 (98%)	481 (97%)	13 (3%)	1 (0%)	47	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	494/504 (98%)	480 (97%)	14 (3%)	0	100	100
1	E	501/504 (99%)	488 (97%)	12 (2%)	1 (0%)	47	33
1	F	494/504 (98%)	479 (97%)	14 (3%)	1 (0%)	47	33
1	G	493/504 (98%)	479 (97%)	13 (3%)	1 (0%)	47	33
1	H	495/504 (98%)	482 (97%)	13 (3%)	0	100	100
All	All	3970/4032 (98%)	3858 (97%)	108 (3%)	4 (0%)	51	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	477	LYS
1	G	425	GLY
1	C	425	GLY
1	F	425	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	377/382 (99%)	376 (100%)	1 (0%)	92	91
1	B	371/382 (97%)	369 (100%)	2 (0%)	88	86
1	C	372/382 (97%)	368 (99%)	4 (1%)	73	65
1	D	364/382 (95%)	361 (99%)	3 (1%)	81	76
1	E	380/382 (100%)	378 (100%)	2 (0%)	88	86
1	F	369/382 (97%)	367 (100%)	2 (0%)	88	86
1	G	367/382 (96%)	366 (100%)	1 (0%)	92	91
1	H	365/382 (96%)	363 (100%)	2 (0%)	88	86
All	All	2965/3056 (97%)	2948 (99%)	17 (1%)	86	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
1	B	191	LYS
1	B	400	PHE
1	C	15	SER
1	C	191	LYS
1	C	390	PRO
1	C	400	PHE
1	D	191	LYS
1	D	212	ILE
1	D	221	PRO
1	E	191	LYS
1	E	212	ILE
1	F	191	LYS
1	F	400	PHE
1	G	191	LYS
1	H	191	LYS
1	H	390	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	ASN
1	B	97	HIS
1	B	257	GLN
1	C	257	GLN
1	E	373	ASN
1	F	257	GLN
1	G	257	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)

15 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	MES	G	502	-	12,12,12	2.04	1 (8%)	14,16,16	2.27	4 (28%)
2	MES	A	501	-	12,12,12	2.25	1 (8%)	14,16,16	2.41	5 (35%)
3	EDO	B	501	-	3,3,3	0.48	0	2,2,2	0.23	0
2	MES	C	502	-	12,12,12	1.97	1 (8%)	14,16,16	1.08	1 (7%)
2	MES	F	502	-	12,12,12	2.02	1 (8%)	14,16,16	1.30	2 (14%)
2	MES	B	502	-	12,12,12	2.07	1 (8%)	14,16,16	3.05	3 (21%)
3	EDO	H	501	-	3,3,3	0.36	0	2,2,2	0.41	0
3	EDO	G	501	-	3,3,3	0.40	0	2,2,2	0.05	0
3	EDO	C	501	-	3,3,3	0.35	0	2,2,2	0.24	0
3	EDO	F	501	-	3,3,3	0.28	0	2,2,2	0.48	0
3	EDO	D	501	-	3,3,3	0.45	0	2,2,2	0.52	0
2	MES	E	501	-	12,12,12	2.08	1 (8%)	14,16,16	3.40	5 (35%)
2	MES	H	503	-	12,12,12	2.26	1 (8%)	14,16,16	2.30	2 (14%)
2	MES	D	502	-	12,12,12	2.40	1 (8%)	14,16,16	2.09	3 (21%)
3	EDO	H	502	-	3,3,3	0.35	0	2,2,2	0.52	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	MES	G	502	-	-	1/6/14/14	0/1/1/1
2	MES	A	501	-	-	4/6/14/14	0/1/1/1
3	EDO	B	501	-	-	0/1/1/1	-
2	MES	C	502	-	-	1/6/14/14	0/1/1/1
2	MES	F	502	-	-	1/6/14/14	0/1/1/1
2	MES	B	502	-	-	0/6/14/14	0/1/1/1
3	EDO	H	501	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	G	501	-	-	0/1/1/1	-
3	EDO	C	501	-	-	0/1/1/1	-
3	EDO	F	501	-	-	0/1/1/1	-
3	EDO	D	501	-	-	1/1/1/1	-
2	MES	E	501	-	-	1/6/14/14	0/1/1/1
2	MES	H	503	-	-	5/6/14/14	0/1/1/1
2	MES	D	502	-	-	4/6/14/14	0/1/1/1
3	EDO	H	502	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	MES	C8-S	-7.76	1.66	1.77
2	H	503	MES	C8-S	-7.33	1.67	1.77
2	A	501	MES	C8-S	-7.27	1.67	1.77
2	E	501	MES	C8-S	-6.72	1.68	1.77
2	G	502	MES	C8-S	-6.60	1.68	1.77
2	C	502	MES	C8-S	-6.51	1.68	1.77
2	F	502	MES	C8-S	-6.38	1.68	1.77
2	B	502	MES	C8-S	-6.36	1.68	1.77

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	MES	O2S-S-C8	9.81	118.73	106.92
2	E	501	MES	O2S-S-C8	8.28	116.88	106.92
2	H	503	MES	O2S-S-C8	7.43	115.86	106.92
2	G	502	MES	O2S-S-C8	6.54	114.79	106.92
2	D	502	MES	O2S-S-C8	6.04	114.19	106.92
2	A	501	MES	O3S-S-C8	5.92	115.34	105.77
2	E	501	MES	O1S-S-C8	-5.80	99.93	106.92
2	E	501	MES	O3S-S-C8	5.51	114.68	105.77
2	E	501	MES	C2-C3-N4	4.16	116.42	110.10
2	A	501	MES	O2S-S-C8	3.99	111.72	106.92
2	G	502	MES	O3S-S-C8	3.43	111.31	105.77
2	B	502	MES	O2S-S-O1S	-3.40	102.19	113.95
2	A	501	MES	O3S-S-O1S	-3.31	103.20	111.27
2	G	502	MES	C2-C3-N4	2.89	114.49	110.10
2	D	502	MES	O2S-S-O1S	-2.85	104.07	113.95
2	F	502	MES	O2S-S-C8	2.64	110.10	106.92
2	D	502	MES	O1S-S-C8	2.56	110.00	106.92
2	F	502	MES	O1S-S-C8	2.50	109.92	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	MES	O1S-S-C8	-2.43	103.98	106.92
2	C	502	MES	O2S-S-C8	2.41	109.82	106.92
2	H	503	MES	O2S-S-O1S	-2.41	105.61	113.95
2	E	501	MES	O2S-S-O1S	-2.34	105.86	113.95
2	A	501	MES	C7-N4-C5	2.16	116.76	111.23
2	A	501	MES	O2S-S-O1S	-2.14	106.53	113.95
2	G	502	MES	O2S-S-O1S	-2.08	106.74	113.95

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MES	C8-C7-N4-C5
2	A	501	MES	N4-C7-C8-S
2	C	502	MES	N4-C7-C8-S
2	D	502	MES	C8-C7-N4-C5
2	D	502	MES	C7-C8-S-O2S
2	E	501	MES	N4-C7-C8-S
2	F	502	MES	N4-C7-C8-S
2	G	502	MES	N4-C7-C8-S
2	H	503	MES	C8-C7-N4-C5
2	H	503	MES	C7-C8-S-O2S
2	A	501	MES	C7-C8-S-O3S
2	A	501	MES	C8-C7-N4-C3
2	H	503	MES	C8-C7-N4-C3
3	H	501	EDO	O1-C1-C2-O2
2	D	502	MES	C7-C8-S-O1S
2	H	503	MES	C7-C8-S-O1S
2	D	502	MES	C7-C8-S-O3S
2	H	503	MES	C7-C8-S-O3S
3	D	501	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MES	1	0
2	C	502	MES	1	0
2	B	502	MES	4	0
2	E	501	MES	1	0
2	H	503	MES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	MES	2	0
3	H	502	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	494/504 (98%)	-0.22	2 (0%) 92 92	7, 12, 22, 35	0
1	B	493/504 (97%)	-0.21	2 (0%) 92 92	8, 13, 24, 42	0
1	C	493/504 (97%)	-0.06	2 (0%) 92 92	8, 15, 28, 37	0
1	D	494/504 (98%)	-0.07	2 (0%) 92 92	8, 15, 28, 39	0
1	E	493/504 (97%)	-0.20	2 (0%) 92 92	7, 12, 23, 29	0
1	F	493/504 (97%)	-0.20	0 100 100	8, 14, 25, 34	0
1	G	493/504 (97%)	-0.06	2 (0%) 92 92	8, 15, 29, 42	0
1	H	494/504 (98%)	0.16	8 (1%) 72 72	8, 20, 36, 50	0
All	All	3947/4032 (97%)	-0.11	20 (0%) 91 91	7, 14, 28, 50	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	SER	2.7
1	B	4	LEU	2.6
1	C	14	ALA	2.6
1	H	11	HIS	2.6
1	E	4	LEU	2.5
1	A	246	ALA	2.4
1	G	315	ASP	2.4
1	H	4	LEU	2.4
1	D	4	LEU	2.3
1	D	14	ALA	2.3
1	C	318	ILE	2.3
1	H	375	GLU	2.3
1	H	5	THR	2.2
1	H	366	VAL	2.2
1	H	9	TRP	2.2
1	A	252[A]	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	327	ALA	2.1
1	H	7	ALA	2.1
1	G	327	ALA	2.1
1	H	153	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 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
3	EDO	H	502	4/4	0.86	0.17	20,20,20,21	0
2	MES	H	503	12/12	0.89	0.17	38,40,42,43	0
2	MES	D	502	12/12	0.89	0.21	32,34,38,42	0
3	EDO	C	501	4/4	0.90	0.12	22,22,22,23	0
2	MES	A	501	12/12	0.90	0.20	21,30,33,33	0
2	MES	G	502	12/12	0.91	0.14	29,34,36,36	0
2	MES	B	502	12/12	0.91	0.15	24,30,33,33	0
2	MES	E	501	12/12	0.93	0.15	20,26,29,32	0
2	MES	C	502	12/12	0.94	0.12	26,32,35,36	0
3	EDO	F	501	4/4	0.94	0.10	19,20,20,21	0
3	EDO	G	501	4/4	0.94	0.11	20,22,23,23	0
2	MES	F	502	12/12	0.94	0.13	25,30,32,33	0
3	EDO	B	501	4/4	0.95	0.10	18,19,19,20	0
3	EDO	H	501	4/4	0.96	0.08	18,18,19,20	0
3	EDO	D	501	4/4	0.96	0.09	16,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.