Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 09:36 am GMT

PDB ID	:	5N6U
Title	:	Crystal structure of Beta-D-Mannosidase from Dictyoglomus thermophilum.
Authors	:	Richet, N.; Lafite, P.
Deposited on	:	2017-02-16
Resolution	:	3.08 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:

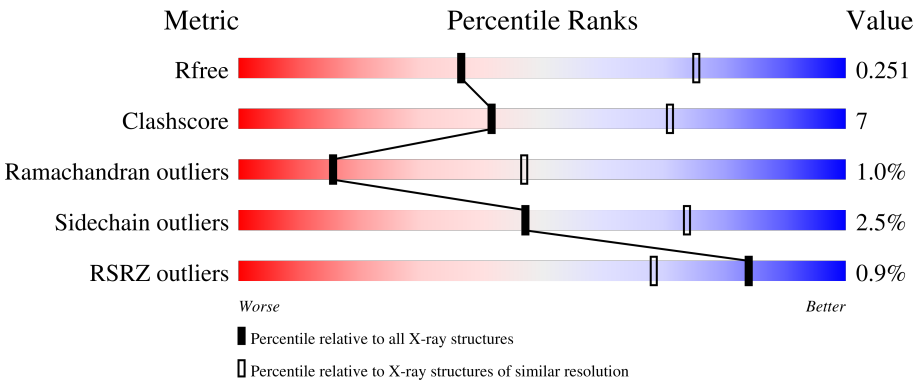
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	836	% 80% 15% • •
1	B	836	% 79% 17% • •
1	C	836	% 77% 18% • •
1	D	836	79% 15% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27265 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 Beta-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	811	6800	4431	1129	1224	16	0	0	0
1	B	811	6800	4431	1129	1224	16	0	0	0
1	C	811	6800	4431	1129	1224	16	0	0	0
1	D	811	6800	4431	1129	1224	16	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP B5YAN4
A	-21	GLY	-	expression tag	UNP B5YAN4
A	-20	SER	-	expression tag	UNP B5YAN4
A	-19	SER	-	expression tag	UNP B5YAN4
A	-18	HIS	-	expression tag	UNP B5YAN4
A	-17	HIS	-	expression tag	UNP B5YAN4
A	-16	HIS	-	expression tag	UNP B5YAN4
A	-15	HIS	-	expression tag	UNP B5YAN4
A	-14	HIS	-	expression tag	UNP B5YAN4
A	-13	HIS	-	expression tag	UNP B5YAN4
A	-12	SER	-	expression tag	UNP B5YAN4
A	-11	SER	-	expression tag	UNP B5YAN4
A	-10	GLY	-	expression tag	UNP B5YAN4
A	-9	LEU	-	expression tag	UNP B5YAN4
A	-8	VAL	-	expression tag	UNP B5YAN4
A	-7	PRO	-	expression tag	UNP B5YAN4
A	-6	ARG	-	expression tag	UNP B5YAN4
A	-5	GLY	-	expression tag	UNP B5YAN4
A	-4	SER	-	expression tag	UNP B5YAN4
A	-3	HIS	-	expression tag	UNP B5YAN4
A	-2	MET	-	expression tag	UNP B5YAN4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP B5YAN4
A	0	SER	-	expression tag	UNP B5YAN4
A	425	CYS	GLU	engineered mutation	UNP B5YAN4
B	-22	MET	-	initiating methionine	UNP B5YAN4
B	-21	GLY	-	expression tag	UNP B5YAN4
B	-20	SER	-	expression tag	UNP B5YAN4
B	-19	SER	-	expression tag	UNP B5YAN4
B	-18	HIS	-	expression tag	UNP B5YAN4
B	-17	HIS	-	expression tag	UNP B5YAN4
B	-16	HIS	-	expression tag	UNP B5YAN4
B	-15	HIS	-	expression tag	UNP B5YAN4
B	-14	HIS	-	expression tag	UNP B5YAN4
B	-13	HIS	-	expression tag	UNP B5YAN4
B	-12	SER	-	expression tag	UNP B5YAN4
B	-11	SER	-	expression tag	UNP B5YAN4
B	-10	GLY	-	expression tag	UNP B5YAN4
B	-9	LEU	-	expression tag	UNP B5YAN4
B	-8	VAL	-	expression tag	UNP B5YAN4
B	-7	PRO	-	expression tag	UNP B5YAN4
B	-6	ARG	-	expression tag	UNP B5YAN4
B	-5	GLY	-	expression tag	UNP B5YAN4
B	-4	SER	-	expression tag	UNP B5YAN4
B	-3	HIS	-	expression tag	UNP B5YAN4
B	-2	MET	-	expression tag	UNP B5YAN4
B	-1	ALA	-	expression tag	UNP B5YAN4
B	0	SER	-	expression tag	UNP B5YAN4
B	425	CYS	GLU	engineered mutation	UNP B5YAN4
C	-22	MET	-	initiating methionine	UNP B5YAN4
C	-21	GLY	-	expression tag	UNP B5YAN4
C	-20	SER	-	expression tag	UNP B5YAN4
C	-19	SER	-	expression tag	UNP B5YAN4
C	-18	HIS	-	expression tag	UNP B5YAN4
C	-17	HIS	-	expression tag	UNP B5YAN4
C	-16	HIS	-	expression tag	UNP B5YAN4
C	-15	HIS	-	expression tag	UNP B5YAN4
C	-14	HIS	-	expression tag	UNP B5YAN4
C	-13	HIS	-	expression tag	UNP B5YAN4
C	-12	SER	-	expression tag	UNP B5YAN4
C	-11	SER	-	expression tag	UNP B5YAN4
C	-10	GLY	-	expression tag	UNP B5YAN4
C	-9	LEU	-	expression tag	UNP B5YAN4
C	-8	VAL	-	expression tag	UNP B5YAN4

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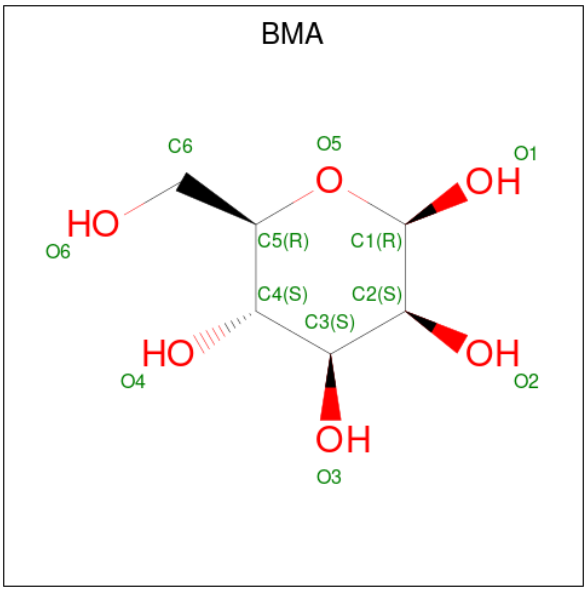
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP B5YAN4
C	-6	ARG	-	expression tag	UNP B5YAN4
C	-5	GLY	-	expression tag	UNP B5YAN4
C	-4	SER	-	expression tag	UNP B5YAN4
C	-3	HIS	-	expression tag	UNP B5YAN4
C	-2	MET	-	expression tag	UNP B5YAN4
C	-1	ALA	-	expression tag	UNP B5YAN4
C	0	SER	-	expression tag	UNP B5YAN4
C	425	CYS	GLU	engineered mutation	UNP B5YAN4
D	-22	MET	-	initiating methionine	UNP B5YAN4
D	-21	GLY	-	expression tag	UNP B5YAN4
D	-20	SER	-	expression tag	UNP B5YAN4
D	-19	SER	-	expression tag	UNP B5YAN4
D	-18	HIS	-	expression tag	UNP B5YAN4
D	-17	HIS	-	expression tag	UNP B5YAN4
D	-16	HIS	-	expression tag	UNP B5YAN4
D	-15	HIS	-	expression tag	UNP B5YAN4
D	-14	HIS	-	expression tag	UNP B5YAN4
D	-13	HIS	-	expression tag	UNP B5YAN4
D	-12	SER	-	expression tag	UNP B5YAN4
D	-11	SER	-	expression tag	UNP B5YAN4
D	-10	GLY	-	expression tag	UNP B5YAN4
D	-9	LEU	-	expression tag	UNP B5YAN4
D	-8	VAL	-	expression tag	UNP B5YAN4
D	-7	PRO	-	expression tag	UNP B5YAN4
D	-6	ARG	-	expression tag	UNP B5YAN4
D	-5	GLY	-	expression tag	UNP B5YAN4
D	-4	SER	-	expression tag	UNP B5YAN4
D	-3	HIS	-	expression tag	UNP B5YAN4
D	-2	MET	-	expression tag	UNP B5YAN4
D	-1	ALA	-	expression tag	UNP B5YAN4
D	0	SER	-	expression tag	UNP B5YAN4
D	425	CYS	GLU	engineered mutation	UNP B5YAN4

- Molecule 2 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	11	6	5	0	0
			Total	C	O		
2	B	1	11	6	5	0	0
			Total	C	O		
2	C	1	11	6	5	0	0
			Total	C	O		
2	D	1	11	6	5	0	0

- Molecule 3 is water.

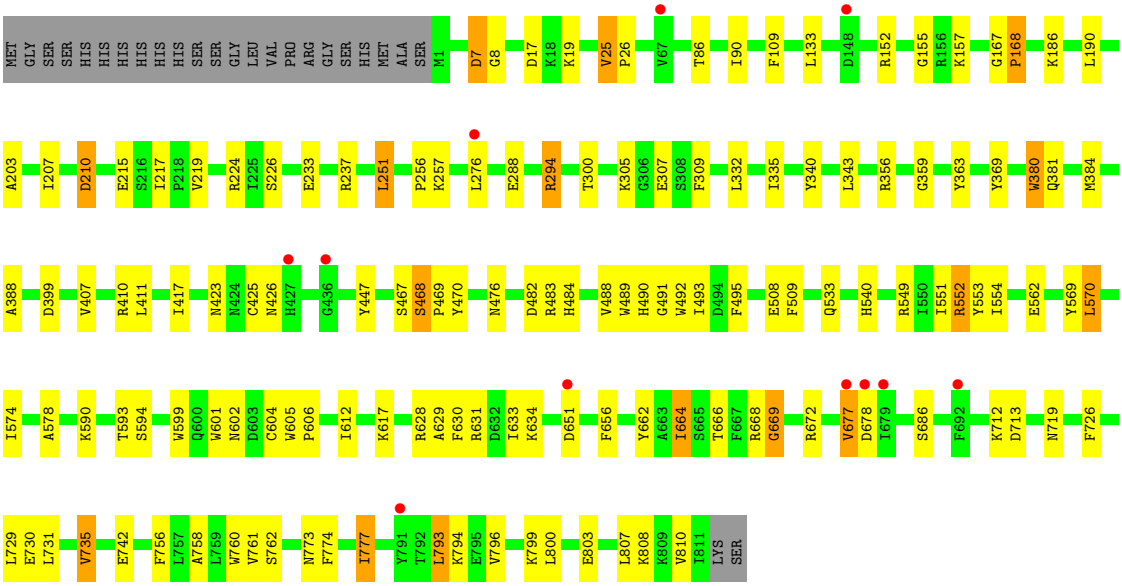
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
			Total	O		
3	B	4	4	4	0	0
			Total	O		
3	C	10	10	10	0	0
			Total	O		
3	D	5	5	5	0	0

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.

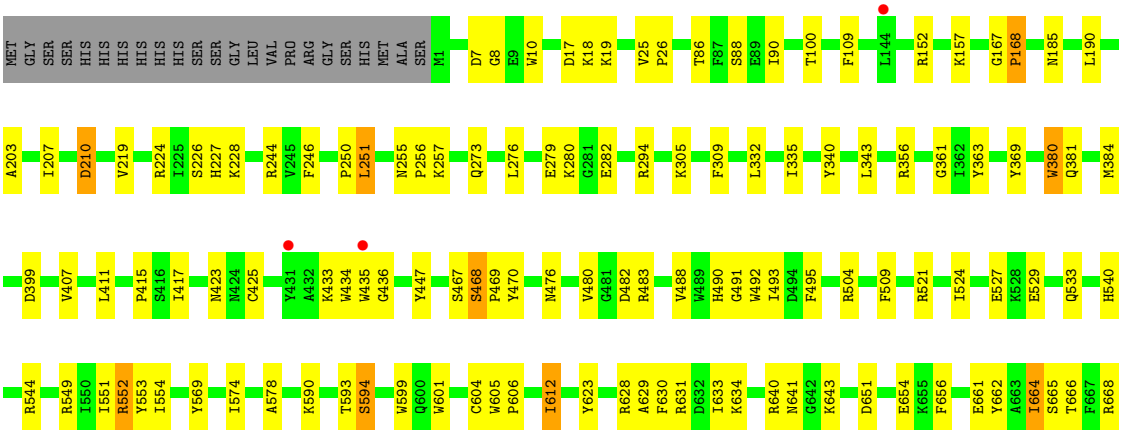
• Molecule 1: Beta-mannosidase

Chain A:



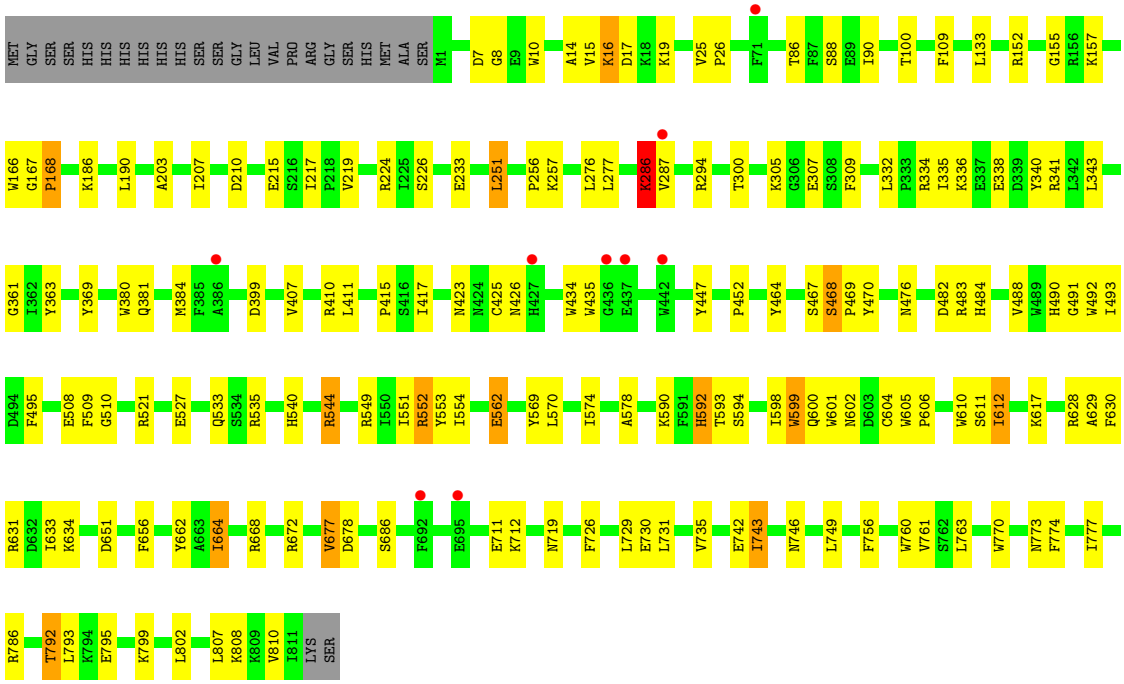
• Molecule 1: Beta-mannosidase

Chain B:



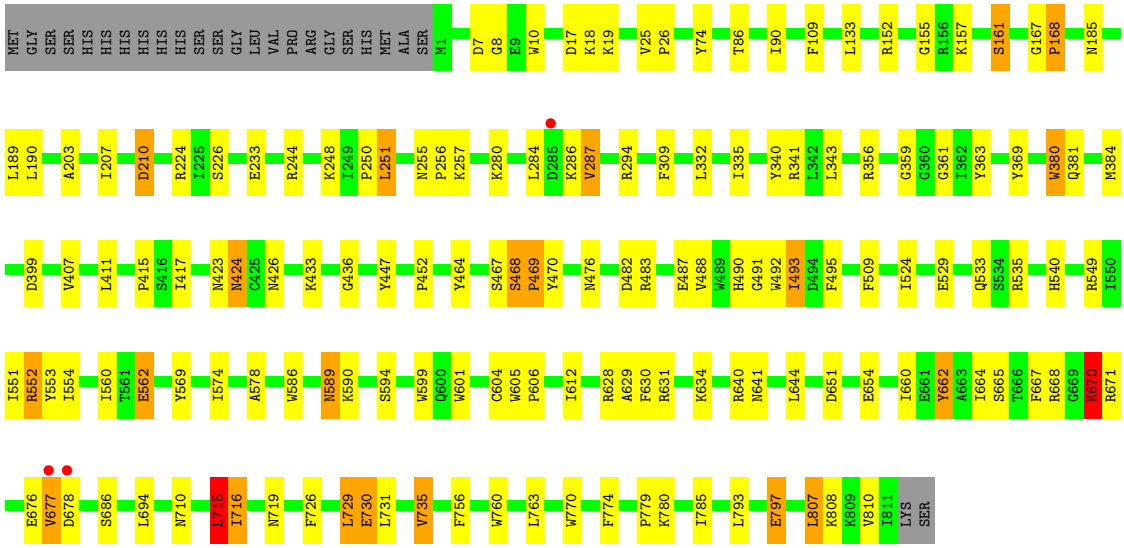
• Molecule 1: Beta-mannosidase

Chain C:



• Molecule 1: Beta-mannosidase

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	139.25Å 75.56Å 217.88Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	49.50 – 3.08 48.48 – 3.19	Depositor EDS
% Data completeness (in resolution range)	88.2 (49.50-3.08) 98.9 (48.48-3.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.204 , 0.255 0.203 , 0.251	Depositor DCC
R_{free} test set	3775 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	81.8	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
Reported twinning fraction	0.913 for H, K, L 0.087 for -h,-k,l	Depositor
Outliers	4 of 75507 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27265	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: BMA

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	0.59	0/6995	0.86	10/9461 (0.1%)
1	B	0.60	0/6995	0.89	13/9461 (0.1%)
1	C	0.61	1/6995 (0.0%)	0.90	16/9461 (0.2%)
1	D	0.62	0/6995	0.91	18/9461 (0.2%)
All	All	0.60	1/27980 (0.0%)	0.89	57/37844 (0.2%)

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	7
1	B	0	7
1	C	0	4
1	D	0	6
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	599	TRP	CG-CD1	6.09	1.45	1.36

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	334	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	C	334	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	C	802	LEU	CA-CB-CG	9.51	137.17	115.30
1	B	552	ARG	NE-CZ-NH1	-8.93	115.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	552	ARG	NE-CZ-NH2	8.49	124.54	120.30
1	C	599	TRP	CA-CB-CG	-7.89	98.71	113.70
1	D	640	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	D	729	LEU	CA-CB-CG	-7.33	98.45	115.30
1	C	277	LEU	CA-CB-CG	7.15	131.74	115.30
1	D	715	LEU	C-N-CA	-6.75	104.84	121.70
1	B	640	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	343	LEU	CB-CG-CD1	6.43	121.93	111.00
1	D	343	LEU	CB-CG-CD1	6.39	121.86	111.00
1	D	662	TYR	CA-CB-CG	6.34	125.44	113.40
1	B	491	GLY	N-CA-C	-6.33	97.27	113.10
1	B	694	LEU	CA-CB-CG	6.24	129.66	115.30
1	B	544	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	544	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	640	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	491	GLY	N-CA-C	-5.99	98.12	113.10
1	D	552	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	552	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	491	GLY	N-CA-C	-5.89	98.38	113.10
1	B	737	VAL	CA-CB-CG1	5.88	119.73	110.90
1	D	535	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	589	ASN	CB-CA-C	-5.82	98.76	110.40
1	D	552	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	424	ASN	CB-CA-C	5.60	121.59	110.40
1	C	552	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	672	ARG	N-CA-C	5.57	126.03	111.00
1	D	341	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	286	LYS	N-CA-C	-5.54	96.04	111.00
1	B	794	LYS	CB-CG-CD	5.54	126.00	111.60
1	C	491	GLY	N-CA-C	-5.49	99.38	113.10
1	D	670	LYS	CA-CB-CG	5.46	125.42	113.40
1	D	716	ILE	N-CA-CB	5.45	123.33	110.80
1	A	410	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	662	TYR	CB-CA-C	5.43	121.25	110.40
1	C	599	TRP	N-CA-CB	5.42	120.35	110.60
1	D	640	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	712	LYS	CA-CB-CG	5.40	125.28	113.40
1	C	410	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	535	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	161	SER	N-CA-CB	5.33	118.50	110.50
1	A	288	GLU	N-CA-CB	5.29	120.12	110.60
1	A	793	LEU	CB-CG-CD1	5.27	119.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	786	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	294	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	294	ARG	CG-CD-NE	-5.25	100.77	111.80
1	A	777	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	B	594	SER	N-CA-C	5.22	125.10	111.00
1	C	341	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	C	277	LEU	CB-CG-CD1	5.17	119.80	111.00
1	D	671	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	294	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	C	434	TRP	N-CA-C	5.05	124.64	111.00
1	A	570	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	VAL	Peptide
1	A	257	LYS	Peptide
1	A	468	SER	Peptide
1	A	669	GLY	Peptide
1	A	713	ASP	Peptide
1	A	799	LYS	Peptide
1	A	807	LEU	Peptide
1	B	227	HIS	Mainchain,Peptide
1	B	228	LYS	Peptide
1	B	257	LYS	Peptide
1	B	468	SER	Peptide
1	B	671	ARG	Peptide
1	B	799	LYS	Peptide
1	C	257	LYS	Peptide
1	C	286	LYS	Peptide
1	C	468	SER	Peptide
1	C	807	LEU	Peptide
1	D	257	LYS	Peptide
1	D	287	VAL	Peptide
1	D	468	SER	Peptide
1	D	670	LYS	Peptide
1	D	715	LEU	Peptide
1	D	807	LEU	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	6800	0	6675	87	1
1	B	6800	0	6675	89	2
1	C	6800	0	6675	112	10
1	D	6800	0	6675	99	2
2	A	11	0	10	0	0
2	B	11	0	10	0	0
2	C	11	0	10	0	0
2	D	11	0	10	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
All	All	27265	0	26740	378	13

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 7.

All (378) 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:305:LYS:HE2	1:C:592:HIS:CE1	1.85	1.11
1:B:590:LYS:NZ	1:B:651:ASP:OD1	2.01	0.94
1:A:590:LYS:NZ	1:A:651:ASP:OD1	2.01	0.94
1:C:600:GLN:HG3	1:C:610:TRP:O	1.66	0.94
1:D:590:LYS:NZ	1:D:651:ASP:OD1	2.02	0.93
1:C:590:LYS:NZ	1:C:651:ASP:OD1	2.01	0.92
1:C:10:TRP:CD1	1:C:25:VAL:HG22	2.07	0.89
1:B:10:TRP:CD1	1:B:25:VAL:HG22	2.08	0.88
1:A:388:ALA:O	1:A:426:ASN:ND2	2.07	0.88
1:B:643:LYS:NZ	1:B:691:GLU:OE2	2.06	0.87
1:D:10:TRP:CD1	1:D:25:VAL:HG22	2.10	0.86
1:C:743:ILE:HD11	1:C:749:LEU:HB2	1.61	0.81
1:B:488:VAL:O	1:B:553:TYR:OH	2.00	0.80
1:C:488:VAL:O	1:C:553:TYR:OH	2.00	0.80
1:C:305:LYS:HE2	1:C:592:HIS:ND1	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:O	1:A:553:TYR:OH	1.99	0.78
1:D:488:VAL:O	1:D:553:TYR:OH	2.00	0.78
1:C:166:TRP:NE1	1:C:599:TRP:HH2	1.82	0.78
1:A:599:TRP:O	1:A:599:TRP:CD2	2.38	0.76
1:C:599:TRP:CG	1:C:599:TRP:O	2.40	0.75
1:B:599:TRP:CD2	1:B:599:TRP:O	2.39	0.75
1:D:726:PHE:HA	1:D:729:LEU:HD12	1.68	0.75
1:D:715:LEU:O	1:D:716:ILE:C	2.24	0.74
1:D:694:LEU:HD12	1:D:694:LEU:O	1.88	0.74
1:B:604:CYS:HG	1:B:605:TRP:HD1	1.36	0.73
1:C:305:LYS:CE	1:C:592:HIS:CE1	2.68	0.73
1:D:599:TRP:CD2	1:D:599:TRP:O	2.41	0.72
1:C:599:TRP:O	1:C:599:TRP:CD2	2.43	0.72
1:B:86:THR:CG2	1:B:157:LYS:HB3	2.21	0.71
1:B:599:TRP:O	1:B:599:TRP:CG	2.44	0.71
1:A:25:VAL:HG13	1:A:26:PRO:HD3	1.73	0.70
1:C:10:TRP:CD1	1:C:25:VAL:CG2	2.74	0.70
1:C:86:THR:CG2	1:C:157:LYS:HB3	2.22	0.70
1:A:86:THR:CG2	1:A:157:LYS:HB3	2.21	0.70
1:D:86:THR:CG2	1:D:157:LYS:HB3	2.21	0.69
1:A:224:ARG:HG2	1:A:233:GLU:HG2	1.73	0.69
1:C:604:CYS:HG	1:C:605:TRP:HD1	1.40	0.69
1:D:599:TRP:O	1:D:599:TRP:CG	2.45	0.69
1:A:599:TRP:O	1:A:599:TRP:CG	2.45	0.69
1:A:167:GLY:HA2	1:A:605:TRP:HE1	1.59	0.68
1:A:758:ALA:HB3	1:A:777:ILE:HG13	1.75	0.68
1:B:10:TRP:CD1	1:B:25:VAL:CG2	2.74	0.68
1:D:763:LEU:HD23	1:D:770:TRP:CZ3	2.28	0.68
1:B:665:SER:HB2	1:B:670:LYS:HA	1.75	0.68
1:C:332:LEU:O	1:C:335:ILE:HG12	1.94	0.68
1:A:332:LEU:O	1:A:335:ILE:HG12	1.94	0.68
1:D:10:TRP:CD1	1:D:25:VAL:CG2	2.76	0.68
1:D:715:LEU:CD1	1:D:785:ILE:HG22	2.25	0.67
1:B:332:LEU:O	1:B:335:ILE:HG12	1.95	0.66
1:C:167:GLY:HA2	1:C:605:TRP:HE1	1.60	0.66
1:D:335:ILE:HD13	1:D:340:TYR:CE2	2.31	0.66
1:A:604:CYS:HG	1:A:605:TRP:HD1	1.43	0.66
1:C:598:ILE:HG22	1:C:600:GLN:H	1.60	0.66
1:B:167:GLY:HA2	1:B:605:TRP:HE1	1.61	0.65
1:C:763:LEU:HD23	1:C:770:TRP:CZ3	2.32	0.65
1:D:601:TRP:CZ3	1:D:612:ILE:HD11	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:TRP:CH2	1:C:612:ILE:HD11	2.32	0.64
1:C:761:VAL:CG2	1:C:777:ILE:HD11	2.28	0.64
1:D:644:LEU:HD13	1:D:694:LEU:HD21	1.78	0.64
1:D:167:GLY:HA2	1:D:605:TRP:HE1	1.61	0.64
1:B:733:ASN:HB3	1:B:808:LYS:HG3	1.77	0.64
1:C:601:TRP:CZ3	1:C:612:ILE:HD11	2.33	0.64
1:B:661:GLU:HG2	1:B:676:GLU:HG2	1.81	0.63
1:B:601:TRP:CZ3	1:B:612:ILE:HD11	2.34	0.63
1:A:305:LYS:HG3	1:A:305:LYS:O	1.99	0.63
1:A:8:GLY:O	1:A:25:VAL:HG12	1.98	0.63
1:B:569:TYR:OH	1:B:760:TRP:HB2	1.99	0.62
1:C:86:THR:HG21	1:C:157:LYS:HD2	1.81	0.62
1:B:86:THR:HG21	1:B:157:LYS:HD2	1.80	0.62
1:D:424:ASN:O	1:D:469:PRO:HD2	1.99	0.62
1:A:601:TRP:CZ3	1:A:612:ILE:HD11	2.35	0.62
1:D:369:TYR:OH	1:D:381:GLN:NE2	2.32	0.62
1:A:86:THR:HG21	1:A:157:LYS:HD2	1.79	0.62
1:D:86:THR:HG21	1:D:157:LYS:HB3	1.81	0.62
1:B:86:THR:HG21	1:B:157:LYS:HB3	1.81	0.62
1:D:601:TRP:CH2	1:D:612:ILE:HD11	2.35	0.62
1:D:604:CYS:HG	1:D:605:TRP:HD1	1.47	0.62
1:C:305:LYS:O	1:C:305:LYS:HG3	1.99	0.61
1:A:86:THR:HG21	1:A:157:LYS:HB3	1.81	0.61
1:A:601:TRP:CH2	1:A:612:ILE:HD11	2.36	0.61
1:B:369:TYR:OH	1:B:381:GLN:NE2	2.33	0.61
1:C:224:ARG:HB3	1:C:233:GLU:HG2	1.82	0.61
1:B:601:TRP:CH2	1:B:612:ILE:HD11	2.35	0.61
1:D:284:LEU:HD11	1:D:286:LYS:HB2	1.83	0.60
1:D:715:LEU:HD11	1:D:785:ILE:HG22	1.82	0.60
1:C:86:THR:HG21	1:C:157:LYS:HB3	1.81	0.60
1:D:86:THR:HG21	1:D:157:LYS:HD2	1.81	0.60
1:B:794:LYS:O	1:B:794:LYS:HG2	2.00	0.60
1:D:294:ARG:HE	1:D:415:PRO:HA	1.66	0.60
1:D:332:LEU:O	1:D:335:ILE:HG13	2.01	0.60
1:B:305:LYS:O	1:B:305:LYS:HG3	2.01	0.60
1:C:369:TYR:OH	1:C:381:GLN:NE2	2.35	0.60
1:C:544:ARG:HG2	3:C:1005:HOH:O	2.02	0.59
1:C:25:VAL:HB	1:C:26:PRO:HD3	1.84	0.59
1:C:88:SER:HG	1:C:100:THR:HG1	1.44	0.59
1:C:773:ASN:OD1	1:C:774:PHE:N	2.36	0.59
1:A:369:TYR:OH	1:A:381:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ARG:O	1:D:250:PRO:HG3	2.03	0.58
1:C:8:GLY:O	1:C:25:VAL:HG23	2.04	0.58
1:B:25:VAL:HB	1:B:26:PRO:HD3	1.86	0.58
1:A:7:ASP:HA	1:A:25:VAL:HG11	1.86	0.57
1:B:8:GLY:O	1:B:25:VAL:HG23	2.04	0.57
1:C:664:ILE:HG23	1:C:672:ARG:HB3	1.85	0.57
1:A:664:ILE:HG23	1:A:672:ARG:HB3	1.85	0.57
1:C:761:VAL:HG22	1:C:777:ILE:HD11	1.86	0.57
1:D:8:GLY:O	1:D:25:VAL:HG23	2.04	0.57
1:C:294:ARG:HE	1:C:415:PRO:HA	1.70	0.57
1:B:17:ASP:OD2	1:B:19:LYS:NZ	2.37	0.56
1:C:343:LEU:HD23	1:C:602:ASN:HB3	1.87	0.56
1:B:664:ILE:HG23	1:B:672:ARG:HB2	1.86	0.56
1:D:25:VAL:HB	1:D:26:PRO:HD3	1.88	0.56
1:A:90:ILE:HD11	1:A:109:PHE:CE2	2.41	0.56
1:C:600:GLN:HB2	1:C:611:SER:HA	1.88	0.56
1:B:294:ARG:HE	1:B:415:PRO:HA	1.69	0.56
1:D:17:ASP:OD2	1:D:19:LYS:NZ	2.37	0.56
1:A:343:LEU:HD23	1:A:602:ASN:HB3	1.87	0.55
1:A:668:ARG:HG2	1:A:756:PHE:CD1	2.41	0.55
1:B:504:ARG:O	1:B:593:THR:O	2.23	0.55
1:D:90:ILE:HD11	1:D:109:PHE:CE2	2.42	0.55
1:A:773:ASN:OD1	1:A:774:PHE:N	2.36	0.55
1:C:17:ASP:OD2	1:C:19:LYS:NZ	2.39	0.55
1:B:88:SER:HG	1:B:100:THR:HG1	1.43	0.55
1:C:668:ARG:HG2	1:C:756:PHE:CD1	2.41	0.55
1:A:8:GLY:N	1:A:25:VAL:CG1	2.70	0.55
1:B:90:ILE:HD11	1:B:109:PHE:CE2	2.42	0.55
1:C:590:LYS:O	1:C:593:THR:O	2.24	0.55
1:D:668:ARG:HG2	1:D:756:PHE:CD1	2.42	0.55
1:B:668:ARG:HG2	1:B:756:PHE:CD1	2.42	0.55
1:A:590:LYS:O	1:A:593:THR:O	2.25	0.55
1:C:90:ILE:HD11	1:C:109:PHE:CE2	2.42	0.55
1:D:424:ASN:O	1:D:468:SER:HB3	2.06	0.55
1:A:17:ASP:OD2	1:A:19:LYS:NZ	2.39	0.54
1:D:490:HIS:O	1:D:549:ARG:NH1	2.41	0.54
1:D:335:ILE:HD13	1:D:340:TYR:HE2	1.70	0.54
1:C:166:TRP:CD1	1:C:599:TRP:HH2	2.26	0.54
1:A:490:HIS:O	1:A:549:ARG:NH1	2.40	0.54
1:B:203:ALA:HB2	1:B:256:PRO:HG3	1.90	0.54
1:D:203:ALA:HB2	1:D:256:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:HIS:O	1:C:549:ARG:NH1	2.40	0.53
1:A:8:GLY:H	1:A:25:VAL:CG1	2.21	0.53
1:A:363:TYR:CZ	1:A:384:MET:HG2	2.44	0.53
1:B:363:TYR:CZ	1:B:384:MET:HG2	2.44	0.53
1:B:490:HIS:O	1:B:549:ARG:NH1	2.41	0.53
1:C:15:VAL:HG13	1:C:16:LYS:HD2	1.90	0.53
1:C:203:ALA:HB2	1:C:256:PRO:HG3	1.90	0.53
1:D:363:TYR:CZ	1:D:384:MET:HG2	2.44	0.53
1:B:733:ASN:CB	1:B:808:LYS:HG3	2.38	0.53
1:C:600:GLN:CG	1:C:610:TRP:O	2.49	0.53
1:D:224:ARG:HB3	1:D:233:GLU:HG3	1.90	0.53
1:D:488:VAL:HA	1:D:493:ILE:HG23	1.91	0.52
1:A:492:TRP:HE3	1:A:552:ARG:HD3	1.75	0.52
1:D:540:HIS:CD2	1:D:605:TRP:CZ3	2.97	0.52
1:C:735:VAL:HA	1:C:808:LYS:O	2.08	0.52
1:A:605:TRP:HB2	1:A:606:PRO:CD	2.40	0.52
1:A:726:PHE:HA	1:A:729:LEU:HD13	1.91	0.52
1:C:605:TRP:HB2	1:C:606:PRO:CD	2.40	0.52
1:A:203:ALA:HB2	1:A:256:PRO:HG3	1.91	0.52
1:B:726:PHE:HA	1:B:729:LEU:HD13	1.91	0.52
1:C:363:TYR:CZ	1:C:384:MET:HG2	2.45	0.52
1:A:735:VAL:HA	1:A:808:LYS:O	2.10	0.51
1:D:487:GLU:O	1:D:493:ILE:CG2	2.58	0.51
1:A:742:GLU:OE1	1:A:794:LYS:HD2	2.11	0.51
1:C:726:PHE:HA	1:C:729:LEU:HD13	1.92	0.51
1:C:286:LYS:O	1:C:287:VAL:C	2.48	0.51
1:A:677:VAL:HG12	1:A:678:ASP:H	1.76	0.50
1:C:540:HIS:CD2	1:C:605:TRP:CZ3	2.98	0.50
1:A:540:HIS:CD2	1:A:605:TRP:CZ3	3.00	0.50
1:C:562:GLU:HG2	1:D:562:GLU:HG2	1.92	0.50
1:D:284:LEU:CD1	1:D:286:LYS:HB2	2.42	0.50
1:D:677:VAL:HG12	1:D:678:ASP:H	1.76	0.50
1:C:677:VAL:HG12	1:C:678:ASP:H	1.76	0.50
1:D:509:PHE:O	1:D:599:TRP:N	2.45	0.50
1:B:629:ALA:HA	1:B:634:LYS:HE2	1.94	0.50
1:D:735:VAL:HA	1:D:808:LYS:O	2.12	0.50
1:C:749:LEU:HG	1:C:786:ARG:HG2	1.94	0.50
1:D:586:TRP:O	1:D:589:ASN:O	2.30	0.50
1:A:604:CYS:SG	1:A:605:TRP:HD1	2.35	0.49
1:D:411:LEU:HB3	1:D:417:ILE:CD1	2.42	0.49
1:D:730:GLU:HA	1:D:730:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:HIS:CD2	1:B:605:TRP:CZ3	3.00	0.49
1:B:628:ARG:NH2	1:B:774:PHE:O	2.44	0.49
1:C:423:ASN:HB3	1:C:447:TYR:CE1	2.47	0.49
1:C:509:PHE:O	1:C:599:TRP:N	2.44	0.49
1:C:742:GLU:HB2	1:C:793:LEU:CD1	2.42	0.49
1:B:604:CYS:SG	1:B:605:TRP:HD1	2.33	0.49
1:A:761:VAL:HG11	1:A:777:ILE:HD11	1.93	0.49
1:D:605:TRP:HB2	1:D:606:PRO:CD	2.42	0.49
1:A:423:ASN:HB3	1:A:447:TYR:CE1	2.48	0.49
1:D:604:CYS:SG	1:D:605:TRP:HD1	2.35	0.49
1:B:467:SER:HB3	1:B:470:TYR:HB2	1.95	0.49
1:B:605:TRP:HB2	1:B:606:PRO:CD	2.43	0.49
1:A:793:LEU:HD12	1:A:796:VAL:HG21	1.94	0.49
1:D:495:PHE:CD1	1:D:578:ALA:HA	2.48	0.48
1:C:335:ILE:HD12	1:C:340:TYR:OH	2.14	0.48
1:D:629:ALA:HA	1:D:634:LYS:HE2	1.96	0.48
1:B:411:LEU:HB3	1:B:417:ILE:CD1	2.43	0.48
1:C:411:LEU:HB3	1:C:417:ILE:CD1	2.43	0.48
1:B:335:ILE:HD12	1:B:340:TYR:OH	2.13	0.48
1:B:551:ILE:O	1:B:554:ILE:HG22	2.14	0.48
1:C:294:ARG:HG3	1:C:294:ARG:O	2.13	0.48
1:D:644:LEU:HD13	1:D:694:LEU:CD2	2.43	0.48
1:B:294:ARG:O	1:B:294:ARG:HG3	2.12	0.48
1:C:604:CYS:SG	1:C:605:TRP:HD1	2.36	0.48
1:A:629:ALA:HA	1:A:634:LYS:HE2	1.95	0.48
1:B:495:PHE:CD1	1:B:578:ALA:HA	2.49	0.48
1:C:629:ALA:HA	1:C:634:LYS:HE2	1.95	0.48
1:A:628:ARG:NH2	1:A:774:PHE:O	2.47	0.48
1:C:224:ARG:CB	1:C:233:GLU:HG2	2.44	0.48
1:D:467:SER:HB3	1:D:470:TYR:HB2	1.96	0.48
1:D:423:ASN:HB3	1:D:447:TYR:CE1	2.48	0.48
1:D:551:ILE:O	1:D:554:ILE:HG22	2.13	0.48
1:D:807:LEU:O	1:D:808:LYS:HG2	2.14	0.48
1:B:524:ILE:HD11	1:B:529:GLU:C	2.35	0.47
1:C:305:LYS:CE	1:C:592:HIS:ND1	2.74	0.47
1:C:540:HIS:CD2	1:C:605:TRP:HZ3	2.33	0.47
1:C:495:PHE:CD1	1:C:578:ALA:HA	2.49	0.47
1:B:279:GLU:O	1:B:279:GLU:HG3	2.14	0.47
1:C:452:PRO:HG3	1:C:464:TYR:CE2	2.50	0.47
1:D:294:ARG:O	1:D:294:ARG:HG3	2.14	0.47
1:A:294:ARG:O	1:A:294:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:HG11	1:B:276:LEU:HD11	1.97	0.47
1:B:509:PHE:O	1:B:599:TRP:N	2.45	0.47
1:C:335:ILE:HD12	1:C:340:TYR:CZ	2.50	0.47
1:C:628:ARG:NH2	1:C:774:PHE:O	2.48	0.47
1:C:729:LEU:O	1:C:731:LEU:N	2.48	0.47
1:A:411:LEU:HB3	1:A:417:ILE:CD1	2.44	0.47
1:B:794:LYS:O	1:B:794:LYS:CG	2.61	0.47
1:A:335:ILE:HD12	1:A:340:TYR:OH	2.14	0.47
1:C:215:GLU:HB2	1:C:217:ILE:HD11	1.97	0.47
1:D:74:TYR:CD1	1:D:185:ASN:OD1	2.68	0.47
1:A:492:TRP:CD1	1:B:492:TRP:HB2	2.50	0.47
1:D:628:ARG:NH2	1:D:774:PHE:O	2.48	0.47
1:A:335:ILE:HD12	1:A:340:TYR:CZ	2.50	0.46
1:C:219:VAL:HG11	1:C:276:LEU:HD11	1.96	0.46
1:A:219:VAL:HG11	1:A:276:LEU:HD11	1.97	0.46
1:A:551:ILE:O	1:A:554:ILE:HG22	2.15	0.46
1:B:335:ILE:HD12	1:B:340:TYR:CZ	2.50	0.46
1:B:423:ASN:HB3	1:B:447:TYR:CE1	2.49	0.46
1:C:508:GLU:CG	1:C:599:TRP:CD1	2.99	0.46
1:A:7:ASP:HA	1:A:25:VAL:CG1	2.44	0.46
1:A:509:PHE:O	1:A:599:TRP:N	2.45	0.46
1:D:540:HIS:CD2	1:D:605:TRP:HZ3	2.34	0.46
1:C:467:SER:HB3	1:C:470:TYR:HB2	1.97	0.46
1:C:551:ILE:O	1:C:554:ILE:HG22	2.15	0.46
1:C:600:GLN:CG	1:C:600:GLN:O	2.60	0.46
1:B:630:PHE:O	1:B:631:ARG:C	2.54	0.46
1:A:168:PRO:HD3	1:A:605:TRP:NE1	2.31	0.45
1:B:361:GLY:C	1:B:384:MET:HE2	2.36	0.45
1:C:336:LYS:HG3	1:C:338:GLU:HB2	1.99	0.45
1:A:729:LEU:O	1:A:731:LEU:N	2.49	0.45
1:C:361:GLY:C	1:C:384:MET:HE2	2.37	0.45
1:D:726:PHE:CA	1:D:729:LEU:HD12	2.44	0.45
1:B:468:SER:O	1:B:482:ASP:OD2	2.34	0.45
1:C:166:TRP:NE1	1:C:599:TRP:CH2	2.73	0.45
1:C:510:GLY:HA2	1:C:600:GLN:HE22	1.82	0.45
1:C:633:ILE:CD1	1:C:656:PHE:CG	3.00	0.45
1:A:215:GLU:HB2	1:A:217:ILE:HD11	1.97	0.45
1:D:665:SER:HA	1:D:670:LYS:HB3	1.98	0.45
1:A:633:ILE:CD1	1:A:656:PHE:CG	3.00	0.45
1:A:495:PHE:CD1	1:A:578:ALA:HA	2.51	0.45
1:A:666:THR:OG1	1:A:669:GLY:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ASN:O	1:A:483:ARG:NH1	2.49	0.45
1:B:670:LYS:HD3	1:B:779:PRO:HB2	1.98	0.45
1:C:168:PRO:HD3	1:C:605:TRP:NE1	2.32	0.45
1:D:667:PHE:HZ	1:D:729:LEU:HD22	1.81	0.45
1:A:309:PHE:O	1:A:594:SER:OG	2.35	0.45
1:A:468:SER:O	1:A:482:ASP:OD2	2.35	0.45
1:A:540:HIS:CD2	1:A:605:TRP:HZ3	2.35	0.45
1:C:468:SER:O	1:C:482:ASP:OD2	2.35	0.45
1:D:424:ASN:O	1:D:469:PRO:CD	2.64	0.45
1:C:166:TRP:CD1	1:C:599:TRP:CH2	3.05	0.45
1:C:476:ASN:O	1:C:483:ARG:NH1	2.49	0.45
1:D:361:GLY:C	1:D:384:MET:HE2	2.37	0.45
1:A:467:SER:HB3	1:A:470:TYR:HB2	1.99	0.45
1:B:309:PHE:O	1:B:594:SER:OG	2.35	0.45
1:C:343:LEU:HD11	1:C:617:LYS:HG2	1.98	0.45
1:B:476:ASN:O	1:B:483:ARG:NH1	2.49	0.44
1:D:468:SER:O	1:D:482:ASP:OD2	2.35	0.44
1:D:569:TYR:OH	1:D:760:TRP:HB2	2.17	0.44
1:B:521:ARG:NH1	1:B:527:GLU:OE1	2.51	0.44
1:B:623:TYR:CD1	1:B:623:TYR:C	2.90	0.44
1:B:729:LEU:O	1:B:731:LEU:N	2.50	0.44
1:C:309:PHE:O	1:C:594:SER:OG	2.35	0.44
1:D:309:PHE:O	1:D:594:SER:OG	2.35	0.44
1:D:524:ILE:HD11	1:D:529:GLU:C	2.38	0.44
1:A:569:TYR:OH	1:A:760:TRP:HB2	2.18	0.44
1:D:363:TYR:CE2	1:D:407:VAL:HG21	2.53	0.44
1:A:492:TRP:HB2	1:B:492:TRP:CD1	2.52	0.44
1:B:246:PHE:HB3	1:D:248:LYS:HB2	1.98	0.44
1:C:492:TRP:CD1	1:D:492:TRP:HB2	2.52	0.44
1:C:761:VAL:HG21	1:C:777:ILE:HD11	1.99	0.44
1:D:729:LEU:O	1:D:731:LEU:N	2.50	0.44
1:A:343:LEU:HD11	1:A:617:LYS:HG2	1.99	0.44
1:A:363:TYR:CE2	1:A:407:VAL:HG21	2.52	0.44
1:D:476:ASN:O	1:D:483:ARG:NH1	2.48	0.44
1:B:633:ILE:CD1	1:B:656:PHE:CG	3.01	0.43
1:D:710:ASN:HB2	1:D:716:ILE:HG21	1.99	0.43
1:B:168:PRO:HD3	1:B:605:TRP:NE1	2.32	0.43
1:A:359:GLY:C	1:A:384:MET:HE3	2.39	0.43
1:C:363:TYR:CE2	1:C:407:VAL:HG21	2.53	0.43
1:C:569:TYR:OH	1:C:760:TRP:HB2	2.18	0.43
1:D:433:LYS:O	1:D:436:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:LYS:HB2	1:B:686:SER:HB3	2.00	0.43
1:C:15:VAL:HG13	1:C:16:LYS:HG3	1.99	0.43
1:B:250:PRO:HG3	1:D:244:ARG:O	2.19	0.43
1:C:492:TRP:HB2	1:D:492:TRP:CD1	2.54	0.43
1:B:224:ARG:NH1	1:B:273:GLN:OE1	2.52	0.43
1:D:668:ARG:HG2	1:D:756:PHE:CE1	2.54	0.43
1:B:540:HIS:CD2	1:B:605:TRP:HZ3	2.37	0.42
1:D:779:PRO:O	1:D:780:LYS:HG2	2.19	0.42
1:D:207:ILE:HD11	1:D:251:LEU:HD21	2.01	0.42
1:A:633:ILE:HD11	1:A:656:PHE:CD1	2.54	0.42
1:A:590:LYS:HB2	1:A:686:SER:HB3	2.02	0.42
1:A:668:ARG:HG2	1:A:756:PHE:CE1	2.55	0.42
1:B:433:LYS:O	1:B:436:GLY:N	2.50	0.42
1:C:207:ILE:HD11	1:C:251:LEU:HD21	2.00	0.42
1:C:630:PHE:O	1:C:631:ARG:C	2.57	0.42
1:D:294:ARG:HE	1:D:415:PRO:CA	2.32	0.42
1:C:508:GLU:HG2	1:C:599:TRP:CD1	2.54	0.42
1:D:487:GLU:O	1:D:493:ILE:HG22	2.20	0.42
1:C:426:ASN:ND2	1:C:447:TYR:OH	2.52	0.42
1:D:189:LEU:HD13	1:D:287:VAL:HG22	2.01	0.42
1:D:630:PHE:O	1:D:631:ARG:C	2.58	0.42
1:C:14:ALA:O	1:C:15:VAL:C	2.58	0.42
1:A:133:LEU:HD21	1:A:155:GLY:HA3	2.00	0.42
1:A:489:TRP:CZ2	1:A:549:ARG:HD2	2.55	0.42
1:A:630:PHE:O	1:A:631:ARG:C	2.58	0.42
1:C:668:ARG:HG2	1:C:756:PHE:CE1	2.55	0.42
1:B:190:LEU:HB3	1:B:210:ASP:HB3	2.02	0.41
1:C:133:LEU:HD21	1:C:155:GLY:HA3	2.02	0.41
1:C:521:ARG:NH1	1:C:527:GLU:OE1	2.53	0.41
1:C:633:ILE:HD11	1:C:656:PHE:CD1	2.55	0.41
1:D:168:PRO:HD3	1:D:605:TRP:NE1	2.35	0.41
1:A:186:LYS:CD	1:A:217:ILE:HD13	2.50	0.41
1:C:590:LYS:HB2	1:C:686:SER:HB3	2.02	0.41
1:B:207:ILE:HD11	1:B:251:LEU:HD21	2.03	0.41
1:B:356:ARG:HA	1:B:380:TRP:HB3	2.02	0.41
1:C:186:LYS:CD	1:C:217:ILE:HD13	2.50	0.41
1:A:552:ARG:HG3	1:A:552:ARG:HH11	1.85	0.41
1:B:335:ILE:HD12	1:B:340:TYR:CE2	2.56	0.41
1:B:363:TYR:CE2	1:B:407:VAL:HG21	2.54	0.41
1:B:434:TRP:HD1	1:B:435:TRP:CZ3	2.39	0.41
1:C:598:ILE:HG22	1:C:600:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:LEU:O	1:D:797:GLU:HG3	2.20	0.41
1:A:207:ILE:HD11	1:A:251:LEU:HD21	2.01	0.41
1:B:668:ARG:HG2	1:B:756:PHE:CE1	2.55	0.41
1:D:335:ILE:CD1	1:D:340:TYR:HE2	2.34	0.41
1:A:190:LEU:HB3	1:A:210:ASP:HB3	2.03	0.41
1:B:280:LYS:HD3	1:B:282:GLU:HB2	2.01	0.41
1:D:660:ILE:HG22	1:D:676:GLU:OE1	2.21	0.41
1:A:356:ARG:HA	1:A:380:TRP:HB3	2.03	0.41
1:A:552:ARG:HD2	1:B:492:TRP:CH2	2.56	0.41
1:B:361:GLY:O	1:B:384:MET:HE2	2.21	0.41
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.98	0.41
1:D:590:LYS:HB2	1:D:686:SER:HB3	2.02	0.41
1:D:763:LEU:HB3	1:D:770:TRP:CZ2	2.56	0.41
1:A:484:HIS:CD2	1:A:508:GLU:HB2	2.56	0.41
1:C:598:ILE:CG2	1:C:600:GLN:HG2	2.51	0.41
1:C:792:THR:HG23	1:C:795:GLU:CB	2.51	0.41
1:D:426:ASN:ND2	1:D:447:TYR:OH	2.53	0.41
1:C:795:GLU:O	1:C:799:LYS:HB2	2.21	0.40
1:C:484:HIS:CD2	1:C:508:GLU:HB2	2.56	0.40
1:D:133:LEU:HD21	1:D:155:GLY:HA3	2.03	0.40
1:D:356:ARG:HA	1:D:380:TRP:HB3	2.02	0.40
1:D:359:GLY:C	1:D:384:MET:HE3	2.42	0.40
1:D:452:PRO:HG3	1:D:464:TYR:CE1	2.57	0.40
1:A:762:SER:N	1:A:803:GLU:O	2.55	0.40
1:B:666:THR:OG1	1:B:669:GLY:N	2.46	0.40
1:B:762:SER:N	1:B:803:GLU:O	2.54	0.40
1:C:190:LEU:HB3	1:C:210:ASP:HB3	2.04	0.40
1:C:335:ILE:HD12	1:C:340:TYR:CE2	2.57	0.40
1:D:190:LEU:HB3	1:D:210:ASP:HB3	2.03	0.40
1:A:605:TRP:CD1	1:A:605:TRP:N	2.89	0.40
1:B:633:ILE:HD11	1:B:656:PHE:CD1	2.55	0.40
1:A:8:GLY:N	1:A:25:VAL:HG11	2.35	0.40
1:A:300:THR:OG1	1:A:307:GLU:OE1	2.39	0.40
1:B:802:LEU:HD11	1:B:810:VAL:CG2	2.51	0.40
1:C:300:THR:OG1	1:C:307:GLU:OE1	2.39	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:NZ	1:C:711:GLU:C[1_545]	0.73	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:CE	1:C:711:GLU:C[1_545]	1.10	1.10
1:C:16:LYS:NZ	1:C:712:LYS:N[1_545]	1.17	1.03
1:C:16:LYS:CE	1:C:711:GLU:O[1_545]	1.39	0.81
1:C:16:LYS:CE	1:C:712:LYS:N[1_545]	1.47	0.73
1:C:16:LYS:NZ	1:C:711:GLU:O[1_545]	1.51	0.69
1:C:16:LYS:CD	1:C:711:GLU:O[1_545]	1.91	0.29
1:D:18:LYS:NZ	1:D:654:GLU:OE1[1_565]	1.94	0.26
1:C:16:LYS:NZ	1:C:711:GLU:CA[1_545]	1.96	0.24
1:B:18:LYS:NZ	1:B:654:GLU:OE1[1_545]	2.12	0.08
1:C:16:LYS:CD	1:C:712:LYS:CA[1_545]	2.16	0.04
1:C:233:GLU:OE1	1:D:280:LYS:NZ[1_455]	2.16	0.04
1:A:237:ARG:NH2	1:B:279:GLU:OE2[1_455]	2.17	0.03

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	809/836 (97%)	723 (89%)	78 (10%)	8 (1%)	15 47
1	B	809/836 (97%)	715 (88%)	86 (11%)	8 (1%)	15 47
1	C	809/836 (97%)	723 (89%)	78 (10%)	8 (1%)	15 47
1	D	809/836 (97%)	725 (90%)	76 (9%)	8 (1%)	15 47
All	All	3236/3344 (97%)	2886 (89%)	318 (10%)	32 (1%)	15 47

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	664	ILE
1	B	152	ARG
1	B	664	ILE
1	B	730	GLU

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Mol	Chain	Res	Type
1	C	152	ARG
1	C	664	ILE
1	D	152	ARG
1	D	664	ILE
1	D	730	GLU
1	A	730	GLU
1	C	730	GLU
1	B	641	ASN
1	D	641	ASN
1	A	469	PRO
1	B	469	PRO
1	B	779	PRO
1	C	469	PRO
1	D	469	PRO
1	A	800	LEU
1	B	168	PRO
1	C	168	PRO
1	A	168	PRO
1	A	677	VAL
1	C	677	VAL
1	D	168	PRO
1	D	677	VAL
1	A	493	ILE
1	B	493	ILE
1	C	493	ILE
1	D	493	ILE
1	C	743	ILE

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	727/748 (97%)	711 (98%)	16 (2%)	52	76
1	B	727/748 (97%)	709 (98%)	18 (2%)	47	74
1	C	727/748 (97%)	707 (97%)	20 (3%)	43	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	727/748 (97%)	708 (97%)	19 (3%)	46	72
All	All	2908/2992 (97%)	2835 (98%)	73 (2%)	47	74

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	210	ASP
1	A	226	SER
1	A	251	LEU
1	A	380	TRP
1	A	399	ASP
1	A	425	CYS
1	A	533	GLN
1	A	552	ARG
1	A	562	GLU
1	A	570	LEU
1	A	574	ILE
1	A	662	TYR
1	A	719	ASN
1	A	735	VAL
1	A	810	VAL
1	B	7	ASP
1	B	185	ASN
1	B	210	ASP
1	B	226	SER
1	B	251	LEU
1	B	255	ASN
1	B	380	TRP
1	B	399	ASP
1	B	425	CYS
1	B	480	VAL
1	B	533	GLN
1	B	552	ARG
1	B	574	ILE
1	B	612	ILE
1	B	662	TYR
1	B	719	ASN
1	B	735	VAL
1	B	810	VAL
1	C	7	ASP
1	C	16	LYS

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Mol	Chain	Res	Type
1	C	226	SER
1	C	251	LEU
1	C	380	TRP
1	C	399	ASP
1	C	425	CYS
1	C	435	TRP
1	C	533	GLN
1	C	552	ARG
1	C	562	GLU
1	C	570	LEU
1	C	574	ILE
1	C	592	HIS
1	C	612	ILE
1	C	662	TYR
1	C	719	ASN
1	C	746	ASN
1	C	792	THR
1	C	810	VAL
1	D	7	ASP
1	D	161	SER
1	D	210	ASP
1	D	226	SER
1	D	251	LEU
1	D	255	ASN
1	D	380	TRP
1	D	399	ASP
1	D	533	GLN
1	D	552	ARG
1	D	560	ILE
1	D	562	GLU
1	D	574	ILE
1	D	662	TYR
1	D	715	LEU
1	D	719	ASN
1	D	735	VAL
1	D	797	GLU
1	D	810	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN

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Mol	Chain	Res	Type
1	A	314	ASN
1	A	381	GLN
1	A	413	ASN
1	A	478	GLN
1	A	502	ASN
1	A	589	ASN
1	A	751	ASN
1	B	314	ASN
1	B	381	GLN
1	B	413	ASN
1	B	478	GLN
1	B	502	ASN
1	B	589	ASN
1	C	185	ASN
1	C	314	ASN
1	C	381	GLN
1	C	413	ASN
1	C	478	GLN
1	C	502	ASN
1	C	589	ASN
1	C	751	ASN
1	C	776	ASN
1	D	314	ASN
1	D	381	GLN
1	D	413	ASN
1	D	478	GLN
1	D	502	ASN
1	D	589	ASN
1	D	751	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)

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)

4 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	BMA	C	901	-	11,11,12	1.68	4 (36%)	15,15,17	1.42	3 (20%)
2	BMA	B	901	-	11,11,12	2.89	5 (45%)	15,15,17	2.40	3 (20%)
2	BMA	D	901	-	11,11,12	2.09	3 (27%)	15,15,17	1.89	3 (20%)
2	BMA	A	901	-	11,11,12	2.14	5 (45%)	15,15,17	1.57	3 (20%)

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	BMA	C	901	-	-	2/2/19/22	0/1/1/1
2	BMA	B	901	-	-	2/2/19/22	0/1/1/1
2	BMA	D	901	-	-	0/2/19/22	0/1/1/1
2	BMA	A	901	-	-	2/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	BMA	O5-C1	6.99	1.54	1.43
2	A	901	BMA	C2-C3	4.59	1.59	1.52
2	D	901	BMA	C2-C3	4.39	1.59	1.52
2	B	901	BMA	C2-C3	3.95	1.58	1.52
2	D	901	BMA	O5-C1	3.72	1.49	1.43
2	A	901	BMA	O5-C1	3.34	1.49	1.43
2	B	901	BMA	O5-C5	3.34	1.50	1.43
2	C	901	BMA	O5-C1	2.85	1.48	1.43
2	B	901	BMA	C1-C2	2.67	1.58	1.52
2	C	901	BMA	C2-C3	2.49	1.56	1.52
2	D	901	BMA	O5-C5	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	BMA	C4-C3	2.20	1.57	1.52
2	C	901	BMA	O5-C5	2.17	1.47	1.43
2	C	901	BMA	C1-C2	2.15	1.57	1.52
2	A	901	BMA	O5-C5	2.14	1.47	1.43
2	B	901	BMA	C4-C3	2.06	1.57	1.52
2	A	901	BMA	C1-C2	2.02	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	BMA	O5-C5-C6	7.94	119.66	107.20
2	D	901	BMA	O5-C5-C6	5.05	115.12	107.20
2	A	901	BMA	O5-C5-C6	3.56	112.78	107.20
2	A	901	BMA	C1-O5-C5	3.26	116.61	112.19
2	C	901	BMA	O6-C6-C5	-3.11	100.64	111.29
2	D	901	BMA	C1-O5-C5	2.88	116.10	112.19
2	A	901	BMA	C1-C2-C3	2.73	113.02	109.67
2	C	901	BMA	C1-C2-C3	2.62	112.89	109.67
2	B	901	BMA	O5-C1-C2	2.57	114.74	110.77
2	B	901	BMA	C1-C2-C3	2.48	112.72	109.67
2	C	901	BMA	C1-O5-C5	2.39	115.43	112.19
2	D	901	BMA	C1-C2-C3	2.11	112.26	109.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	BMA	O5-C5-C6-O6
2	B	901	BMA	C4-C5-C6-O6
2	A	901	BMA	O5-C5-C6-O6
2	A	901	BMA	C4-C5-C6-O6
2	C	901	BMA	O5-C5-C6-O6
2	C	901	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 (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	811/836 (97%)	0.08	11 (1%)	75	55	53, 86, 130, 161	1 (0%)
1	B	811/836 (97%)	0.02	6 (0%)	87	74	45, 81, 124, 160	1 (0%)
1	C	811/836 (97%)	0.08	9 (1%)	80	62	46, 86, 127, 181	1 (0%)
1	D	811/836 (97%)	0.01	3 (0%)	92	84	47, 82, 123, 175	1 (0%)
All	All	3244/3344 (97%)	0.05	29 (0%)	84	68	45, 84, 126, 181	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	790	PRO	4.5
1	C	695	GLU	3.7
1	D	678	ASP	3.7
1	C	287	VAL	3.7
1	B	435	TRP	3.4
1	A	436	GLY	3.3
1	C	71	PHE	3.3
1	A	148	ASP	3.3
1	B	791	TYR	3.2
1	D	677	VAL	2.9
1	A	692	PHE	2.9
1	B	144	LEU	2.7
1	A	791	TYR	2.7
1	A	678	ASP	2.7
1	C	442	TRP	2.7
1	A	679	ILE	2.6
1	A	651	ASP	2.6
1	D	285	ASP	2.6
1	C	427	HIS	2.5
1	C	437	GLU	2.5
1	B	431	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	67	VAL	2.4
1	A	677	VAL	2.3
1	A	276	LEU	2.2
1	C	386	ALA	2.2
1	C	692	PHE	2.2
1	B	797	GLU	2.1
1	A	427	HIS	2.0
1	C	436	GLY	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, 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	BMA	B	901	11/12	0.86	0.23	58,69,79,82	0
2	BMA	D	901	11/12	0.86	0.24	75,94,105,123	0
2	BMA	C	901	11/12	0.88	0.35	87,103,115,116	0
2	BMA	A	901	11/12	0.91	0.27	71,87,95,98	0

6.5 Other polymers (i)

There are no such residues in this entry.