



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:50 AM 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

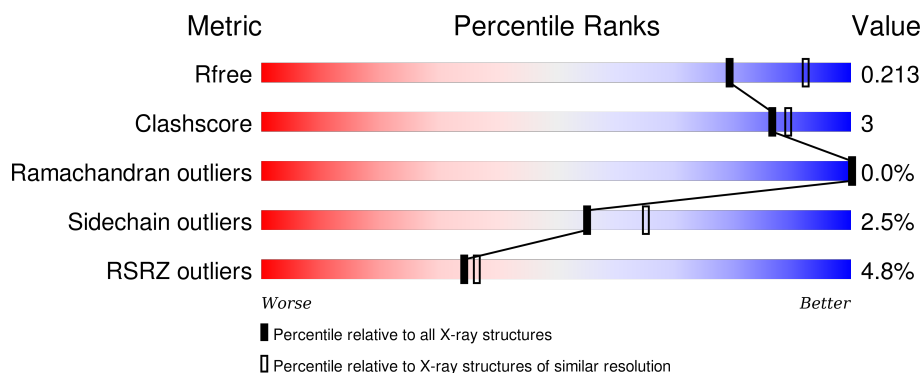
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	705	<div> <div>5%</div> <div>85%</div> <div>5% • 9%</div> </div>
1	B	705	<div> <div>5%</div> <div>83%</div> <div>9% • 8%</div> </div>
1	C	705	<div> <div>4%</div> <div>83%</div> <div>9% • 8%</div> </div>
1	D	705	<div> <div>4%</div> <div>85%</div> <div>6% • 9%</div> </div>

2 Entry composition

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

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: C₂H₆OS).



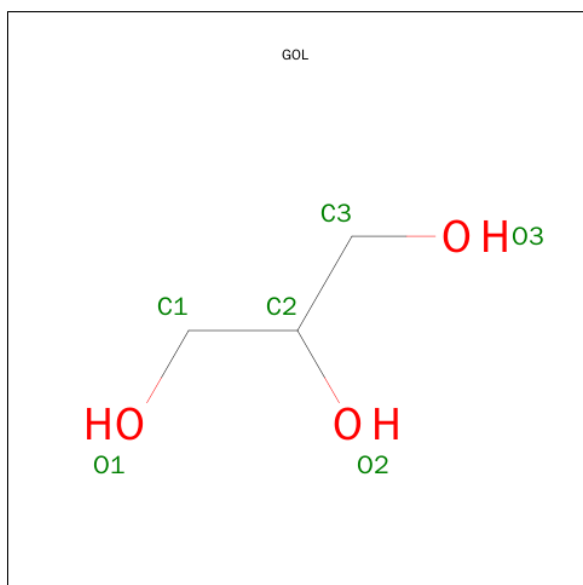
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

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



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

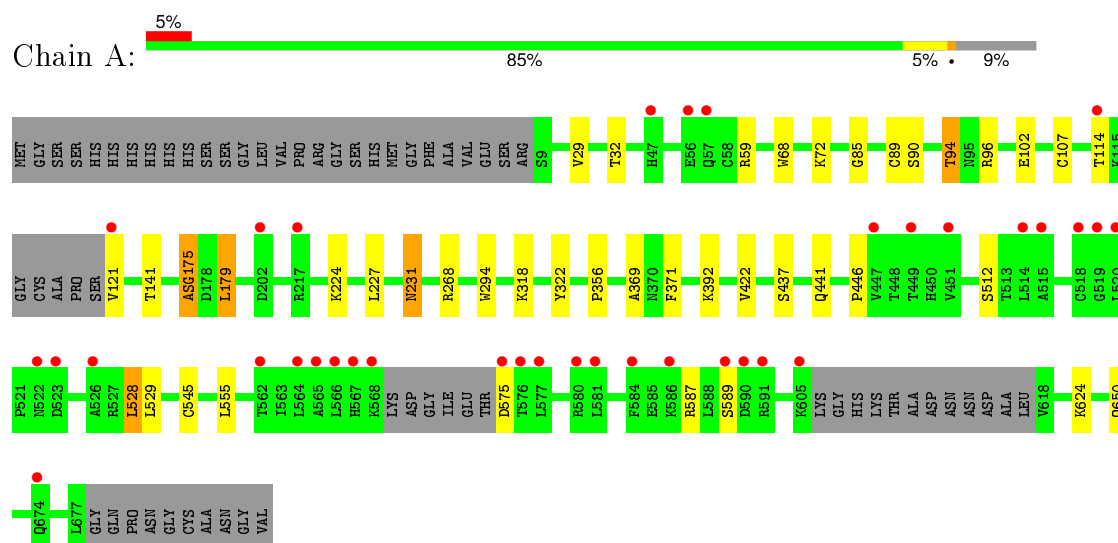
- Molecule 5 is water.

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

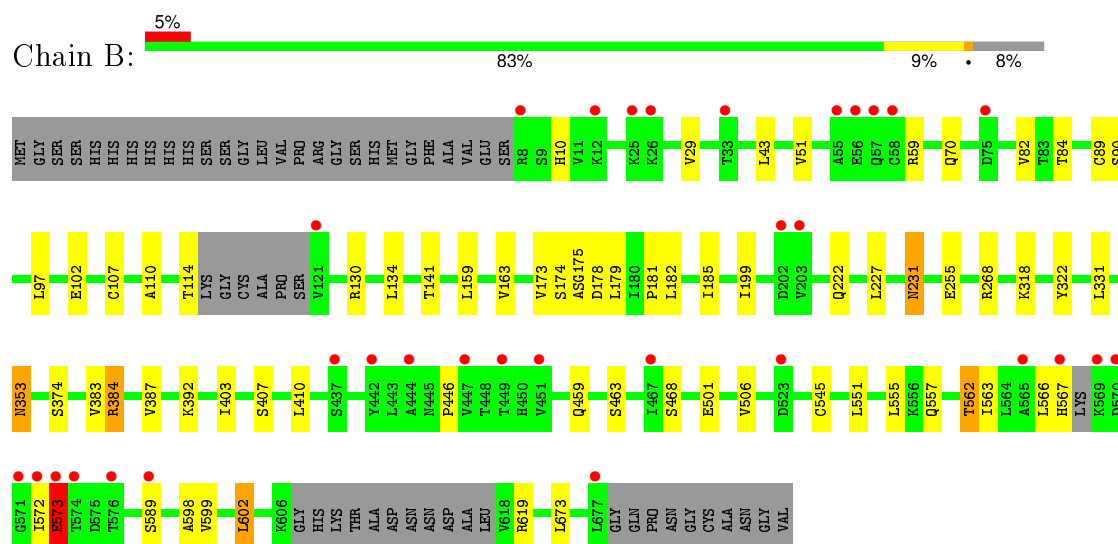
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

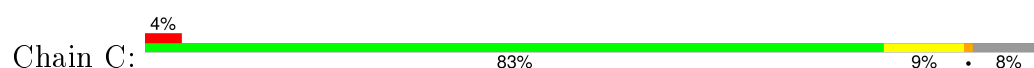
• Molecule 1: PHENYLALANINE AMMONIA-LYASE

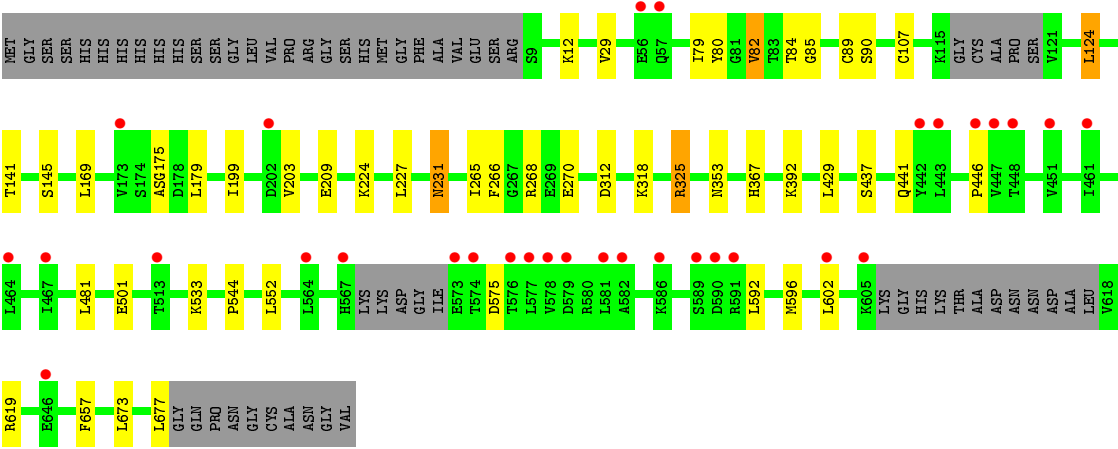
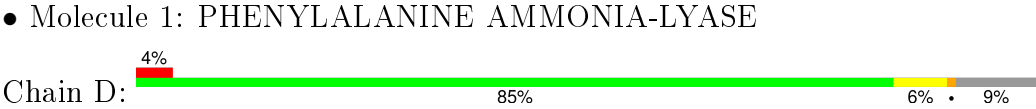
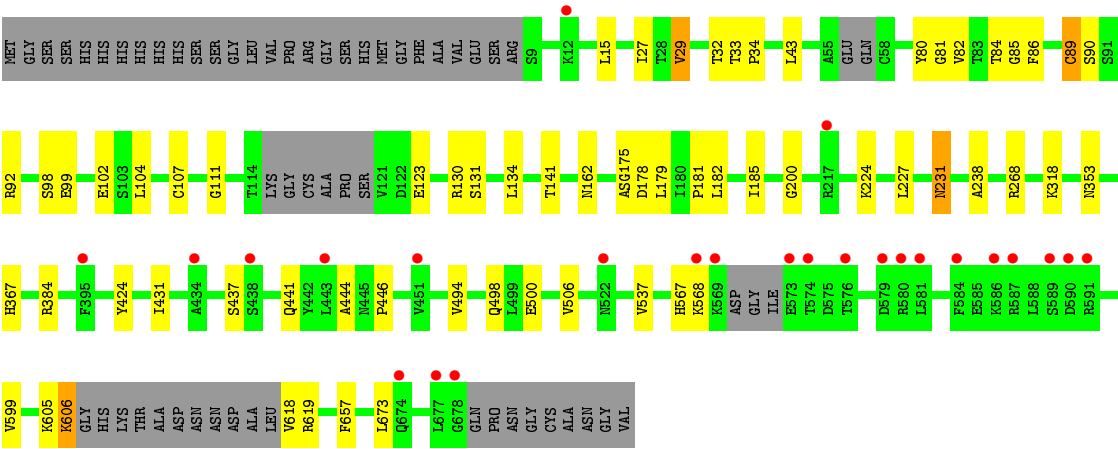


• Molecule 1: PHENYLALANINE AMMONIA-LYASE



• Molecule 1: PHENYLALANINE AMMONIA-LYASE





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.26%)	DCC
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
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 142819 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, FMT, MDO, 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	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%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

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(°)	Ideal(°)
1	B	384	ARG	NE-CZ-NH2	-5.61	117.50	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	MDO	Mainchain,Peptide
1	B	175	MDO	Mainchain,Peptide
1	C	175	MDO	Mainchain,Peptide
1	D	175	MDO	Mainchain,Peptide

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	5004	0	5072	26	0
1	B	5051	0	5114	37	0
1	C	5015	0	5085	36	0
1	D	5011	0	5072	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	20395	110	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 (110) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:SER:O	1:D:224:LYS:HE3	2.10	0.51
1:B:110:ALA:HB1	1:D:429:LEU:HD23	1.92	0.51
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.94	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:B:130:ARG:HD2	5:B:2044:HOH:O	2.13	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:D:227:LEU:O	1:D:231:ASN:HB2	2.14	0.48
1:C:179:LEU:HD11	2:C:1175:BME:S2	2.53	0.48
1:C:43:LEU:HG	1:C:134:LEU:HD22	1.95	0.48
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:179:LEU:HD23	1:C:431:ILE:HD13	1.99	0.45
1:A:85:GLY:HA2	1:C:424:TYR:OH	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:80:TYR:HB3	1:C:367:HIS:CD2	2.55	0.41
1:B:353:ASN:H	1:B:353:ASN:ND2	2.18	0.41
1:B:70:GLN:OE1	1:B:222:GLN:HB3	2.21	0.41
1:A:68:TRP:O	1:A:72:LYS:HG2	2.20	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:C:33:THR:HA	1:C:34:PRO:HD3	1.91	0.41
1:B:383:VAL:O	1:B:387:VAL:HG23	2.21	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:A:175:MDO:HB1	1:B:322:TYR:HE2	1.86	0.40
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:HA	1:B:231:ASN:HD22	1.73	0.40
1:C:81:GLY:HA3	1:C:227:LEU:HD22	2.03	0.40
1:B:10:HIS:NE2	1:B:255:GLU:OE2	2.55	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 ⓘ

5.3.1 Protein backbone ⓘ

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	633/705 (90%)	621 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	637/705 (90%)	623 (98%)	13 (2%)	1 (0%)	52	57
1	C	635/705 (90%)	623 (98%)	12 (2%)	0	100	100
1	D	634/705 (90%)	620 (98%)	14 (2%)	0	100	100
All	All	2539/2820 (90%)	2487 (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 ⓘ

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%)	60	70
1	B	551/592 (93%)	536 (97%)	15 (3%)	52	62
1	C	547/592 (92%)	536 (98%)	11 (2%)	63	74
1	D	547/592 (92%)	531 (97%)	16 (3%)	50	59
All	All	2191/2368 (92%)	2137 (98%)	54 (2%)	55	65

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	D	602	LEU
1	D	673	LEU

Some 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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	A	175	1,2	11,13,14	2.74	5 (45%)	13,18,20	3.28	3 (23%)
1	MDO	B	175	1,2	11,13,14	2.68	5 (45%)	13,18,20	3.13	3 (23%)
1	MDO	C	175	1,2	11,13,14	2.77	5 (45%)	13,18,20	3.18	3 (23%)
1	MDO	D	175	1,2	11,13,14	2.80	5 (45%)	13,18,20	2.58	3 (23%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	MDO	C2-N3	-3.55	1.32	1.39
1	B	175	MDO	C2-N3	-3.39	1.32	1.39
1	D	175	MDO	C2-N3	-3.38	1.32	1.39
1	A	175	MDO	C2-N3	-3.26	1.32	1.39
1	B	175	MDO	CA2-N2	-2.51	1.33	1.39
1	C	175	MDO	CA2-N2	-2.39	1.33	1.39
1	A	175	MDO	CA2-N2	-2.25	1.34	1.39
1	D	175	MDO	CA2-N2	-2.18	1.34	1.39
1	D	175	MDO	CA-C1	2.74	1.55	1.51
1	B	175	MDO	CA-C1	3.08	1.55	1.51
1	A	175	MDO	CA-C1	3.15	1.55	1.51
1	C	175	MDO	CA-C1	3.50	1.56	1.51
1	A	175	MDO	O-C	3.61	1.43	1.19
1	C	175	MDO	O-C	3.63	1.43	1.19
1	B	175	MDO	O-C	3.66	1.43	1.19
1	D	175	MDO	O-C	3.74	1.44	1.19
1	B	175	MDO	O2-C2	5.79	1.35	1.23
1	C	175	MDO	O2-C2	5.91	1.35	1.23
1	A	175	MDO	O2-C2	6.24	1.36	1.23
1	D	175	MDO	O2-C2	6.45	1.36	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	MDO	O2-C2-CA2	-8.98	126.10	130.95
1	C	175	MDO	O2-C2-CA2	-7.62	126.83	130.95
1	B	175	MDO	O2-C2-CA2	-7.15	127.09	130.95
1	D	175	MDO	O2-C2-CA2	-4.94	128.28	130.95
1	C	175	MDO	N3-C1-N2	-2.69	109.48	111.56
1	D	175	MDO	N3-C1-N2	-2.58	109.56	111.56
1	B	175	MDO	N3-C1-N2	-2.53	109.60	111.56
1	A	175	MDO	N3-C1-N2	-2.12	109.92	111.56
1	D	175	MDO	CA2-C2-N3	7.01	107.05	103.39
1	A	175	MDO	CA2-C2-N3	7.11	107.11	103.39
1	B	175	MDO	CA2-C2-N3	7.97	107.56	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	175	MDO	CA2-C2-N3	7.98	107.56	103.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	MDO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	1089	1	3,3,3	0.71	0	2,2,2	0.18	0
2	BME	A	1175	1	3,3,3	0.65	0	2,2,2	0.17	0
3	FMT	A	1679	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BME	B	1089	1	3,3,3	0.81	0	2,2,2	0.27	0
2	BME	B	1175	1	3,3,3	0.68	0	2,2,2	0.28	0
4	GOL	B	1679	-	5,5,5	0.36	0	5,5,5	0.34	0
3	FMT	B	1680	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BME	C	1089	1	3,3,3	0.54	0	2,2,2	0.14	0
2	BME	C	1175	1	3,3,3	0.61	0	2,2,2	0.22	0
3	FMT	C	1680	-	0,2,2	0.00	-	0,1,1	0.00	-
2	BME	D	1089	1	3,3,3	0.65	0	2,2,2	0.19	0
2	BME	D	1175	1	3,3,3	0.65	0	2,2,2	0.24	0
3	FMT	D	1679	-	0,2,2	0.00	-	0,1,1	0.00	-

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	1089	1	-	0/1/1/1	0/0/0/0
2	BME	A	1175	1	-	0/1/1/1	0/0/0/0
3	FMT	A	1679	-	-	0/0/0/0	0/0/0/0
2	BME	B	1089	1	-	0/1/1/1	0/0/0/0
2	BME	B	1175	1	-	0/1/1/1	0/0/0/0
4	GOL	B	1679	-	-	0/4/4/4	0/0/0/0
3	FMT	B	1680	-	-	0/0/0/0	0/0/0/0
2	BME	C	1089	1	-	0/1/1/1	0/0/0/0
2	BME	C	1175	1	-	0/1/1/1	0/0/0/0
3	FMT	C	1680	-	-	0/0/0/0	0/0/0/0
2	BME	D	1089	1	-	0/1/1/1	0/0/0/0
2	BME	D	1175	1	-	0/1/1/1	0/0/0/0
3	FMT	D	1679	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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
3	C	1680	FMT	1	0
2	D	1175	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	643/705 (91%)	0.24	36 (5%) 28 30	16, 31, 54, 67	0
1	B	649/705 (92%)	0.29	32 (4%) 33 36	17, 32, 47, 68	0
1	C	645/705 (91%)	0.16	25 (3%) 43 45	16, 30, 47, 61	0
1	D	644/705 (91%)	0.24	31 (4%) 34 36	17, 31, 54, 71	0
All	All	2581/2820 (91%)	0.23	124 (4%) 34 36	16, 31, 50, 71	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLN	6.0
1	B	571	GLY	4.7
1	D	576	THR	4.6
1	B	570	ASP	4.6
1	C	678	GLY	4.6
1	A	520	LEU	4.6
1	D	57	GLN	4.3
1	D	56	GLU	4.3
1	B	56	GLU	4.2
1	B	572	ILE	4.1
1	D	577	LEU	4.1
1	A	576	THR	4.1
1	A	584	PHE	3.9
1	A	566	LEU	3.8
1	A	589	SER	3.8
1	B	202	ASP	3.8
1	C	591	ARG	3.7
1	C	573	GLU	3.7
1	B	574	THR	3.7
1	A	202	ASP	3.7
1	A	564	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	573	GLU	3.7
1	C	569	LYS	3.6
1	D	574	THR	3.6
1	B	573	GLU	3.6
1	A	47	HIS	3.3
1	A	523	ASP	3.3
1	B	75	ASP	3.3
1	D	451	VAL	3.3
1	D	605	LYS	3.2
1	B	523	ASP	3.2
1	D	591	ARG	3.2
1	A	581	LEU	3.2
1	A	522	ASN	3.1
1	B	567	HIS	3.0
1	C	574	THR	3.0
1	C	677	LEU	3.0
1	A	519	GLY	3.0
1	A	605	LYS	3.0
1	A	451	VAL	3.0
1	A	568	LYS	3.0
1	B	55	ALA	3.0
1	C	576	THR	2.9
1	C	586	LYS	2.9
1	D	586	LYS	2.9
1	A	57	GLN	2.9
1	A	447	VAL	2.9
1	B	677	LEU	2.8
1	A	580	ARG	2.8
1	A	121	VAL	2.8
1	C	451	VAL	2.8
1	D	564	LEU	2.8
1	B	447	VAL	2.7
1	B	589	SER	2.7
1	C	568	LYS	2.7
1	A	567	HIS	2.7
1	D	467	ILE	2.7
1	C	590	ASP	2.6
1	D	202	ASP	2.6
1	A	565	ALA	2.6
1	A	56	GLU	2.6
1	A	518	CYS	2.6
1	B	8	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	579	ASP	2.6
1	A	217	ARG	2.5
1	B	12	LYS	2.5
1	B	25	LYS	2.5
1	B	121	VAL	2.5
1	A	590	ASP	2.5
1	A	577	LEU	2.5
1	D	602	LEU	2.5
1	C	522	ASN	2.5
1	D	443	LEU	2.5
1	B	569	LYS	2.5
1	D	581	LEU	2.5
1	D	447	VAL	2.5
1	C	217	ARG	2.5
1	C	12	LYS	2.4
1	A	514	LEU	2.4
1	D	461	ILE	2.4
1	D	589	SER	2.4
1	B	437	SER	2.3
1	B	576	THR	2.3
1	B	565	ALA	2.3
1	D	578	VAL	2.3
1	A	449	THR	2.3
1	D	582	ALA	2.3
1	C	581	LEU	2.3
1	D	464	LEU	2.3
1	C	589	SER	2.2
1	A	591	ARG	2.2
1	B	449	THR	2.2
1	A	515	ALA	2.2
1	C	579	ASP	2.2
1	C	443	LEU	2.2
1	B	451	VAL	2.2
1	B	58	CYS	2.2
1	D	442	TYR	2.2
1	B	444	ALA	2.2
1	C	434	ALA	2.2
1	B	442	TYR	2.1
1	D	446	PRO	2.1
1	A	586	LYS	2.1
1	A	562	THR	2.1
1	D	646	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	114	THR	2.1
1	D	448	THR	2.1
1	A	575	ASP	2.1
1	C	395	PHE	2.1
1	D	590	ASP	2.1
1	B	203	VAL	2.1
1	A	526	ALA	2.1
1	A	674	GLN	2.1
1	B	33	THR	2.1
1	D	513	THR	2.0
1	C	587	ARG	2.0
1	C	674	GLN	2.0
1	C	438	SER	2.0
1	B	26	LYS	2.0
1	C	580	ARG	2.0
1	C	584	PHE	2.0
1	D	567	HIS	2.0
1	D	173	VAL	2.0
1	B	467	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	MDO	A	175	13/14	0.93	0.12	-	22,24,27,32	0
1	MDO	B	175	13/14	0.92	0.13	-	26,27,31,35	0
1	MDO	C	175	13/14	0.94	0.13	-	22,24,27,32	0
1	MDO	D	175	13/14	0.93	0.15	-	22,23,26,31	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	BME	C	1175	4/4	0.91	0.16	1.73	41,43,43,43	0
2	BME	D	1175	4/4	0.85	0.17	1.49	43,44,44,44	0
2	BME	B	1175	4/4	0.87	0.16	1.46	45,45,46,46	0
3	FMT	B	1680	3/3	0.96	0.14	0.96	43,43,43,44	0
2	BME	A	1089	4/4	0.94	0.13	0.37	33,34,35,35	0
3	FMT	A	1679	3/3	0.97	0.12	-0.05	31,31,32,33	0
2	BME	C	1089	4/4	0.95	0.13	-0.06	31,31,32,34	0
4	GOL	B	1679	6/6	0.93	0.10	-0.19	37,38,38,39	0
2	BME	A	1175	4/4	0.94	0.13	-0.24	43,43,43,43	0
3	FMT	C	1680	3/3	0.95	0.10	-0.40	37,37,37,38	0
2	BME	B	1089	4/4	0.97	0.11	-0.48	39,39,39,40	0
2	BME	D	1089	4/4	0.94	0.10	-1.07	30,31,32,34	0
3	FMT	D	1679	3/3	0.97	0.09	-2.06	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.