Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 11:07 am BST

PDB ID	:	6YMN
Title	:	Crystal structure of the Diels Alderase AbmU from Streptomyces koyangensis
Authors	:	Back, C.R.; Burton, N.; Race, P.R.
Deposited on	:	2020-04-09
Resolution	:	2.05 Å(reported)

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

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

The following versions of software and data (see references ①) were used in the production of this report:

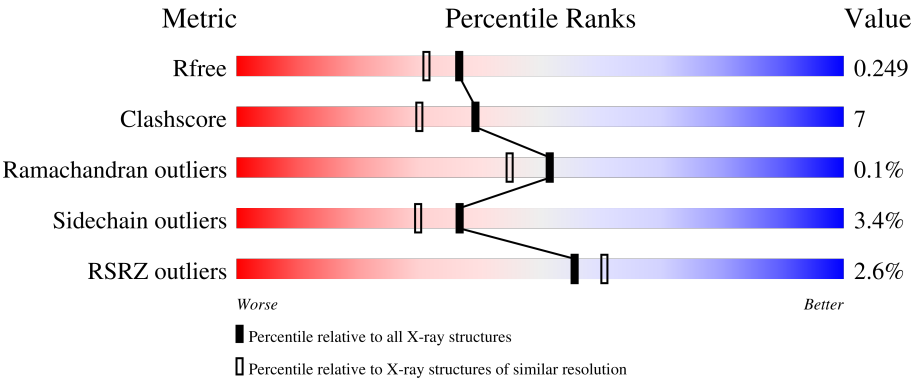
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	AAA	237	4% 77% 10% • 12%
1	BBB	237	2% 80% 6% • 13%
1	CCC	237	2% 73% 13% • 14%
1	DDD	237	% 66% 14% • 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	AAA	302	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12772 atoms, of which 6023 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 AbmU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	209	Total	C	H	N	O	S	69	2	0
			3175	1031	1559	279	301	5			
1	BBB	206	Total	C	H	N	O	S	66	0	0
			3091	999	1514	276	298	4			
1	CCC	204	Total	C	H	N	O	S	65	2	0
			3097	1003	1519	276	296	3			
1	DDD	193	Total	C	H	N	O	S	62	0	0
			2917	946	1431	258	279	3			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP A0A2P1BT29
AAA	-17	ALA	-	expression tag	UNP A0A2P1BT29
AAA	-16	HIS	-	expression tag	UNP A0A2P1BT29
AAA	-15	HIS	-	expression tag	UNP A0A2P1BT29
AAA	-14	HIS	-	expression tag	UNP A0A2P1BT29
AAA	-13	HIS	-	expression tag	UNP A0A2P1BT29
AAA	-12	HIS	-	expression tag	UNP A0A2P1BT29
AAA	-11	HIS	-	expression tag	UNP A0A2P1BT29
AAA	-10	SER	-	expression tag	UNP A0A2P1BT29
AAA	-9	SER	-	expression tag	UNP A0A2P1BT29
AAA	-8	GLY	-	expression tag	UNP A0A2P1BT29
AAA	-7	LEU	-	expression tag	UNP A0A2P1BT29
AAA	-6	GLU	-	expression tag	UNP A0A2P1BT29
AAA	-5	VAL	-	expression tag	UNP A0A2P1BT29
AAA	-4	LEU	-	expression tag	UNP A0A2P1BT29
AAA	-3	PHE	-	expression tag	UNP A0A2P1BT29
AAA	-2	GLN	-	expression tag	UNP A0A2P1BT29
AAA	-1	GLY	-	expression tag	UNP A0A2P1BT29
AAA	0	PRO	-	expression tag	UNP A0A2P1BT29
BBB	-18	MET	-	initiating methionine	UNP A0A2P1BT29
BBB	-17	ALA	-	expression tag	UNP A0A2P1BT29

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-16	HIS	-	expression tag	UNP A0A2P1BT29
BBB	-15	HIS	-	expression tag	UNP A0A2P1BT29
BBB	-14	HIS	-	expression tag	UNP A0A2P1BT29
BBB	-13	HIS	-	expression tag	UNP A0A2P1BT29
BBB	-12	HIS	-	expression tag	UNP A0A2P1BT29
BBB	-11	HIS	-	expression tag	UNP A0A2P1BT29
BBB	-10	SER	-	expression tag	UNP A0A2P1BT29
BBB	-9	SER	-	expression tag	UNP A0A2P1BT29
BBB	-8	GLY	-	expression tag	UNP A0A2P1BT29
BBB	-7	LEU	-	expression tag	UNP A0A2P1BT29
BBB	-6	GLU	-	expression tag	UNP A0A2P1BT29
BBB	-5	VAL	-	expression tag	UNP A0A2P1BT29
BBB	-4	LEU	-	expression tag	UNP A0A2P1BT29
BBB	-3	PHE	-	expression tag	UNP A0A2P1BT29
BBB	-2	GLN	-	expression tag	UNP A0A2P1BT29
BBB	-1	GLY	-	expression tag	UNP A0A2P1BT29
BBB	0	PRO	-	expression tag	UNP A0A2P1BT29
CCC	-18	MET	-	initiating methionine	UNP A0A2P1BT29
CCC	-17	ALA	-	expression tag	UNP A0A2P1BT29
CCC	-16	HIS	-	expression tag	UNP A0A2P1BT29
CCC	-15	HIS	-	expression tag	UNP A0A2P1BT29
CCC	-14	HIS	-	expression tag	UNP A0A2P1BT29
CCC	-13	HIS	-	expression tag	UNP A0A2P1BT29
CCC	-12	HIS	-	expression tag	UNP A0A2P1BT29
CCC	-11	HIS	-	expression tag	UNP A0A2P1BT29
CCC	-10	SER	-	expression tag	UNP A0A2P1BT29
CCC	-9	SER	-	expression tag	UNP A0A2P1BT29
CCC	-8	GLY	-	expression tag	UNP A0A2P1BT29
CCC	-7	LEU	-	expression tag	UNP A0A2P1BT29
CCC	-6	GLU	-	expression tag	UNP A0A2P1BT29
CCC	-5	VAL	-	expression tag	UNP A0A2P1BT29
CCC	-4	LEU	-	expression tag	UNP A0A2P1BT29
CCC	-3	PHE	-	expression tag	UNP A0A2P1BT29
CCC	-2	GLN	-	expression tag	UNP A0A2P1BT29
CCC	-1	GLY	-	expression tag	UNP A0A2P1BT29
CCC	0	PRO	-	expression tag	UNP A0A2P1BT29
DDD	-18	MET	-	initiating methionine	UNP A0A2P1BT29
DDD	-17	ALA	-	expression tag	UNP A0A2P1BT29
DDD	-16	HIS	-	expression tag	UNP A0A2P1BT29
DDD	-15	HIS	-	expression tag	UNP A0A2P1BT29
DDD	-14	HIS	-	expression tag	UNP A0A2P1BT29
DDD	-13	HIS	-	expression tag	UNP A0A2P1BT29

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-12	HIS	-	expression tag	UNP A0A2P1BT29
DDD	-11	HIS	-	expression tag	UNP A0A2P1BT29
DDD	-10	SER	-	expression tag	UNP A0A2P1BT29
DDD	-9	SER	-	expression tag	UNP A0A2P1BT29
DDD	-8	GLY	-	expression tag	UNP A0A2P1BT29
DDD	-7	LEU	-	expression tag	UNP A0A2P1BT29
DDD	-6	GLU	-	expression tag	UNP A0A2P1BT29
DDD	-5	VAL	-	expression tag	UNP A0A2P1BT29
DDD	-4	LEU	-	expression tag	UNP A0A2P1BT29
DDD	-3	PHE	-	expression tag	UNP A0A2P1BT29
DDD	-2	GLN	-	expression tag	UNP A0A2P1BT29
DDD	-1	GLY	-	expression tag	UNP A0A2P1BT29
DDD	0	PRO	-	expression tag	UNP A0A2P1BT29

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	2	Total Br 2 2	0	0
2	BBB	2	Total Br 2 2	0	0
2	CCC	1	Total Br 1 1	0	0
2	DDD	2	Total Br 2 2	0	0

- Molecule 3 is water.

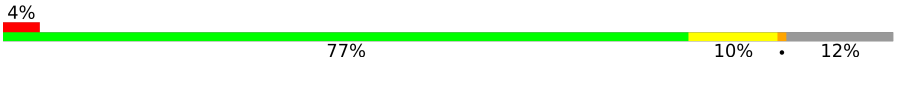
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	115	Total O 115 115	0	0
3	BBB	138	Total O 138 138	0	0
3	CCC	119	Total O 119 119	0	0
3	DDD	113	Total O 113 113	0	0

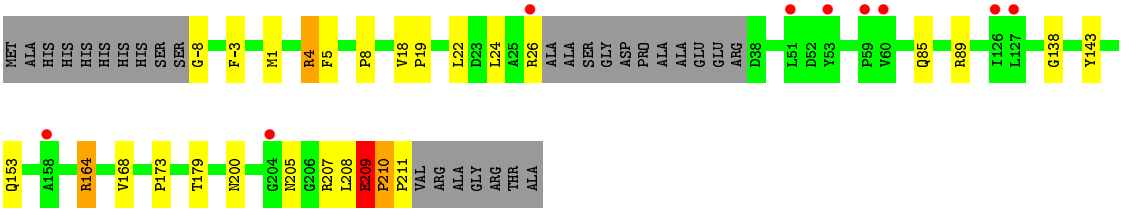
3 Residue-property plots (i)

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: AbmU

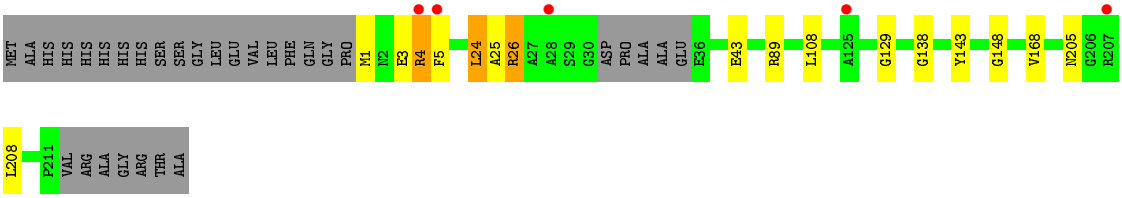
Chain AAA:





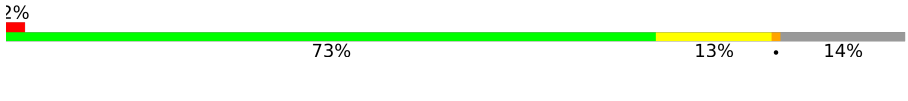
- Molecule 1: AbmU

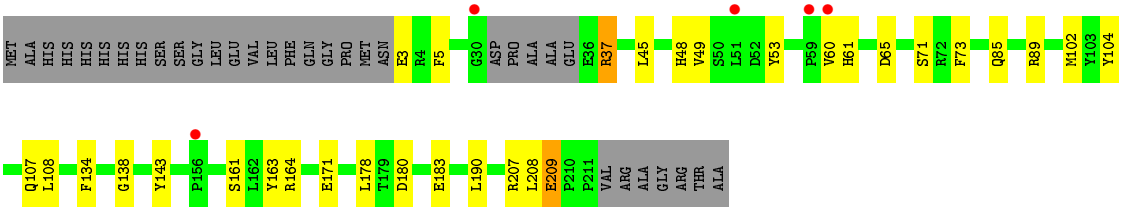
Chain BBB:



- Molecule 1: AbmU

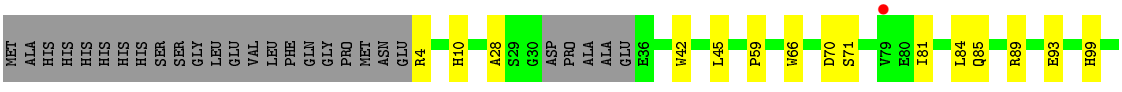
Chain CCC:





- Molecule 1: AbmU

Chain DDD:




M102
Y103
Y104
R105
E106
D112
T117
G123
T124
A125
I126
L127
GLY
GLY
A130
G138
Y143
L149
E157
V168
L169
D180
L190
S198
V199
N200
P201
A202
T203
GLY
ASN
GLY
ARG
LEU
GLU
PRO
PRO
VAL
ARG
ALA
GLY
ARG
THR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.13Å 65.00Å 97.86Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	56.44 – 2.05 56.44 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (56.44-2.05) 99.5 (56.44-2.05)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.189 , 0.243 0.198 , 0.249	Depositor DCC
R_{free} test set	2613 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12772	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	AAA	0.78	2/1671 (0.1%)	0.92	3/2282 (0.1%)
1	BBB	0.70	0/1623	0.89	0/2216
1	CCC	0.70	1/1631 (0.1%)	0.87	0/2227
1	DDD	0.66	0/1529	0.86	0/2088
All	All	0.71	3/6454 (0.0%)	0.89	3/8813 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	210	PRO	N-CA	12.65	1.68	1.47
1	CCC	209	GLU	C-N	7.66	1.48	1.34
1	AAA	209	GLU	C-N	6.27	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	210	PRO	N-CA-C	-7.26	93.23	112.10
1	AAA	210	PRO	CA-N-CD	-6.85	101.92	111.50
1	AAA	211	PRO	N-CA-C	5.11	125.39	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1616	1559	1554	31	0
1	BBB	1577	1514	1508	19	0
1	CCC	1578	1519	1512	23	0
1	DDD	1486	1431	1421	35	0
2	AAA	2	0	0	2	0
2	BBB	2	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	2	0	0	0	0
3	AAA	115	0	0	6	0
3	BBB	138	0	0	3	0
3	CCC	119	0	0	8	0
3	DDD	113	0	0	11	0
All	All	6749	6023	5995	91	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 7.

All (91) 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:AAA:210:PRO:N	1:AAA:210:PRO:CA	1.68	1.36
1:AAA:4:ARG:NE	1:BBB:43:GLU:OE2	1.65	1.29
1:AAA:168:VAL:HG23	3:BBB:492:HOH:O	1.75	0.85
1:AAA:210:PRO:N	1:AAA:210:PRO:C	2.34	0.81
1:DDD:89:ARG:CD	3:DDD:448:HOH:O	2.30	0.78
1:BBB:129:GLY:HA2	3:BBB:449:HOH:O	1.84	0.76
1:DDD:89:ARG:HD2	3:DDD:448:HOH:O	1.86	0.74
3:CCC:419:HOH:O	1:DDD:10:HIS:HE1	1.72	0.72
1:AAA:153:GLN:NE2	3:AAA:401:HOH:O	2.20	0.71
1:AAA:138:GLY:HA3	1:AAA:143:TYR:O	1.91	0.71
1:CCC:61:HIS:HA	1:CCC:65:ASP:OD2	1.93	0.68
1:CCC:208:LEU:O	1:DDD:89:ARG:HG3	1.93	0.68
1:CCC:164:ARG:HD3	3:CCC:506:HOH:O	1.94	0.68
1:AAA:-3:PHE:CZ	1:BBB:26:ARG:HB3	2.29	0.67
1:AAA:168:VAL:CG2	3:BBB:492:HOH:O	2.39	0.67
1:DDD:126:ILE:HG12	3:DDD:438:HOH:O	1.95	0.65
1:CCC:61:HIS:HB2	3:CCC:411:HOH:O	1.98	0.64
1:CCC:138:GLY:HA3	1:CCC:143:TYR:O	1.99	0.63
1:AAA:1[B]:MET:H	1:AAA:1[B]:MET:CE	2.13	0.61
1:AAA:4:ARG:HE	1:BBB:43:GLU:CD	1.88	0.60
1:AAA:8:PRO:HG2	3:AAA:444:HOH:O	2.03	0.59
1:AAA:5:PHE:CE2	1:BBB:24:LEU:HD13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:24:LEU:HB2	1:BBB:5:PHE:CZ	2.39	0.58
1:AAA:208:LEU:HB3	1:BBB:89:ARG:HG3	1.86	0.58
1:AAA:1[B]:MET:H	1:AAA:1[B]:MET:HE2	1.70	0.56
1:DDD:124:THR:O	1:DDD:124:THR:HG22	2.05	0.55
1:CCC:45:LEU:HD13	1:CCC:73:PHE:HB3	1.90	0.53
1:BBB:138:GLY:HA3	1:BBB:143:TYR:O	2.08	0.53
1:CCC:209:GLU:HG3	1:DDD:66:TRP:CZ2	2.45	0.51
1:DDD:126:ILE:O	1:DDD:126:ILE:HG23	2.10	0.51
1:CCC:49:VAL:HG21	1:CCC:163:TYR:CE2	2.45	0.51
1:DDD:200:ASN:HB2	3:DDD:441:HOH:O	2.10	0.50
1:CCC:104[A]:TYR:CZ	1:CCC:134:PHE:CG	3.00	0.50
1:BBB:4:ARG:HD2	1:BBB:4:ARG:H	1.77	0.49
1:CCC:190:LEU:HD12	1:DDD:190:LEU:HD12	1.94	0.49
1:CCC:3:GLU:HB2	3:CCC:460:HOH:O	2.12	0.49
1:DDD:169:LEU:HD12	1:DDD:169:LEU:N	2.27	0.48
1:DDD:10:HIS:CD2	3:DDD:452:HOH:O	2.65	0.48
1:AAA:173:PRO:HD2	3:AAA:447:HOH:O	2.14	0.47
1:AAA:4:ARG:CZ	1:BBB:43:GLU:OE2	2.51	0.47
1:DDD:180:ASP:OD1	3:DDD:401:HOH:O	2.20	0.47
1:BBB:3:GLU:HB2	1:BBB:4:ARG:NH1	2.30	0.46
1:DDD:89:ARG:HG2	3:DDD:448:HOH:O	2.14	0.46
1:DDD:4:ARG:NE	1:DDD:4:ARG:HA	2.31	0.46
1:CCC:178:LEU:HD22	1:CCC:183:GLU:HB3	1.98	0.46
1:DDD:66:TRP:HB3	1:DDD:89:ARG:HG2	1.97	0.46
1:CCC:61:HIS:CA	1:CCC:65:ASP:OD2	2.63	0.45
1:DDD:138:GLY:HA3	1:DDD:143:TYR:O	2.16	0.45
1:AAA:-8:GLY:N	3:AAA:410:HOH:O	2.48	0.45
1:AAA:1[B]:MET:CE	2:AAA:302:BR:BR	3.20	0.45
1:AAA:18:VAL:HB	1:AAA:19:PRO:HD3	1.98	0.45
1:DDD:123:GLY:O	1:DDD:126:ILE:HG22	2.17	0.45
1:CCC:102:MET:SD	1:CCC:104[B]:TYR:HE1	2.40	0.45
1:AAA:-3:PHE:CE2	1:BBB:26:ARG:HB3	2.52	0.44
1:CCC:53:TYR:HE2	3:CCC:411:HOH:O	1.96	0.44
1:DDD:42:TRP:HB3	1:DDD:45:LEU:HD21	1.99	0.44
1:DDD:89:ARG:CG	3:DDD:448:HOH:O	2.61	0.44
1:AAA:5:PHE:CD1	1:BBB:25:ALA:HA	2.52	0.44
1:DDD:81:ILE:C	1:DDD:81:ILE:HD12	2.38	0.44
3:CCC:419:HOH:O	1:DDD:10:HIS:CE1	2.58	0.44
1:DDD:112:ASP:OD1	1:DDD:112:ASP:N	2.44	0.43
1:DDD:70:ASP:OD1	1:DDD:85:GLN:OE1	2.36	0.43
1:DDD:102:MET:CE	1:DDD:104:TYR:OH	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:37:ARG:HB3	1:CCC:171:GLU:HB3	1.99	0.43
1:DDD:28:ALA:HB3	3:DDD:402:HOH:O	2.19	0.43
1:AAA:164:ARG:HD3	3:AAA:401:HOH:O	2.18	0.43
1:BBB:108:LEU:HD12	1:BBB:108:LEU:N	2.33	0.43
1:CCC:5:PHE:HA	1:DDD:149:LEU:HD23	1.99	0.43
1:DDD:93:GLU:HA	1:DDD:99:HIS:O	2.18	0.43
1:AAA:26:ARG:HB3	1:AAA:26:ARG:CZ	2.47	0.43
1:BBB:148:GLY:HA3	1:BBB:168:VAL:O	2.18	0.43
1:AAA:89:ARG:CG	1:BBB:208:LEU:O	2.67	0.42
1:AAA:89:ARG:HG3	1:BBB:208:LEU:HB3	2.01	0.42
1:AAA:208:LEU:O	1:BBB:89:ARG:HD2	2.19	0.42
1:CCC:60:VAL:HA	3:CCC:469:HOH:O	2.19	0.42
1:DDD:106:GLU:HB2	1:DDD:117:THR:OG1	2.20	0.42
1:AAA:85:GLN:NE2	3:AAA:413:HOH:O	2.52	0.42
1:AAA:207:ARG:HB3	1:AAA:209:GLU:HG2	2.02	0.42
1:CCC:48:HIS:O	1:CCC:71:SER:HA	2.19	0.42
1:CCC:108:LEU:HD12	1:CCC:108:LEU:N	2.35	0.42
1:DDD:202:ALA:O	1:DDD:203:THR:HB	2.20	0.42
1:AAA:1[B]:MET:HE2	2:AAA:302:BR:BR	2.75	0.41
1:AAA:208:LEU:O	1:BBB:89:ARG:CG	2.68	0.41
1:DDD:168:VAL:C	1:DDD:169:LEU:HD12	2.41	0.41
1:CCC:104[A]:TYR:CE1	1:CCC:134:PHE:CD2	3.08	0.41
1:DDD:10:HIS:CE1	3:DDD:442:HOH:O	2.74	0.41
1:DDD:202:ALA:HB2	3:DDD:511:HOH:O	2.20	0.41
1:CCC:85:GLN:HE21	1:CCC:85:GLN:HB2	1.74	0.40
1:DDD:71:SER:HB2	1:DDD:84:LEU:HB3	2.02	0.40
1:CCC:107:GLN:HB3	3:CCC:471:HOH:O	2.21	0.40
1:DDD:42:TRP:HZ3	1:DDD:169:LEU:HD13	1.86	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	AAA	207/237 (87%)	200 (97%)	7 (3%)	0	100	100
1	BBB	202/237 (85%)	195 (96%)	7 (4%)	0	100	100
1	CCC	202/237 (85%)	195 (96%)	7 (4%)	0	100	100
1	DDD	187/237 (79%)	179 (96%)	7 (4%)	1 (0%)	29	18
All	All	798/948 (84%)	769 (96%)	28 (4%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	125	ALA

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	AAA	168/185 (91%)	161 (96%)	7 (4%)	30	22
1	BBB	162/185 (88%)	157 (97%)	5 (3%)	40	33
1	CCC	162/185 (88%)	156 (96%)	6 (4%)	34	27
1	DDD	153/185 (83%)	148 (97%)	5 (3%)	38	31
All	All	645/740 (87%)	622 (96%)	23 (4%)	37	28

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	ARG
1	AAA	22	LEU
1	AAA	164	ARG
1	AAA	179	THR
1	AAA	200	ASN
1	AAA	205	ASN
1	AAA	209	GLU
1	BBB	1	MET
1	BBB	4	ARG
1	BBB	24	LEU

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Mol	Chain	Res	Type
1	BBB	26	ARG
1	BBB	205	ASN
1	CCC	37	ARG
1	CCC	89[A]	ARG
1	CCC	89[B]	ARG
1	CCC	161	SER
1	CCC	180	ASP
1	CCC	207	ARG
1	DDD	59	PRO
1	DDD	157	GLU
1	DDD	180	ASP
1	DDD	198	SER
1	DDD	203	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	209/237 (88%)	0.17	9 (4%)	35	38	22, 41, 72, 87	0
1	BBB	206/237 (86%)	0.07	5 (2%)	59	63	20, 35, 69, 92	0
1	CCC	204/237 (86%)	0.10	5 (2%)	57	61	25, 39, 72, 90	0
1	DDD	193/237 (81%)	0.10	2 (1%)	82	84	25, 42, 66, 91	0
All	All	812/948 (85%)	0.11	21 (2%)	56	60	20, 39, 72, 92	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	4	ARG	4.7
1	AAA	127	LEU	4.5
1	BBB	5	PHE	3.4
1	CCC	30	GLY	3.3
1	BBB	28	ALA	3.3
1	AAA	60	VAL	3.2
1	CCC	59	PRO	3.1
1	AAA	51	LEU	3.0
1	CCC	156	PRO	2.8
1	AAA	126	ILE	2.6
1	AAA	53	TYR	2.5
1	AAA	26	ARG	2.5
1	AAA	204	GLY	2.5
1	BBB	207	ARG	2.5
1	BBB	125	ALA	2.5
1	AAA	158	ALA	2.2
1	CCC	51	LEU	2.2
1	DDD	127	LEU	2.1
1	CCC	60	VAL	2.1
1	DDD	79	VAL	2.1
1	AAA	59	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BR	DDD	301	1/1	0.60	0.18	85,85,85,85	0
2	BR	BBB	302	1/1	0.76	0.11	80,80,80,80	0
2	BR	AAA	302	1/1	0.89	0.24	82,82,82,82	0
2	BR	AAA	301	1/1	0.91	0.13	60,60,60,60	0
2	BR	CCC	301	1/1	0.94	0.09	41,41,41,41	0
2	BR	BBB	301	1/1	0.97	0.15	53,53,53,53	0
2	BR	DDD	302	1/1	0.99	0.23	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.