Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 10:31 pm GMT

PDB ID	:	2YII
Title	:	Manipulating the regioselectivity of phenylalanine aminomutase: new insights into the reaction mechanism of MIO-dependent enzymes from structure-guided directed evolution
Authors	:	Wu, B.; Szymanski, W.; Wybenga, G.G.; Heberling, M.M.; Bartsch, S.; Wildeman, S.; Poelarends, G.J.; Feringa, B.L.; Dijkstra, B.W.; Janssen, D.B.
Deposited on	:	2011-05-13
Resolution	:	2.18 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

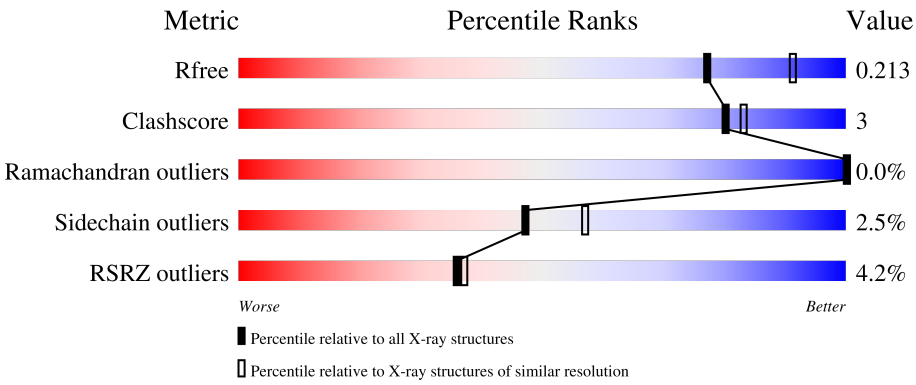
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	705	5% 85% 5% • 9%
1	B	705	4% 83% 9% • 8%
1	C	705	3% 83% 9% • 8%
1	D	705	4% 85% 6% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20965 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 PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	644	5004	3176	862	943	23	0	0	0
1	B	650	5051	3203	871	954	23	0	0	0
1	C	646	5015	3183	864	945	23	0	0	0
1	D	645	5011	3179	862	947	23	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q68G84
A	-18	GLY	-	expression tag	UNP Q68G84
A	-17	SER	-	expression tag	UNP Q68G84
A	-16	SER	-	expression tag	UNP Q68G84
A	-15	HIS	-	expression tag	UNP Q68G84
A	-14	HIS	-	expression tag	UNP Q68G84
A	-13	HIS	-	expression tag	UNP Q68G84
A	-12	HIS	-	expression tag	UNP Q68G84
A	-11	HIS	-	expression tag	UNP Q68G84
A	-10	HIS	-	expression tag	UNP Q68G84
A	-9	SER	-	expression tag	UNP Q68G84
A	-8	SER	-	expression tag	UNP Q68G84
A	-7	GLY	-	expression tag	UNP Q68G84
A	-6	LEU	-	expression tag	UNP Q68G84
A	-5	VAL	-	expression tag	UNP Q68G84
A	-4	PRO	-	expression tag	UNP Q68G84
A	-3	ARG	-	expression tag	UNP Q68G84
A	-2	GLY	-	expression tag	UNP Q68G84
A	-1	SER	-	expression tag	UNP Q68G84
A	0	HIS	-	expression tag	UNP Q68G84
A	175	MDO	ALA	chromophore	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MDO	SER	chromophore	UNP Q68G84
A	175	MDO	GLY	chromophore	UNP Q68G84
B	-19	MET	-	expression tag	UNP Q68G84
B	-18	GLY	-	expression tag	UNP Q68G84
B	-17	SER	-	expression tag	UNP Q68G84
B	-16	SER	-	expression tag	UNP Q68G84
B	-15	HIS	-	expression tag	UNP Q68G84
B	-14	HIS	-	expression tag	UNP Q68G84
B	-13	HIS	-	expression tag	UNP Q68G84
B	-12	HIS	-	expression tag	UNP Q68G84
B	-11	HIS	-	expression tag	UNP Q68G84
B	-10	HIS	-	expression tag	UNP Q68G84
B	-9	SER	-	expression tag	UNP Q68G84
B	-8	SER	-	expression tag	UNP Q68G84
B	-7	GLY	-	expression tag	UNP Q68G84
B	-6	LEU	-	expression tag	UNP Q68G84
B	-5	VAL	-	expression tag	UNP Q68G84
B	-4	PRO	-	expression tag	UNP Q68G84
B	-3	ARG	-	expression tag	UNP Q68G84
B	-2	GLY	-	expression tag	UNP Q68G84
B	-1	SER	-	expression tag	UNP Q68G84
B	0	HIS	-	expression tag	UNP Q68G84
B	175	MDO	ALA	chromophore	UNP Q68G84
B	175	MDO	SER	chromophore	UNP Q68G84
B	175	MDO	GLY	chromophore	UNP Q68G84
C	-19	MET	-	expression tag	UNP Q68G84
C	-18	GLY	-	expression tag	UNP Q68G84
C	-17	SER	-	expression tag	UNP Q68G84
C	-16	SER	-	expression tag	UNP Q68G84
C	-15	HIS	-	expression tag	UNP Q68G84
C	-14	HIS	-	expression tag	UNP Q68G84
C	-13	HIS	-	expression tag	UNP Q68G84
C	-12	HIS	-	expression tag	UNP Q68G84
C	-11	HIS	-	expression tag	UNP Q68G84
C	-10	HIS	-	expression tag	UNP Q68G84
C	-9	SER	-	expression tag	UNP Q68G84
C	-8	SER	-	expression tag	UNP Q68G84
C	-7	GLY	-	expression tag	UNP Q68G84
C	-6	LEU	-	expression tag	UNP Q68G84
C	-5	VAL	-	expression tag	UNP Q68G84
C	-4	PRO	-	expression tag	UNP Q68G84
C	-3	ARG	-	expression tag	UNP Q68G84

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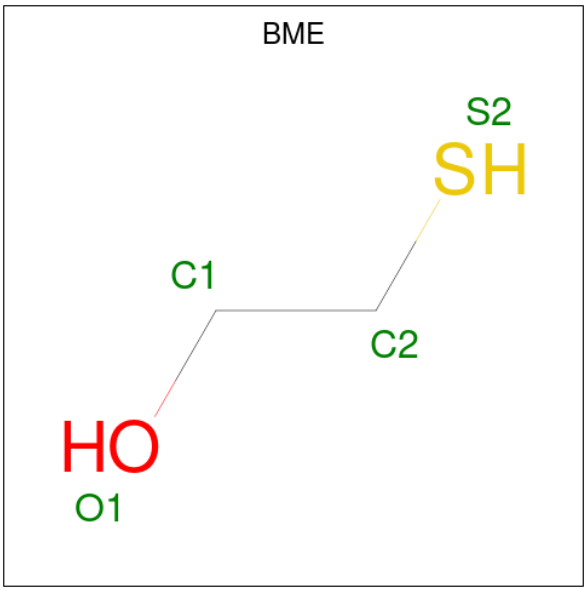
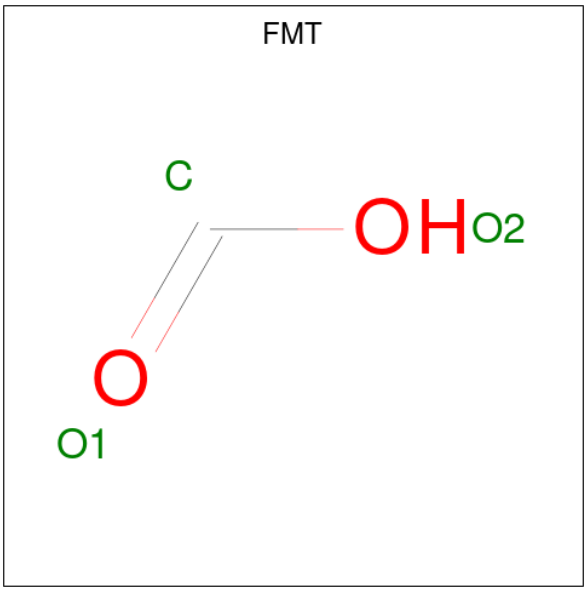
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q68G84
C	-1	SER	-	expression tag	UNP Q68G84
C	0	HIS	-	expression tag	UNP Q68G84
C	175	MDO	ALA	chromophore	UNP Q68G84
C	175	MDO	SER	chromophore	UNP Q68G84
C	175	MDO	GLY	chromophore	UNP Q68G84
D	-19	MET	-	expression tag	UNP Q68G84
D	-18	GLY	-	expression tag	UNP Q68G84
D	-17	SER	-	expression tag	UNP Q68G84
D	-16	SER	-	expression tag	UNP Q68G84
D	-15	HIS	-	expression tag	UNP Q68G84
D	-14	HIS	-	expression tag	UNP Q68G84
D	-13	HIS	-	expression tag	UNP Q68G84
D	-12	HIS	-	expression tag	UNP Q68G84
D	-11	HIS	-	expression tag	UNP Q68G84
D	-10	HIS	-	expression tag	UNP Q68G84
D	-9	SER	-	expression tag	UNP Q68G84
D	-8	SER	-	expression tag	UNP Q68G84
D	-7	GLY	-	expression tag	UNP Q68G84
D	-6	LEU	-	expression tag	UNP Q68G84
D	-5	VAL	-	expression tag	UNP Q68G84
D	-4	PRO	-	expression tag	UNP Q68G84
D	-3	ARG	-	expression tag	UNP Q68G84
D	-2	GLY	-	expression tag	UNP Q68G84
D	-1	SER	-	expression tag	UNP Q68G84
D	0	HIS	-	expression tag	UNP Q68G84
D	175	MDO	ALA	chromophore	UNP Q68G84
D	175	MDO	SER	chromophore	UNP Q68G84
D	175	MDO	GLY	chromophore	UNP Q68G84

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



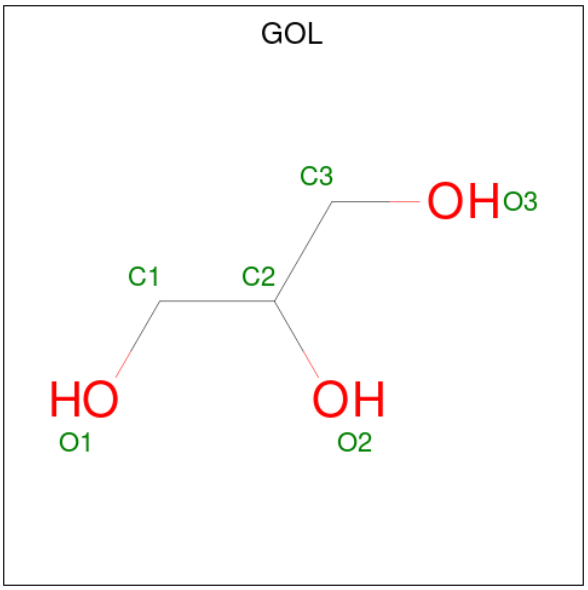
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	4	2	1	1	0	0
2	A	1	4	2	1	1	0	0
2	B	1	4	2	1	1	0	0
2	B	1	4	2	1	1	0	0
2	C	1	4	2	1	1	0	0
2	C	1	4	2	1	1	0	0
2	D	1	4	2	1	1	0	0
2	D	1	4	2	1	1	0	0

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



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is water.

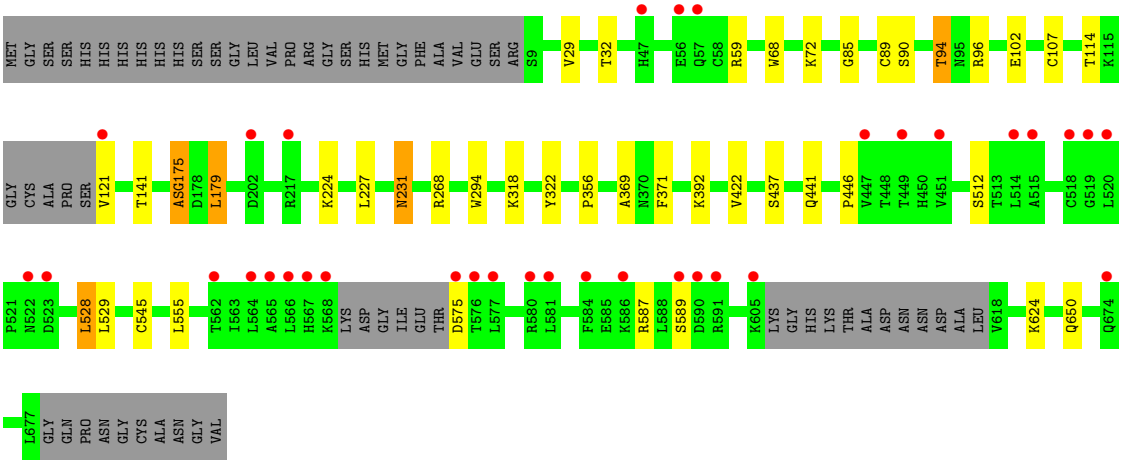
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	241	241	241	0	0
			Total	O		
5	B	193	193	193	0	0
			Total	O		
5	C	228	228	228	0	0
			Total	O		
5	D	172	172	172	0	0

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.

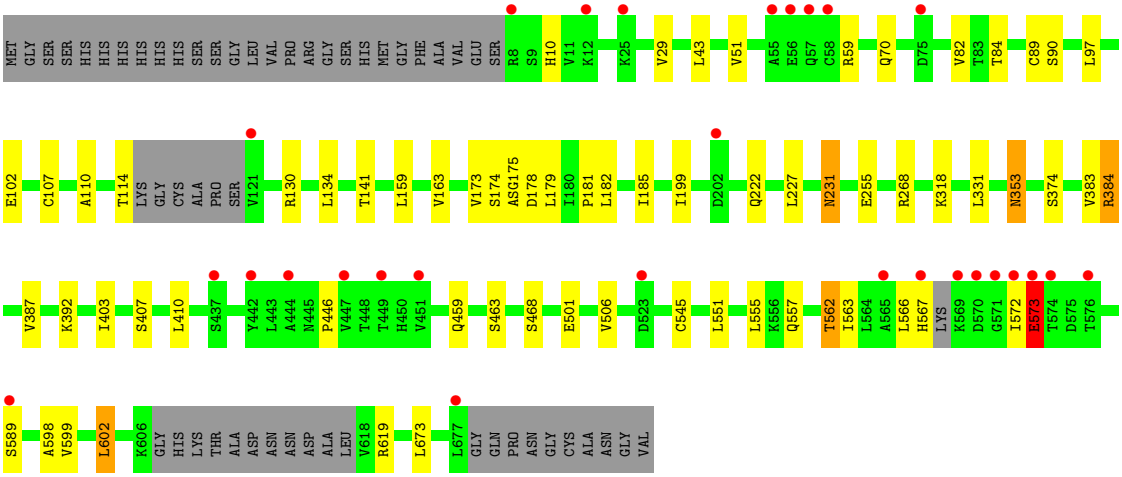
• Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain A:



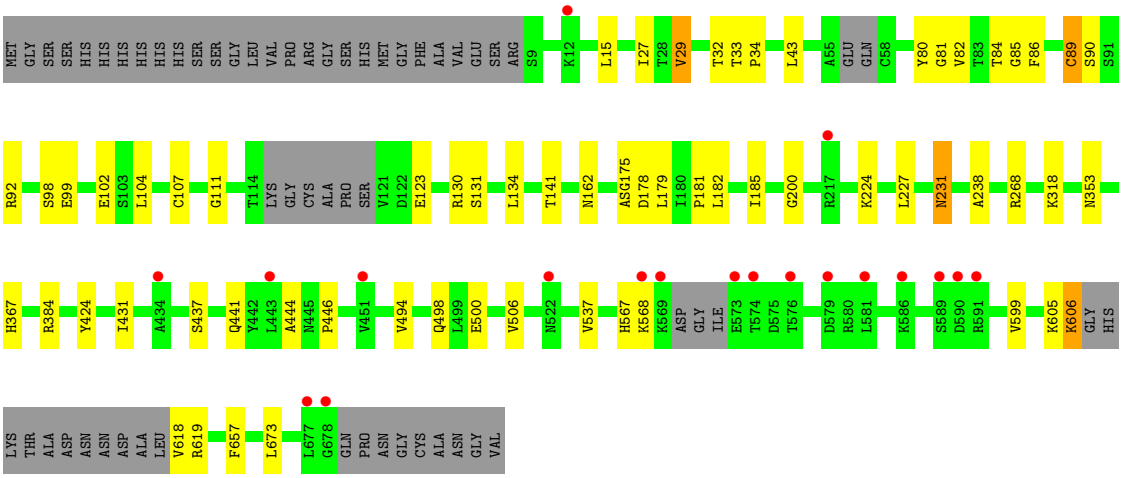
• Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain B:



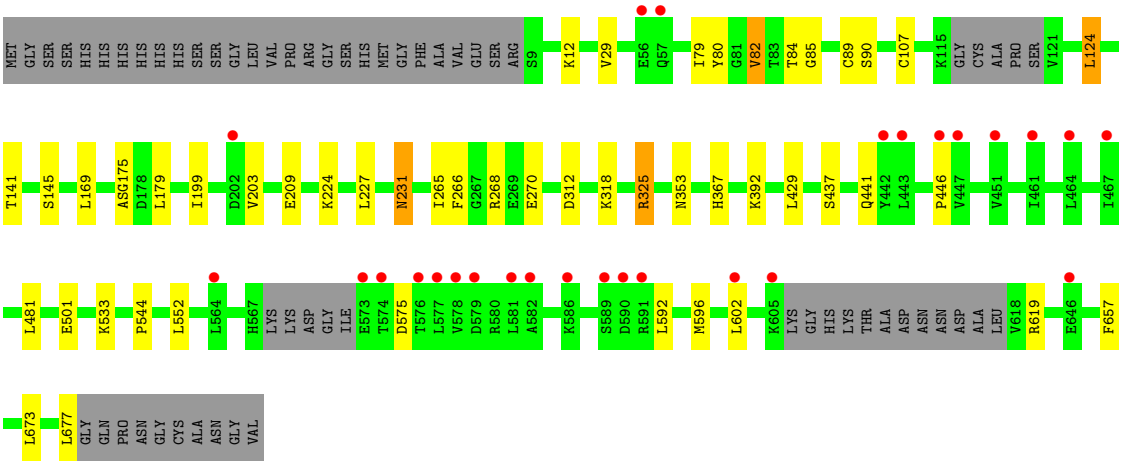
• Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain C:



- Molecule 1: PHENYLALANINE AMMONIA-LYASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.45Å 146.00Å 99.68Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	98.31 – 2.18 48.26 – 2.18	Depositor EDS
% Data completeness (in resolution range)	97.9 (98.31-2.18) 98.0 (48.26-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.179 , 0.214 0.180 , 0.213	Depositor DCC
R_{free} test set	7140 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20965	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 (i)

5.1 Standard geometry (i)

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

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	0.38	0/5075	0.52	0/6882
1	B	0.39	0/5121	0.53	1/6942 (0.0%)
1	C	0.55	1/5086 (0.0%)	0.53	0/6896
1	D	0.39	0/5082	0.53	0/6893
All	All	0.44	1/20364 (0.0%)	0.53	1/27613 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	CYS	C-N	28.00	1.98	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	384	ARG	NE-CZ-NH2	-5.61	117.50	120.30

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	5004	0	5065	25	0
1	B	5051	0	5107	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5015	0	5078	36	0
1	D	5011	0	5065	26	0
2	A	8	0	10	0	0
2	B	8	0	10	1	0
2	C	8	0	10	2	0
2	D	8	0	10	1	0
3	A	3	0	1	0	0
3	B	3	0	1	0	0
3	C	3	0	1	1	0
3	D	3	0	1	0	0
4	B	6	0	8	0	0
5	A	241	0	0	1	0
5	B	193	0	0	1	0
5	C	228	0	0	1	0
5	D	172	0	0	1	0
All	All	20965	0	20367	109	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 (109) 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:C:89:CYS:C	1:C:90:SER:N	1.98	1.17
1:A:89:CYS:C	1:A:90:SER:N	2.02	1.11
1:D:89:CYS:C	1:D:90:SER:N	2.03	1.10
1:B:173:VAL:C	1:B:174:SER:N	2.11	1.04
1:C:506:VAL:HG21	1:C:599:VAL:HG21	1.39	1.02
1:B:89:CYS:C	1:B:90:SER:N	2.14	1.00
1:C:82:VAL:HG22	1:C:224:LYS:HB2	1.66	0.77
1:C:605:LYS:O	1:C:606:LYS:HB3	1.84	0.74
1:A:587:ARG:HH11	1:A:587:ARG:HG2	1.52	0.73
1:B:407:SER:OG	1:B:410:LEU:HB2	1.90	0.71
1:D:199:ILE:HB	1:D:203:VAL:HG22	1.76	0.68
1:B:384:ARG:NH2	1:B:468:SER:OG	2.27	0.67
1:D:592:LEU:HG	1:D:596:MET:CE	2.24	0.67
1:B:179:LEU:HD11	2:B:1175:BME:S2	2.35	0.65
1:A:318:LYS:HB3	1:B:90:SER:HB2	1.78	0.64
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.80	0.63
1:C:437:SER:O	1:C:441:GLN:HG2	1.98	0.63
1:D:592:LEU:HG	1:D:596:MET:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HG23	1:C:141:THR:HG21	1.80	0.62
1:A:224:LYS:HE2	1:A:356:PRO:HD2	1.83	0.60
1:C:90:SER:HB2	1:D:318:LYS:HB3	1.83	0.60
1:D:501:GLU:OE1	1:D:619:ARG:HD2	2.03	0.59
1:A:294:TRP:CH2	1:A:624:LYS:HE2	2.38	0.57
3:C:1680:FMT:O1	1:D:325:ARG:NH2	2.37	0.57
1:A:227:LEU:O	1:A:231:ASN:HB2	2.03	0.57
1:A:587:ARG:HG2	1:A:587:ARG:NH1	2.19	0.57
1:A:587:ARG:HD2	5:A:2216:HOH:O	2.05	0.57
1:D:544:PRO:HG2	1:D:596:MET:HE3	1.87	0.57
1:B:506:VAL:HG21	1:B:599:VAL:HG11	1.88	0.56
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.88	0.55
1:A:545:CYS:SG	1:A:589:SER:HA	2.46	0.55
1:C:84:THR:HG22	1:C:85:GLY:O	2.06	0.55
1:D:12:LYS:HE2	1:D:677:LEU:HB3	1.88	0.54
1:C:182:LEU:HD23	1:C:185:ILE:HD12	1.90	0.54
1:C:98:SER:O	1:C:102:GLU:HG3	2.07	0.54
1:B:403:ILE:O	1:B:407:SER:HB2	2.07	0.54
1:B:563:ILE:O	1:B:567:HIS:HB3	2.09	0.53
1:C:318:LYS:HB3	1:D:90:SER:HB2	1.91	0.53
1:A:29:VAL:HG12	1:A:141:THR:HG21	1.91	0.52
1:C:506:VAL:CG2	1:C:599:VAL:HG21	2.27	0.52
1:B:227:LEU:O	1:B:231:ASN:HB2	2.09	0.52
1:D:79:ILE:HB	1:D:82:VAL:HG22	1.92	0.52
1:B:545:CYS:SG	1:B:589:SER:HA	2.49	0.52
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.91	0.51
1:D:145:SER:O	1:D:224:LYS:HE3	2.10	0.51
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.94	0.51
1:B:110:ALA:HB1	1:D:429:LEU:HD23	1.92	0.51
1:B:572:ILE:HG13	1:B:573:GLU:H	1.77	0.50
1:D:592:LEU:HG	1:D:596:MET:HE1	1.92	0.50
1:B:43:LEU:O	1:B:130:ARG:NH2	2.45	0.50
1:B:501:GLU:OE1	1:B:619:ARG:HD2	2.11	0.49
1:C:178:ASP:HB3	1:C:181:PRO:HG2	1.92	0.49
1:B:178:ASP:HB3	1:B:181:PRO:HG2	1.93	0.49
1:A:94:THR:HG22	1:A:96:ARG:H	1.78	0.49
1:A:650:GLN:HG3	1:C:111:GLY:O	2.13	0.49
1:B:130:ARG:HD2	5:B:2044:HOH:O	2.13	0.49
1:C:43:LEU:HG	1:C:134:LEU:HD22	1.95	0.48
1:C:179:LEU:HD11	2:C:1175:BME:S2	2.53	0.48
1:D:227:LEU:O	1:D:231:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:SER:HA	1:B:463:SER:HB2	1.95	0.48
1:C:227:LEU:O	1:C:231:ASN:HB2	2.14	0.48
1:D:80:TYR:HB3	1:D:367:HIS:CD2	2.50	0.47
1:B:51:VAL:HG21	1:B:159:LEU:HD13	1.96	0.47
1:D:437:SER:O	1:D:441:GLN:HG2	2.15	0.47
1:A:512:SER:HB2	1:A:529:LEU:HD21	1.96	0.47
1:D:544:PRO:CG	1:D:596:MET:HE3	2.45	0.46
1:C:27:ILE:CD1	1:C:43:LEU:HB2	2.45	0.46
1:A:369:ALA:HA	1:A:371:PHE:CE2	2.50	0.46
1:A:437:SER:O	1:A:441:GLN:HG2	2.17	0.45
1:D:124:LEU:HD13	1:D:169:LEU:HD12	1.98	0.45
1:B:255:GLU:HG2	1:B:331:LEU:HD13	1.99	0.45
1:A:85:GLY:HA2	1:C:424:TYR:OH	2.17	0.45
1:A:179:LEU:HD23	1:C:431:ILE:HD13	1.99	0.45
1:A:528:LEU:HG	1:A:555:LEU:HD22	1.98	0.44
1:C:567:HIS:O	1:C:568:LYS:HB2	2.18	0.44
1:B:598:ALA:O	1:B:602:LEU:HB2	2.17	0.44
1:C:130:ARG:HD2	5:C:2052:HOH:O	2.16	0.44
1:D:270:GLU:HB2	5:D:2071:HOH:O	2.17	0.44
1:D:179:LEU:HD11	2:D:1175:BME:S2	2.58	0.44
1:C:131:SER:HB2	1:C:238:ALA:HB1	1.99	0.43
1:C:384:ARG:HG2	1:C:444:ALA:HA	2.00	0.43
1:C:15:LEU:HD21	1:C:673:LEU:HD12	2.01	0.43
1:B:163:VAL:HG13	1:B:199:ILE:HD13	2.01	0.43
1:A:422:VAL:HG11	1:C:99:GLU:HG3	2.00	0.43
1:B:182:LEU:HD23	1:B:185:ILE:HD12	2.01	0.43
1:B:551:LEU:O	1:B:555:LEU:HG	2.19	0.43
1:A:175:MDO:O2	1:A:179:LEU:HD13	2.20	0.42
1:A:114:THR:HG1	1:C:657:PHE:HZ	1.67	0.42
1:A:90:SER:HB2	1:B:318:LYS:HB3	2.01	0.42
1:B:562:THR:HG23	1:B:566:LEU:HD12	2.00	0.42
1:C:162:ASN:ND2	1:C:200:GLY:HA2	2.34	0.42
1:B:353:ASN:H	1:B:353:ASN:ND2	2.18	0.41
1:C:80:TYR:HB3	1:C:367:HIS:CD2	2.55	0.41
1:A:68:TRP:O	1:A:72:LYS:HG2	2.20	0.41
1:B:70:GLN:OE1	1:B:222:GLN:HB3	2.21	0.41
1:D:265:ILE:O	1:D:266:PHE:HB2	2.21	0.41
1:B:43:LEU:HD22	1:B:134:LEU:HD22	2.01	0.41
1:C:86:PHE:CE2	1:C:104:LEU:HB2	2.55	0.41
1:A:322:TYR:CZ	1:B:459:GLN:HG2	2.55	0.41
1:B:383:VAL:O	1:B:387:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HA	1:C:34:PRO:HD3	1.91	0.41
1:C:86:PHE:HB3	2:C:1175:BME:H11	2.03	0.41
1:D:84:THR:HG22	1:D:85:GLY:O	2.20	0.41
1:B:114:THR:HG22	1:D:657:PHE:CZ	2.56	0.40
1:C:494:VAL:O	1:C:498:GLN:HG3	2.20	0.40
1:B:231:ASN:HD22	1:B:231:ASN:HA	1.73	0.40
1:B:10:HIS:NE2	1:B:255:GLU:OE2	2.55	0.40
1:C:81:GLY:HA3	1:C:227:LEU:HD22	2.03	0.40
1:C:500:GLU:HG3	1:C:537:VAL:HG12	2.03	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	631/705 (90%)	619 (98%)	12 (2%)	0	100	100
1	B	636/705 (90%)	622 (98%)	13 (2%)	1 (0%)	47	52
1	C	633/705 (90%)	621 (98%)	12 (2%)	0	100	100
1	D	632/705 (90%)	618 (98%)	14 (2%)	0	100	100
All	All	2532/2820 (90%)	2480 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	573	GLU

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	546/592 (92%)	534 (98%)	12 (2%)	52	62
1	B	551/592 (93%)	536 (97%)	15 (3%)	44	54
1	C	547/592 (92%)	536 (98%)	11 (2%)	55	66
1	D	547/592 (92%)	531 (97%)	16 (3%)	42	51
All	All	2191/2368 (92%)	2137 (98%)	54 (2%)	47	57

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	59	ARG
1	A	94	THR
1	A	102	GLU
1	A	107	CYS
1	A	121	VAL
1	A	179	LEU
1	A	231	ASN
1	A	268	ARG
1	A	392	LYS
1	A	528	LEU
1	A	575	ASP
1	B	59	ARG
1	B	82	VAL
1	B	84	THR
1	B	97	LEU
1	B	102	GLU
1	B	107	CYS
1	B	231	ASN
1	B	268	ARG
1	B	353	ASN
1	B	392	LYS
1	B	557	GLN
1	B	562	THR
1	B	573	GLU
1	B	602	LEU
1	B	673	LEU
1	C	29	VAL

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Mol	Chain	Res	Type
1	C	32	THR
1	C	92	ARG
1	C	107	CYS
1	C	123	GLU
1	C	231	ASN
1	C	268	ARG
1	C	353	ASN
1	C	606	LYS
1	C	618	VAL
1	C	619	ARG
1	D	82	VAL
1	D	107	CYS
1	D	124	LEU
1	D	209	GLU
1	D	231	ASN
1	D	268	ARG
1	D	312	ASP
1	D	325	ARG
1	D	353	ASN
1	D	392	LYS
1	D	481	LEU
1	D	533	LYS
1	D	552	LEU
1	D	575	ASP
1	D	602	LEU
1	D	673	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	B	231	ASN
1	B	557	GLN
1	C	231	ASN
1	D	231	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)

4 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	$\#\|Z\| > 2$
1	MDO	D	175	2,1	12,13,14	2.80	5 (41%)	15,18,20	2.92	4 (26%)
1	MDO	C	175	2,1	12,13,14	2.81	6 (50%)	15,18,20	3.43	4 (26%)
1	MDO	A	175	2,1	12,13,14	2.77	6 (50%)	15,18,20	3.51	4 (26%)
1	MDO	B	175	2,1	12,13,14	2.72	6 (50%)	15,18,20	3.48	4 (26%)

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
1	MDO	D	175	2,1	-	3/4/23/24	0/1/1/1
1	MDO	C	175	2,1	-	2/4/23/24	0/1/1/1
1	MDO	A	175	2,1	-	0/4/23/24	0/1/1/1
1	MDO	B	175	2,1	-	2/4/23/24	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	MDO	O2-C2	6.46	1.36	1.23
1	A	175	MDO	O2-C2	6.25	1.36	1.23
1	C	175	MDO	O2-C2	5.92	1.35	1.23
1	B	175	MDO	O2-C2	5.80	1.35	1.23
1	D	175	MDO	O3-C3	4.25	1.44	1.19
1	B	175	MDO	O3-C3	4.15	1.43	1.19
1	C	175	MDO	O3-C3	4.12	1.43	1.19
1	A	175	MDO	O3-C3	4.10	1.43	1.19
1	C	175	MDO	CA1-C1	3.39	1.56	1.51
1	C	175	MDO	C2-N3	-3.24	1.32	1.39
1	B	175	MDO	C2-N3	-3.10	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	MDO	C2-N3	-3.10	1.32	1.39
1	B	175	MDO	CA2-N2	-3.06	1.33	1.39
1	A	175	MDO	CA1-C1	3.03	1.55	1.51
1	A	175	MDO	C2-N3	-2.98	1.32	1.39
1	B	175	MDO	CA1-C1	2.96	1.55	1.51
1	C	175	MDO	CA2-N2	-2.92	1.33	1.39
1	A	175	MDO	CA2-N2	-2.75	1.34	1.39
1	D	175	MDO	CA2-N2	-2.67	1.34	1.39
1	D	175	MDO	CA1-C1	2.60	1.55	1.51
1	C	175	MDO	CA2-C2	-2.33	1.38	1.43
1	B	175	MDO	CA2-C2	-2.27	1.38	1.43
1	A	175	MDO	CA2-C2	-2.18	1.38	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	175	MDO	CA2-C2-N3	8.86	107.56	103.37
1	B	175	MDO	CA2-C2-N3	8.85	107.56	103.37
1	A	175	MDO	O2-C2-CA2	-8.66	126.10	130.96
1	A	175	MDO	CA2-C2-N3	7.90	107.11	103.37
1	D	175	MDO	CA2-C2-N3	7.79	107.05	103.37
1	C	175	MDO	O2-C2-CA2	-7.35	126.83	130.96
1	B	175	MDO	O2-C2-CA2	-6.90	127.09	130.96
1	B	175	MDO	O3-C3-CA3	-5.93	108.47	126.39
1	A	175	MDO	O3-C3-CA3	-5.80	108.87	126.39
1	D	175	MDO	O3-C3-CA3	-5.09	111.03	126.39
1	C	175	MDO	O3-C3-CA3	-5.08	111.05	126.39
1	D	175	MDO	O2-C2-CA2	-4.78	128.28	130.96
1	C	175	MDO	N3-C1-N2	-2.85	109.48	111.45
1	D	175	MDO	N3-C1-N2	-2.73	109.56	111.45
1	B	175	MDO	N3-C1-N2	-2.68	109.60	111.45
1	A	175	MDO	N3-C1-N2	-2.22	109.92	111.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	175	MDO	N2-C1-CA1-CB
1	C	175	MDO	N2-C1-CA1-CB
1	D	175	MDO	N2-C1-CA1-CB
1	B	175	MDO	N3-C1-CA1-CB
1	C	175	MDO	N3-C1-CA1-CB

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Mol	Chain	Res	Type	Atoms
1	D	175	MDO	N3-C1-CA1-CB
1	D	175	MDO	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	MDO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	C	1089	1	3,3,3	0.53	0	1,2,2	0.17	0
3	FMT	A	1679	-	2,2,2	0.70	0	1,1,1	0.09	0
2	BME	A	1175	1	3,3,3	0.65	0	1,2,2	0.26	0
2	BME	B	1175	1	3,3,3	0.68	0	1,2,2	0.37	0
2	BME	C	1175	1	3,3,3	0.61	0	1,2,2	0.04	0
3	FMT	D	1679	-	2,2,2	0.57	0	1,1,1	0.07	0
2	BME	D	1089	1	3,3,3	0.64	0	1,2,2	0.23	0
3	FMT	B	1680	-	2,2,2	0.68	0	1,1,1	0.12	0
2	BME	A	1089	1	3,3,3	0.71	0	1,2,2	0.01	0
2	BME	D	1175	1	3,3,3	0.65	0	1,2,2	0.33	0
2	BME	B	1089	1	3,3,3	0.83	0	1,2,2	0.28	0
4	GOL	B	1679	-	5,5,5	0.36	0	5,5,5	0.40	0
3	FMT	C	1680	-	2,2,2	0.60	0	1,1,1	0.08	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	C	1089	1	-	0/1/1/1	-
2	BME	A	1175	1	-	0/1/1/1	-
2	BME	B	1175	1	-	0/1/1/1	-
2	BME	C	1175	1	-	0/1/1/1	-
2	BME	D	1089	1	-	0/1/1/1	-
2	BME	A	1089	1	-	0/1/1/1	-
2	BME	D	1175	1	-	0/1/1/1	-
2	BME	B	1089	1	-	1/1/1/1	-
4	GOL	B	1679	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1679	GOL	O2-C2-C3-O3
4	B	1679	GOL	C1-C2-C3-O3
2	B	1089	BME	O1-C1-C2-S2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1175	BME	1	0
2	C	1175	BME	2	0
2	D	1175	BME	1	0
3	C	1680	FMT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	D	1
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	89:CYS	C	90:SER	N	2.14
1	B	173:VAL	C	174:SER	N	2.11
1	D	89:CYS	C	90:SER	N	2.03
1	A	89:CYS	C	90:SER	N	2.02
1	C	89:CYS	C	90:SER	N	1.98

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	643/705 (91%)	0.18	34 (5%)	26	27	16, 31, 54, 67	0
1	B	649/705 (92%)	0.23	28 (4%)	35	36	17, 32, 47, 68	0
1	C	645/705 (91%)	0.10	19 (2%)	51	52	16, 30, 47, 61	0
1	D	644/705 (91%)	0.18	27 (4%)	36	37	17, 31, 54, 71	0
All	All	2581/2820 (91%)	0.17	108 (4%)	36	37	16, 31, 50, 71	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLN	5.8
1	B	571	GLY	4.5
1	B	570	ASP	4.4
1	D	576	THR	4.4
1	C	678	GLY	4.3
1	A	520	LEU	4.3
1	D	57	GLN	4.2
1	D	56	GLU	4.1
1	B	56	GLU	4.1
1	D	577	LEU	3.9
1	A	576	THR	3.9
1	B	572	ILE	3.9
1	A	584	PHE	3.7
1	A	589	SER	3.6
1	A	566	LEU	3.6
1	C	573	GLU	3.6
1	C	591	ARG	3.6
1	B	202	ASP	3.6
1	B	574	THR	3.5
1	D	573	GLU	3.5
1	A	202	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	569	LYS	3.5
1	A	564	LEU	3.5
1	B	573	GLU	3.5
1	D	574	THR	3.4
1	A	47	HIS	3.2
1	A	523	ASP	3.2
1	B	75	ASP	3.1
1	D	605	LYS	3.1
1	D	591	ARG	3.0
1	D	451	VAL	3.0
1	B	523	ASP	3.0
1	A	522	ASN	3.0
1	A	581	LEU	3.0
1	B	567	HIS	2.9
1	A	605	LYS	2.9
1	C	574	THR	2.9
1	A	568	LYS	2.9
1	A	519	GLY	2.8
1	C	586	LYS	2.8
1	C	677	LEU	2.8
1	D	586	LYS	2.8
1	A	57	GLN	2.8
1	C	576	THR	2.8
1	B	55	ALA	2.8
1	A	451	VAL	2.7
1	A	580	ARG	2.7
1	A	447	VAL	2.7
1	B	677	LEU	2.7
1	B	589	SER	2.6
1	C	568	LYS	2.6
1	D	564	LEU	2.6
1	A	121	VAL	2.6
1	A	567	HIS	2.6
1	C	451	VAL	2.5
1	B	447	VAL	2.5
1	C	590	ASP	2.5
1	A	56	GLU	2.5
1	D	202	ASP	2.5
1	D	467	ILE	2.5
1	A	217	ARG	2.5
1	B	8	ARG	2.5
1	B	12	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	25	LYS	2.5
1	A	565	ALA	2.5
1	D	579	ASP	2.4
1	A	518	CYS	2.4
1	C	522	ASN	2.4
1	B	569	LYS	2.4
1	A	590	ASP	2.4
1	C	217	ARG	2.4
1	A	577	LEU	2.3
1	D	443	LEU	2.3
1	D	602	LEU	2.3
1	C	12	LYS	2.3
1	D	581	LEU	2.3
1	B	121	VAL	2.3
1	A	514	LEU	2.3
1	D	447	VAL	2.3
1	D	589	SER	2.3
1	B	437	SER	2.2
1	D	461	ILE	2.2
1	B	576	THR	2.2
1	A	449	THR	2.2
1	B	565	ALA	2.2
1	A	591	ARG	2.2
1	C	581	LEU	2.1
1	D	464	LEU	2.1
1	C	589	SER	2.1
1	B	449	THR	2.1
1	D	578	VAL	2.1
1	D	582	ALA	2.1
1	C	579	ASP	2.1
1	A	515	ALA	2.1
1	A	586	LYS	2.1
1	D	442	TYR	2.1
1	C	443	LEU	2.0
1	B	442	TYR	2.0
1	D	646	GLU	2.0
1	B	58	CYS	2.0
1	D	446	PRO	2.0
1	A	562	THR	2.0
1	B	444	ALA	2.0
1	C	434	ALA	2.0
1	A	575	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	674	GLN	2.0
1	B	451	VAL	2.0
1	D	590	ASP	2.0

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, 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
1	MDO	B	175	13/14	0.92	0.13	26,27,31,35	0
1	MDO	A	175	13/14	0.93	0.12	22,24,27,32	0
1	MDO	D	175	13/14	0.93	0.15	22,23,26,31	0
1	MDO	C	175	13/14	0.94	0.13	22,24,27,32	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, 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	D	1175	4/4	0.85	0.17	43,44,44,44	0
2	BME	B	1175	4/4	0.87	0.16	45,45,46,46	0
2	BME	C	1175	4/4	0.91	0.16	41,43,43,43	0
4	GOL	B	1679	6/6	0.93	0.11	37,38,38,39	0
2	BME	D	1089	4/4	0.94	0.10	30,31,32,34	0
2	BME	A	1089	4/4	0.94	0.13	33,34,35,35	0
2	BME	A	1175	4/4	0.94	0.13	43,43,43,43	0
3	FMT	C	1680	3/3	0.95	0.10	37,37,37,38	0
2	BME	C	1089	4/4	0.95	0.13	31,31,32,34	0
3	FMT	B	1680	3/3	0.96	0.14	43,43,43,44	0
3	FMT	A	1679	3/3	0.97	0.12	31,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	D	1679	3/3	0.97	0.09	32,32,32,32	0
2	BME	B	1089	4/4	0.97	0.11	39,39,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.