Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 08:58 pm GMT

PDB ID	:	2IZQ
Title	:	Gramicidin D complex with KI
Authors	:	Olczak, A.; Glowka, M.L.; Szczesio, M.; Bojarska, J.; Duax, W.L.; Burkhart, B.M.; Wawrzak, Z.
Deposited on	:	2006-07-26
Resolution	:	0.80 Å(reported)

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

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

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

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

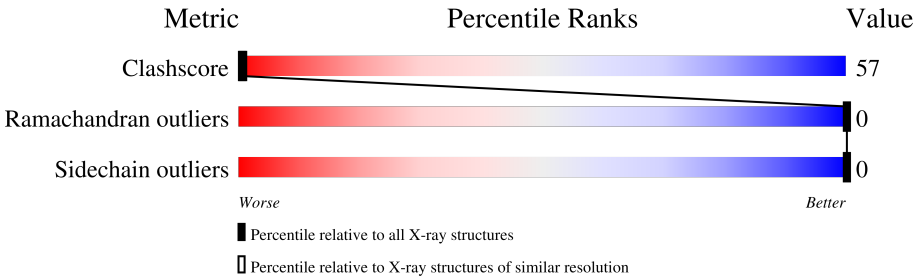
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 0.80 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))
Clashscore	180529	1424 (1.00-0.60)
Ramachandran outliers	177936	1340 (1.00-0.60)
Sidechain outliers	177891	1341 (1.00-0.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	18	28% 56% 17%
1	B	18	39% 39% 22%
1	C	18	33% 44% 22%
1	D	18	33% 56% 11%

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
1	DLE	A	14[B]	-	-	X	-
1	DVA	A	6[B]	-	-	X	-
1	DLE	B	10[A]	-	-	X	-
1	FVA	B	1[A]	-	-	X	-
1	DVA	B	6[B]	-	-	X	-
1	DVA	B	8[B]	-	-	X	-
1	FVA	D	1[B]	-	X	-	-
1	DVA	D	8[B]	-	-	X	-
2	K	A	107	-	-	X	-
2	K	C	106	-	-	X	-
3	IOD	D	101[A]	-	-	X	-
4	MOH	C	103[A]	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1870 atoms, of which 892 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 GRAMICIDIN D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	16	Total	C	H	N	O	0	12	0
			450	175	224	27	24			
1	B	16	Total	C	H	N	O	0	14	0
			404	149	204	22	29			
1	C	16	Total	C	H	N	O	0	12	0
			451	172	227	26	26			
1	D	16	Total	C	H	N	O	0	14	0
			447	162	237	24	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	TYR	TRP	microheterogeneity	NOR NOR00243
A	11	PHE	TRP	microheterogeneity	NOR NOR00243
B	11	TYR	TRP	microheterogeneity	NOR NOR00243
C	11	TYR	TRP	microheterogeneity	NOR NOR00243
C	11	PHE	TRP	microheterogeneity	NOR NOR00243
D	11	TYR	TRP	microheterogeneity	NOR NOR00243

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	K	0	0
			3	3		
2	C	3	Total	K	0	0
			3	3		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

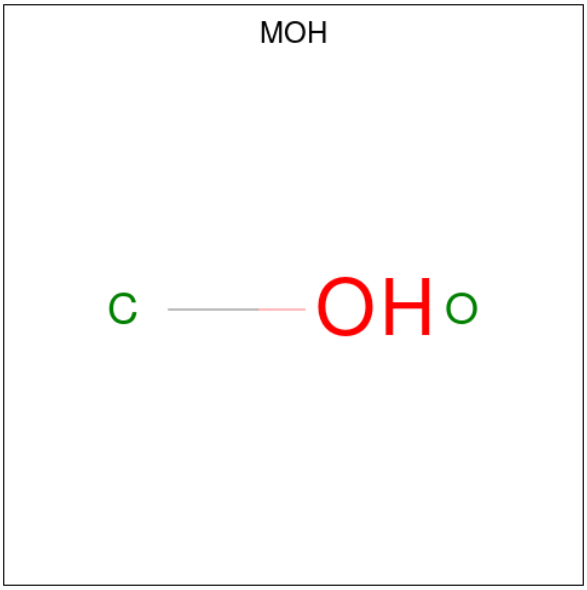
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	I	0	4
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total I 2 2	0	2
3	D	2	Total I 2 2	0	2

- Molecule 4 is METHANOL (three-letter code: MOH) (formula: CH_4O).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	15	Total O 15 15	0	0
5	C	23	Total O 23 23	0	0
5	D	17	Total O 17 17	0	0

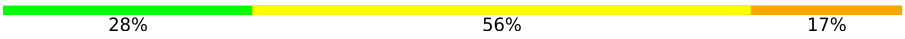
3 Residue-property plots (i)

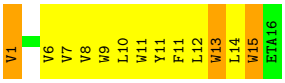
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: GRAMICIDIN D

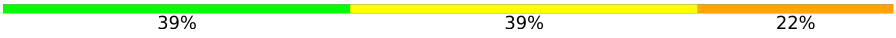
Chain A:





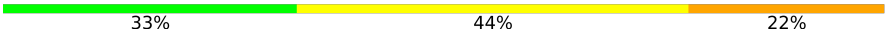
• Molecule 1: GRAMICIDIN D

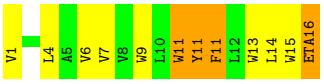
Chain B:



• Molecule 1: GRAMICIDIN D

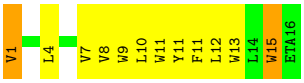
Chain C:





• Molecule 1: GRAMICIDIN D

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	30.14Å 31.32Å 51.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 0.80	Depositor
% Data completeness (in resolution range)	100.0 (28.00-0.80)	Depositor
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.111 , 0.122	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1870	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DVA, DLE, FVA, ETA, K, IOD, MOH

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	1.08	0/152	2.74	9/195 (4.6%)
1	B	1.69	4/134 (3.0%)	1.93	6/171 (3.5%)
1	C	1.16	0/152	2.22	5/195 (2.6%)
1	D	0.95	0/145	1.50	5/186 (2.7%)
All	All	1.24	4/583 (0.7%)	2.16	25/747 (3.3%)

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	3
1	C	0	1
1	D	0	4
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9[A]	TRP	CE2-CZ2	-9.86	1.23	1.39
1	B	9[B]	TRP	CE2-CZ2	-9.86	1.23	1.39
1	B	9[A]	TRP	CZ2-CH2	6.84	1.50	1.37
1	B	9[B]	TRP	CZ2-CH2	6.84	1.50	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11[B]	TYR	CB-CG-CD1	-17.41	110.56	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	11[B]	TYR	CG-CD2-CE2	14.21	132.67	121.30
1	A	11[B]	TYR	CB-CG-CD2	13.16	128.89	121.00
1	C	11[B]	TYR	CB-CG-CD1	9.40	126.64	121.00
1	C	11[B]	TYR	CD1-CE1-CZ	9.12	128.01	119.80
1	C	11[B]	TYR	CZ-CE2-CD2	-8.78	111.89	119.80
1	B	9[A]	TRP	NE1-CE2-CZ2	-7.59	122.05	130.40
1	B	9[B]	TRP	NE1-CE2-CZ2	-7.59	122.05	130.40
1	B	9[A]	TRP	CH2-CZ2-CE2	-7.54	109.86	117.40
1	B	9[B]	TRP	CH2-CZ2-CE2	-7.54	109.86	117.40
1	A	11[B]	TYR	CZ-CE2-CD2	-7.48	113.07	119.80
1	A	13[A]	TRP	CD1-CG-CD2	-7.39	100.38	106.30
1	A	13[B]	TRP	CD1-CG-CD2	-7.39	100.38	106.30
1	B	9[A]	TRP	CD2-CE2-CZ2	6.35	129.92	122.30
1	B	9[B]	TRP	CD2-CE2-CZ2	6.35	129.92	122.30
1	D	11[B]	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	A	13[A]	TRP	CG-CD1-NE1	6.23	116.33	110.10
1	A	13[B]	TRP	CG-CD1-NE1	6.23	116.33	110.10
1	C	11[B]	TYR	CG-CD1-CE1	-6.16	116.37	121.30
1	D	15[A]	TRP	CA-CB-CG	5.57	124.29	113.70
1	D	15[B]	TRP	CA-CB-CG	5.57	124.29	113.70
1	A	13[A]	TRP	CD1-NE1-CE2	-5.48	104.07	109.00
1	A	13[B]	TRP	CD1-NE1-CE2	-5.48	104.07	109.00
1	D	7[A]	VAL	N-CA-CB	5.28	123.11	111.50
1	D	7[B]	VAL	N-CA-CB	5.28	123.11	111.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15[A]	TRP	Mainchain
1	A	15[B]	TRP	Mainchain
1	B	10[A]	DLE	Mainchain
1	B	10[B]	DLE	Mainchain
1	B	4[A]	DLE	Mainchain
1	C	9[B]	TRP	Mainchain
1	D	10[A]	DLE	Peptide
1	D	10[B]	DLE	Peptide
1	D	13[A]	TRP	Mainchain
1	D	13[B]	TRP	Mainchain

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	226	224	236	51	0
1	B	200	204	193	41	0
1	C	224	227	227	13	0
1	D	210	237	220	21	0
2	A	3	0	0	3	0
2	C	3	0	0	3	0
3	A	4	0	0	1	0
3	B	2	0	0	0	0
3	D	2	0	0	3	0
4	A	4	0	0	0	0
4	C	12	0	0	5	0
4	D	2	0	0	0	0
5	A	31	0	0	6	0
5	B	15	0	0	2	0
5	C	23	0	0	4	0
5	D	17	0	0	5	0
All	All	978	892	876	97	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 57.

All (97) 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:A:14[B]:DLE:HD23	1:A:15[B]:TRP:CE3	1.38	1.58
1:A:14[B]:DLE:CD2	1:A:15[B]:TRP:CD2	1.97	1.47
1:A:14[B]:DLE:CD2	1:A:15[B]:TRP:CE3	1.98	1.46
1:D:4[A]:DLE:CD1	3:D:101[A]:IOD:I	2.39	1.41
1:D:4[A]:DLE:HD11	3:D:101[A]:IOD:I	1.91	1.40
1:A:15[A]:TRP:CD1	1:B:1[A]:FVA:HG13	1.67	1.29
2:C:106:K:K	5:D:2004:HOH:O	1.40	1.28
2:A:107:K:K	5:B:208:HOH:O	1.42	1.28
2:C:106:K:K	5:D:2002:HOH:O	1.13	1.19
1:D:4[A]:DLE:HD12	3:D:101[A]:IOD:I	2.08	1.18
1:C:11[A]:TRP:CH2	4:C:103[A]:MOH:C	2.28	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7[B]:VAL:HG23	1:B:8[B]:DVA:CG2	1.74	1.16
1:A:14[B]:DLE:HD21	1:A:15[B]:TRP:CH2	1.81	1.15
5:C:223:HOH:O	1:D:4[A]:DLE:HD11	1.00	1.15
2:A:107:K:K	5:A:206:HOH:O	1.55	1.14
1:A:7[B]:VAL:HG23	1:B:8[B]:DVA:HG22	1.31	1.13
1:A:14[B]:DLE:HD21	1:A:15[B]:TRP:CE2	1.83	1.13
1:A:14[B]:DLE:HD22	1:A:15[B]:TRP:CD2	1.84	1.10
1:A:14[B]:DLE:HD21	1:A:15[B]:TRP:CZ2	1.87	1.08
1:A:14[B]:DLE:CD2	1:A:15[B]:TRP:CE2	2.38	1.07
1:A:15[A]:TRP:CD1	1:B:1[A]:FVA:CG1	2.39	1.06
1:A:14[B]:DLE:CD2	1:A:15[B]:TRP:CZ3	2.39	1.04
1:A:14[B]:DLE:HD21	1:A:15[B]:TRP:CZ3	1.93	1.03
1:A:12[A]:DLE:HD13	1:B:10[A]:DLE:HD22	1.42	0.99
1:A:14[B]:DLE:HD21	1:A:15[B]:TRP:CE3	1.95	0.98
1:D:8[B]:DVA:HG23	1:D:9[B]:TRP:CZ3	1.99	0.98
1:C:11[A]:TRP:HH2	4:C:103[A]:MOH:C	1.74	0.96
1:A:12[A]:DLE:CD1	1:B:10[A]:DLE:HD22	1.99	0.93
1:C:4[B]:DLE:CD1	1:D:12[B]:DLE:HB3	2.01	0.91
4:C:104:MOH:C	5:C:202:HOH:O	2.17	0.90
1:A:15[A]:TRP:HD1	1:B:1[A]:FVA:HG13	1.38	0.88
2:C:105:K:K	5:D:2002:HOH:O	0.79	0.85
1:C:11[A]:TRP:CZ2	4:C:103[A]:MOH:C	2.60	0.84
1:B:12[B]:DLE:HG	1:B:12[B]:DLE:O	1.78	0.84
1:A:14[B]:DLE:HD23	1:A:15[B]:TRP:CD2	1.89	0.80
1:A:15[A]:TRP:NE1	1:B:1[A]:FVA:CG1	2.46	0.78
1:A:9[A]:TRP:CZ3	5:A:230:HOH:O	2.37	0.78
5:C:223:HOH:O	1:D:4[A]:DLE:CD1	1.76	0.76
1:B:8[A]:DVA:HG23	1:B:9[A]:TRP:CE3	2.20	0.75
1:A:7[B]:VAL:HG23	1:B:8[B]:DVA:HG21	1.68	0.74
1:C:4[B]:DLE:HD13	1:D:12[B]:DLE:HB3	1.70	0.73
1:A:14[B]:DLE:HD23	1:A:15[B]:TRP:CZ3	2.08	0.72
1:B:4[B]:DLE:HD22	1:D:4[B]:DLE:HD22	1.72	0.71
1:A:14[B]:DLE:HD22	1:A:15[B]:TRP:CG	2.28	0.69
1:A:14[B]:DLE:HD21	1:A:15[B]:TRP:CD2	1.92	0.69
1:A:12[A]:DLE:CD1	1:B:10[A]:DLE:CD2	2.71	0.69
1:C:7[B]:VAL:HG22	1:D:15[B]:TRP:HE3	1.58	0.67
1:D:8[B]:DVA:CG2	1:D:9[B]:TRP:CZ3	2.77	0.67
1:A:15[A]:TRP:HD1	1:B:1[A]:FVA:CG1	1.97	0.67
1:A:9[A]:TRP:HZ3	5:A:230:HOH:O	1.76	0.66
1:A:7[B]:VAL:CG2	1:B:8[B]:DVA:HG22	2.17	0.66
1:D:8[B]:DVA:CG2	1:D:9[B]:TRP:CH2	2.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15[A]:TRP:HE1	1:B:1[A]:FVA:HG11	1.61	0.65
1:B:12[B]:DLE:HD11	5:D:2014:HOH:O	1.98	0.64
1:A:15[A]:TRP:NE1	1:B:1[A]:FVA:HG13	2.05	0.63
1:B:4[B]:DLE:CD2	1:D:4[B]:DLE:HD22	2.30	0.60
1:A:14[B]:DLE:HD22	1:A:15[B]:TRP:CE2	2.23	0.59
1:A:6[B]:DVA:HG22	1:B:10[B]:DLE:CD2	2.33	0.59
1:A:9[A]:TRP:CH2	5:A:230:HOH:O	2.54	0.59
1:D:8[B]:DVA:HG23	1:D:9[B]:TRP:CH2	2.38	0.58
1:B:12[B]:DLE:O	1:B:12[B]:DLE:CG	2.50	0.58
1:A:10[B]:DLE:HD21	1:B:6[B]:DVA:HG22	1.86	0.58
1:A:6[B]:DVA:O	1:A:6[B]:DVA:HG23	2.04	0.57
1:A:10[B]:DLE:CD2	1:B:6[B]:DVA:CG2	2.82	0.57
1:C:4[B]:DLE:HD11	1:D:12[B]:DLE:HB3	1.81	0.57
1:B:10[A]:DLE:HG	1:B:11[A]:TRP:NE1	2.20	0.55
1:A:15[A]:TRP:HE1	1:B:1[A]:FVA:CG1	2.15	0.55
1:B:12[B]:DLE:CD1	5:D:2014:HOH:O	2.54	0.55
1:C:15[B]:TRP:CD1	1:D:1[B]:FVA:HG13	2.42	0.55
1:D:8[B]:DVA:HG23	1:D:9[B]:TRP:CE3	2.43	0.53
1:A:10[B]:DLE:HD21	1:B:6[B]:DVA:CG2	2.38	0.53
1:A:12[A]:DLE:HD13	1:B:10[A]:DLE:CD2	2.28	0.52
1:A:1[B]:FVA:HG22	1:B:14[B]:DLE:HD12	1.91	0.52
1:A:10[B]:DLE:CD2	1:B:6[B]:DVA:HG23	2.40	0.52
1:A:10[B]:DLE:CD2	1:B:6[B]:DVA:HG22	2.41	0.50
1:C:7[B]:VAL:CG2	1:D:15[B]:TRP:HE3	2.22	0.50
1:C:16:ETA:O	5:C:201:HOH:O	2.20	0.50
1:A:15[A]:TRP:NE1	1:B:1[A]:FVA:HG11	2.19	0.49
1:A:8:DVA:C	5:A:210:HOH:O	2.60	0.49
1:B:8[A]:DVA:HG23	1:B:9[A]:TRP:CZ3	2.48	0.49
1:B:9[B]:TRP:CH2	4:C:103[B]:MOH:O	2.67	0.48
1:A:6[B]:DVA:HG22	1:B:10[B]:DLE:HD22	1.96	0.48
1:D:1[B]:FVA:CN	1:D:1[B]:FVA:CG1	2.93	0.47
1:B:10[A]:DLE:HG	1:B:11[A]:TRP:CD1	2.53	0.44
1:A:6[B]:DVA:O	1:A:6[B]:DVA:CG2	2.66	0.43
1:B:4[B]:DLE:CD2	1:D:4[B]:DLE:CD2	2.96	0.43
1:A:7[A]:VAL:CG1	1:B:9[A]:TRP:CD1	3.03	0.42
3:A:104[A]:IOD:I	5:A:216:HOH:O	2.81	0.41
1:A:10[A]:DLE:CD1	1:B:12[A]:DLE:HD22	2.51	0.41
1:B:8[A]:DVA:CG2	1:B:9[A]:TRP:CE3	2.99	0.41
1:A:13[B]:TRP:CH2	1:B:9[B]:TRP:CH2	2.69	0.41
2:A:107:K:K	5:B:209:HOH:O	0.34	0.41
1:C:6[A]:DVA:HG12	1:C:7[A]:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	11/18 (61%)	11 (100%)	0	0	100	100
1	B	12/18 (67%)	12 (100%)	0	0	100	100
1	C	11/18 (61%)	11 (100%)	0	0	100	100
1	D	12/18 (67%)	12 (100%)	0	0	100	100
All	All	46/72 (64%)	46 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	11/7 (157%)	11 (100%)	0	100	100
1	B	9/7 (129%)	9 (100%)	0	100	100
1	C	11/7 (157%)	11 (100%)	0	100	100
1	D	10/7 (143%)	10 (100%)	0	100	100
All	All	41/28 (146%)	41 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

68 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	FVA	B	1[B]	-	7,8,9	1.18	1 (14%)	8,9,11	2.19	2 (25%)
1	ETA	B	16[A]	-	3,3,3	0.47	0	2,2,2	0.62	0
1	ETA	A	16[A]	1	3,3,3	0.94	0	2,2,2	0.87	0
1	ETA	C	16	1	3,3,3	0.96	0	2,2,2	2.06	1 (50%)
1	ETA	B	16[B]	-	3,3,3	0.42	0	2,2,2	0.23	0
1	ETA	A	16[B]	1	3,3,3	0.64	0	2,2,2	0.96	0
1	FVA	A	1[A]	2	7,8,9	1.05	0	8,9,11	2.02	1 (12%)
1	ETA	D	16[A]	1	3,3,3	0.66	0	2,2,2	0.48	0
1	FVA	D	1[A]	2	7,8,9	1.05	0	8,9,11	4.43	5 (62%)
1	FVA	A	1[B]	-	7,8,9	0.56	0	8,9,11	1.72	3 (37%)
1	FVA	D	1[B]	-	7,8,9	1.30	1 (14%)	8,9,11	4.12	5 (62%)
1	FVA	C	1[A]	-	7,8,9	0.86	0	8,9,11	1.44	1 (12%)
1	FVA	C	1[B]	-	7,8,9	0.45	0	8,9,11	2.15	3 (37%)
1	ETA	D	16[B]	1	3,3,3	0.24	0	2,2,2	0.59	0
1	FVA	B	1[A]	-	7,8,9	1.18	1 (14%)	8,9,11	4.85	4 (50%)

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	FVA	B	1[B]	-	-	2/7/9/11	-
1	ETA	B	16[A]	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ETA	A	16[A]	1	-	1/1/1/1	-
1	ETA	C	16	1	-	0/1/1/1	-
1	ETA	B	16[B]	-	-	0/1/1/1	-
1	ETA	A	16[B]	1	-	0/1/1/1	-
1	FVA	A	1[A]	2	-	0/7/9/11	-
1	ETA	D	16[A]	1	-	0/1/1/1	-
1	FVA	D	1[A]	2	-	1/7/9/11	-
1	FVA	A	1[B]	-	-	1/7/9/11	-
1	FVA	D	1[B]	-	-	5/7/9/11	-
1	FVA	C	1[A]	-	-	0/7/9/11	-
1	FVA	C	1[B]	-	-	2/7/9/11	-
1	ETA	D	16[B]	1	-	1/1/1/1	-
1	FVA	B	1[A]	-	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1[B]	FVA	CG1-CB	2.17	1.60	1.52
1	B	1[A]	FVA	CN-N	-2.03	1.26	1.33
1	B	1[B]	FVA	CN-N	-2.03	1.26	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1[A]	FVA	CB-CA-N	11.99	126.78	111.17
1	D	1[B]	FVA	CG2-CB-CA	9.74	126.13	111.21
1	D	1[A]	FVA	CB-CA-N	-8.56	100.03	111.17
1	D	1[A]	FVA	CG2-CB-CA	-7.12	100.30	111.21
1	B	1[A]	FVA	CB-CA-C	-5.34	106.34	113.04
1	B	1[B]	FVA	CB-CA-N	-5.04	104.61	111.17
1	A	1[A]	FVA	CB-CA-C	-4.99	106.79	113.04
1	D	1[A]	FVA	CG1-CB-CA	3.96	117.27	111.21
1	D	1[B]	FVA	CG2-CB-CG1	-3.89	99.72	110.59
1	C	1[A]	FVA	CB-CA-C	-3.36	108.83	113.04
1	C	1[B]	FVA	CB-CA-C	-3.36	108.83	113.04
1	C	1[B]	FVA	O-C-CA	-3.32	115.58	124.83
1	B	1[B]	FVA	CG2-CB-CA	-3.27	106.21	111.21
1	D	1[B]	FVA	CG1-CB-CA	-2.96	106.67	111.21
1	C	1[B]	FVA	CB-CA-N	-2.96	107.32	111.17
1	C	16	ETA	O-C-CA	-2.90	100.80	111.48
1	D	1[A]	FVA	CG2-CB-CG1	2.82	118.48	110.59
1	D	1[B]	FVA	CB-CA-N	2.52	114.44	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1[B]	FVA	CB-CA-C	-2.50	109.90	113.04
1	D	1[B]	FVA	CB-CA-C	-2.41	110.02	113.04
1	B	1[A]	FVA	O1-CN-N	2.38	131.54	125.27
1	B	1[A]	FVA	O-C-CA	-2.29	118.44	124.83
1	A	1[B]	FVA	CB-CA-N	2.22	114.06	111.17
1	D	1[A]	FVA	CA-N-CN	-2.11	118.85	122.42
1	A	1[B]	FVA	CG1-CB-CA	-2.04	108.08	111.21

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1[B]	FVA	C-CA-CB-CG1
1	B	1[A]	FVA	O-C-CA-CB
1	B	1[B]	FVA	O1-CN-N-CA
1	C	1[B]	FVA	O1-CN-N-CA
1	D	1[A]	FVA	O-C-CA-CB
1	D	1[B]	FVA	O1-CN-N-CA
1	D	1[B]	FVA	C-CA-CB-CG1
1	D	1[B]	FVA	C-CA-CB-CG2
1	D	1[B]	FVA	N-CA-CB-CG1
1	D	1[B]	FVA	N-CA-CB-CG2
1	A	16[A]	ETA	O-C-CA-N
1	D	16[B]	ETA	O-C-CA-N
1	B	1[B]	FVA	O-C-CA-CB
1	C	1[B]	FVA	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	16	ETA	1	0
1	A	1[B]	FVA	1	0
1	D	1[B]	FVA	2	0
1	B	1[A]	FVA	9	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 14 are monoatomic - leaving 9 for Mogul analysis.

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	$\#\|Z\| > 2$
4	MOH	C	104	-	1,1,1	0.19	0	-		
4	MOH	D	103	-	1,1,1	0.66	0	-		
4	MOH	C	103[A]	-	1,1,1	1.13	0	-		
4	MOH	C	102	-	1,1,1	0.01	0	-		
4	MOH	A	108	-	1,1,1	0.19	0	-		
4	MOH	C	101[A]	-	1,1,1	0.96	0	-		
4	MOH	C	103[B]	-	1,1,1	0.20	0	-		
4	MOH	C	101[B]	-	1,1,1	0.84	0	-		
4	MOH	A	106	-	1,1,1	1.09	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	104	MOH	1	0
4	C	103[A]	MOH	3	0
4	C	103[B]	MOH	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	10:DLE	C	11[B]:TYR	N	1.18
1	A	10:DLE	C	11[C]:PHE	N	1.01

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.