



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 12:13 am GMT

PDB ID : 1C4D
Title : GRAMICIDIN CSCL COMPLEX
Authors : Wallace, B.A.
Deposited on : 1999-06-04
Resolution : 2.00 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

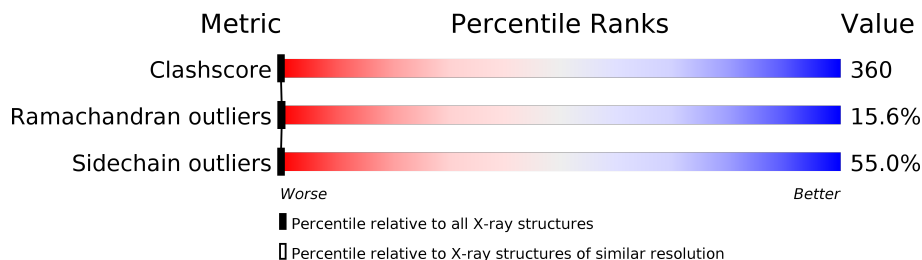
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	122078	8264 (2.00-2.00)
Ramachandran outliers	120005	8163 (2.00-2.00)
Sidechain outliers	119972	8162 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	16	
1	B	16	
1	C	16	
1	D	16	

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	FVA	A	1	-	-	X	-
1	DLE	A	10	-	-	X	-
1	DLE	A	14	-	-	X	-
1	ETA	A	16	-	-	X	-
1	DLE	A	4	-	-	X	-
1	DVA	A	6	X	-	X	-
1	DVA	A	8	-	-	X	-
1	FVA	B	1	-	-	X	-
1	DLE	B	10	-	-	X	-
1	DLE	B	12	-	-	X	-
1	DLE	B	14	-	-	X	-
1	ETA	B	16	-	-	X	-
1	DLE	B	4	-	-	X	-
1	DVA	B	6	-	-	X	-
1	DVA	B	8	-	-	X	-
1	DLE	C	10	-	-	X	-
1	DLE	C	14	-	-	X	-
1	ETA	C	16	-	-	X	-
1	DLE	C	4	-	-	X	-
1	DVA	C	6	-	-	X	-
1	DVA	C	8	X	-	X	-
1	FVA	D	1	-	-	X	-
1	DLE	D	10	-	-	X	-
1	DLE	D	12	-	-	X	-
1	DLE	D	14	-	-	X	-
1	ETA	D	16	-	-	X	-
1	DLE	D	4	-	-	X	-
1	DVA	D	6	-	-	X	-
1	DVA	D	8	X	-	X	-
3	CL	A	119	-	-	X	-
3	CL	C	118	-	-	X	-
3	CL	D	119	-	-	X	-
4	MOH	A	133	-	-	X	-
4	MOH	D	131	-	-	X	-
4	MOH	D	132	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 604 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 GRAMICIDIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	16	Total	C	N	O	0	0	0
			136	99	20	17			
1	B	16	Total	C	N	O	0	0	0
			136	99	20	17			
1	C	16	Total	C	N	O	0	0	0
			136	99	20	17			
1	D	16	Total	C	N	O	0	0	0
			136	99	20	17			

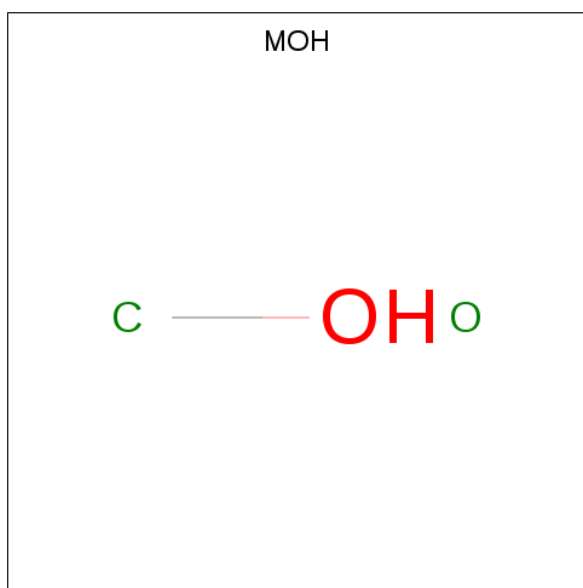
- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is METHANOL (three-letter code: MOH) (formula: CH₄O).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	7	Total 7	O 7	0	0
5	C	7	Total 7	O 7	0	0
5	D	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

• Molecule 1: GRAMICIDIN A

Chain A: 



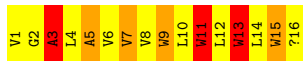
• Molecule 1: GRAMICIDIN A

Chain B: 

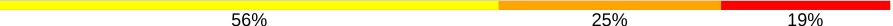


• Molecule 1: GRAMICIDIN A

Chain C: 



• Molecule 1: GRAMICIDIN A

Chain D: 



4 Data and refinement statistics

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	32.12Å 52.10Å 31.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	604	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: DLE, CL, ETA, DVA, FVA, MOH, CS

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	2.42	4/78 (5.1%)	1.63	1/100 (1.0%)
1	B	1.77	1/78 (1.3%)	2.07	3/100 (3.0%)
1	C	2.71	8/78 (10.3%)	1.54	0/100
1	D	1.63	0/78	2.12	4/100 (4.0%)
All	All	2.18	13/312 (4.2%)	1.86	8/400 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
1	C	1	0
1	D	1	2
All	All	3	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	CB-CG	-10.87	1.30	1.50
1	C	13	TRP	CB-CG	-8.24	1.35	1.50
1	C	15	TRP	CB-CG	-8.21	1.35	1.50
1	B	13	TRP	CE3-CZ3	-7.55	1.25	1.38
1	A	11	TRP	CG-CD1	-7.50	1.26	1.36
1	C	3	ALA	CA-CB	-7.17	1.37	1.52
1	C	13	TRP	CG-CD1	-7.07	1.26	1.36
1	A	13	TRP	CB-CG	-6.64	1.38	1.50
1	C	9	TRP	CB-CG	6.19	1.61	1.50
1	C	13	TRP	CD2-CE2	-5.52	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	ALA	CA-CB	5.48	1.64	1.52
1	A	3	ALA	CA-CB	-5.25	1.41	1.52
1	C	11	TRP	CE3-CZ3	-5.21	1.29	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	VAL	CB-CA-C	10.02	130.44	111.40
1	D	7	VAL	CG1-CB-CG2	8.26	124.11	110.90
1	B	9	TRP	N-CA-CB	5.95	121.31	110.60
1	B	9	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	B	13	TRP	CB-CA-C	5.40	121.20	110.40
1	D	7	VAL	N-CA-CB	-5.17	100.12	111.50
1	D	9	TRP	N-CA-CB	5.05	119.70	110.60
1	A	15	TRP	CB-CA-C	-5.01	100.39	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	6	DVA	CA
1	C	8	DVA	CA
1	D	8	DVA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3	ALA	Mainchain
1	D	12	DLE	Mainchain
1	D	15	TRP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	136	0	131	158	1
1	B	136	0	132	154	0
1	C	136	0	131	167	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	136	0	128	173	0
2	A	3	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
3	A	2	0	0	2	0
3	B	1	0	0	1	0
3	C	2	0	0	2	0
3	D	1	0	0	4	0
4	A	8	0	0	3	0
4	B	6	0	0	1	0
4	C	4	0	0	2	0
4	D	8	0	0	11	1
5	A	4	0	0	5	0
5	B	7	0	0	8	0
5	C	7	0	0	2	0
5	D	2	0	0	10	0
All	All	604	0	522	398	2

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 360.

All (398) 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:10:DLE:HB2	1:C:11:TRP:CZ3	1.63	1.31
1:A:9:TRP:NE1	1:B:11:TRP:HB2	1.47	1.28
1:A:6:DVA:CG2	1:B:8:DVA:HA	1.70	1.22
1:A:1:FVA:HG13	1:B:13:TRP:CZ3	1.83	1.13
1:C:7:VAL:HG12	1:D:7:VAL:HG13	1.24	1.13
1:A:11:TRP:CZ2	1:B:4:DLE:HD23	1.83	1.13
1:A:6:DVA:HG21	1:B:8:DVA:CA	1.77	1.13
1:C:7:VAL:HA	5:D:2001:HOH:O	1.46	1.12
1:A:9:TRP:HA	1:B:10:DLE:O	1.51	1.11
1:C:8:DVA:HG22	1:C:9:TRP:H	1.13	1.11
1:A:4:DLE:HB3	1:B:10:DLE:CG	1.81	1.10
1:A:10:DLE:O	1:B:9:TRP:HA	1.49	1.10
1:A:4:DLE:CB	1:B:10:DLE:HG	1.80	1.10
1:C:14:DLE:HA	1:D:1:FVA:O1	1.52	1.09
1:C:10:DLE:O	1:D:9:TRP:HA	1.53	1.08
1:A:14:DLE:HB3	1:B:6:DVA:HB	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:TRP:CE2	1:D:11:TRP:HB2	1.88	1.08
1:C:9:TRP:HA	1:D:10:DLE:O	1.53	1.07
1:C:3:ALA:HB3	1:D:11:TRP:CD1	1.89	1.07
1:A:6:DVA:HG13	1:A:7:VAL:HG12	1.20	1.06
1:D:13:TRP:HA	5:D:2001:HOH:O	1.55	1.06
1:A:11:TRP:HE1	1:B:4:DLE:HD12	1.12	1.05
1:A:5:ALA:O	1:A:6:DVA:HG23	1.55	1.05
1:C:8:DVA:HG21	1:D:6:DVA:CA	1.86	1.05
1:A:16:ETA:O	1:B:4:DLE:HD13	1.55	1.04
1:A:4:DLE:HD22	1:B:16:ETA:HB1	1.38	1.03
1:C:3:ALA:HB3	1:D:11:TRP:NE1	1.73	1.02
1:A:11:TRP:HB3	1:B:9:TRP:CZ3	1.94	1.02
1:C:8:DVA:HG13	4:C:120:MOH:C	1.88	1.02
1:C:8:DVA:HG21	1:D:6:DVA:CB	1.92	1.00
1:A:14:DLE:HD11	1:A:15:TRP:CZ2	1.98	0.99
1:C:5:ALA:O	1:D:8:DVA:HG13	1.63	0.98
1:C:12:DLE:O	1:D:7:VAL:HA	1.64	0.98
1:D:11:TRP:CZ3	1:D:12:DLE:HD23	1.99	0.98
1:C:11:TRP:HB3	1:D:9:TRP:NE1	1.78	0.97
1:C:10:DLE:HD13	1:D:10:DLE:O	1.65	0.96
1:A:11:TRP:HZ2	1:B:4:DLE:HD23	1.15	0.96
1:A:6:DVA:HG21	1:B:8:DVA:HA	0.96	0.95
1:C:9:TRP:NE1	1:D:11:TRP:HB2	1.80	0.95
1:C:7:VAL:O	1:C:8:DVA:HG23	1.69	0.93
1:A:10:DLE:HD13	1:A:10:DLE:N	1.84	0.92
1:C:13:TRP:HA	1:D:6:DVA:O	1.69	0.92
1:C:4:DLE:CA	1:D:10:DLE:HD21	2.00	0.92
1:C:5:ALA:HA	1:D:14:DLE:O	1.69	0.92
1:C:4:DLE:HD13	1:D:16:ETA:HB2	1.53	0.91
1:A:6:DVA:HG11	1:B:8:DVA:CG1	2.01	0.91
1:B:11:TRP:CE3	1:B:12:DLE:HB3	2.06	0.90
1:A:11:TRP:HB3	1:B:9:TRP:CE3	2.06	0.90
1:C:8:DVA:HG23	1:D:7:VAL:H	1.36	0.89
1:C:8:DVA:HG11	1:D:6:DVA:HB	1.54	0.89
1:A:7:VAL:HG13	1:B:7:VAL:HG13	1.54	0.89
1:A:13:TRP:HA	1:B:6:DVA:O	1.73	0.89
1:C:4:DLE:HA	1:D:10:DLE:CG	2.03	0.89
1:A:1:FVA:HG13	1:B:13:TRP:HZ3	1.28	0.89
1:A:9:TRP:HE1	1:B:11:TRP:HB2	1.34	0.88
1:C:6:DVA:HA	1:D:8:DVA:CG1	2.04	0.88
1:A:14:DLE:HD11	1:A:15:TRP:CE2	2.09	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HA	1:B:12:DLE:O	1.75	0.87
1:A:6:DVA:HG11	1:B:8:DVA:HG13	1.56	0.86
1:A:4:DLE:HD22	1:B:16:ETA:CB	2.05	0.86
1:C:8:DVA:HG22	1:C:9:TRP:N	1.82	0.86
1:A:10:DLE:HB3	1:A:11:TRP:CZ3	2.10	0.85
1:A:11:TRP:HZ2	1:B:4:DLE:CD2	1.89	0.85
1:A:14:DLE:HB3	1:B:6:DVA:CB	2.03	0.84
1:A:11:TRP:CD1	1:B:3:ALA:O	2.30	0.84
1:A:14:DLE:HD12	1:B:6:DVA:CG1	2.07	0.84
1:C:16:ETA:HA1	4:D:131:MOH:O	1.78	0.84
1:D:9:TRP:O	1:D:10:DLE:HD22	1.78	0.84
1:A:1:FVA:CG1	1:B:13:TRP:HZ3	1.89	0.83
1:A:16:ETA:HB2	1:B:4:DLE:N	1.93	0.83
1:B:1:FVA:CN	1:B:1:FVA:HG23	2.08	0.83
1:C:10:DLE:HB2	1:C:11:TRP:HZ3	1.43	0.83
1:C:6:DVA:HA	1:D:8:DVA:HG11	1.59	0.83
1:A:14:DLE:CB	1:B:6:DVA:HB	2.04	0.82
1:A:10:DLE:HB3	1:A:11:TRP:CE3	2.15	0.82
1:A:11:TRP:NE1	1:B:4:DLE:HD12	1.93	0.82
1:B:3:ALA:HB1	1:B:4:DLE:CD1	2.10	0.81
1:C:10:DLE:HD13	1:D:10:DLE:C	2.10	0.81
1:A:10:DLE:HG	1:B:10:DLE:CA	2.10	0.81
1:A:9:TRP:CE3	1:A:10:DLE:HD11	2.15	0.80
1:C:4:DLE:HB3	1:D:16:ETA:HB2	1.64	0.79
1:A:12:DLE:O	1:B:7:VAL:HA	1.82	0.79
1:C:10:DLE:HB2	1:C:11:TRP:CE3	2.17	0.79
1:B:5:ALA:O	5:B:2005:HOH:O	2.00	0.79
1:D:13:TRP:H	4:D:132:MOH:C	1.94	0.79
1:A:3:ALA:O	1:B:10:DLE:HD13	1.81	0.79
2:B:116:CS:CS	5:B:2003:HOH:O	2.29	0.79
1:A:7:VAL:HA	1:B:13:TRP:HB3	1.64	0.79
1:A:6:DVA:O	1:B:13:TRP:HA	1.84	0.78
1:C:4:DLE:C	1:D:10:DLE:HD21	2.14	0.78
1:A:5:ALA:HA	1:B:14:DLE:O	1.85	0.77
1:A:1:FVA:CG1	1:B:13:TRP:CZ3	2.64	0.77
1:A:10:DLE:O	1:B:9:TRP:CA	2.33	0.77
1:A:9:TRP:CD1	1:B:11:TRP:HB2	2.20	0.77
1:A:3:ALA:HA	1:B:16:ETA:O	1.85	0.76
1:A:3:ALA:HB3	1:B:11:TRP:NE1	2.00	0.76
1:A:6:DVA:HG22	1:A:7:VAL:H	1.51	0.76
1:D:1:FVA:HG21	4:D:121:MOH:C	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:DLE:O	1:D:6:DVA:N	2.18	0.76
1:C:4:DLE:CA	1:D:10:DLE:HD11	2.14	0.76
1:D:1:FVA:CN	1:D:1:FVA:CG2	2.64	0.76
1:C:4:DLE:CD1	1:D:16:ETA:HB2	2.15	0.76
1:A:6:DVA:HG13	1:A:7:VAL:CG1	2.12	0.76
1:D:12:DLE:O	5:D:2001:HOH:O	2.04	0.75
1:C:2:GLY:HA3	4:D:132:MOH:C	2.16	0.75
1:C:6:DVA:N	1:D:14:DLE:HB3	2.02	0.75
1:A:4:DLE:CD2	1:B:16:ETA:HB1	2.15	0.74
1:C:8:DVA:CG2	1:D:7:VAL:H	2.00	0.74
1:C:8:DVA:HG21	1:D:6:DVA:HB	1.69	0.74
1:A:4:DLE:O	1:B:15:TRP:HA	1.88	0.74
1:C:10:DLE:CB	1:C:11:TRP:CZ3	2.58	0.74
1:C:4:DLE:HA	1:D:10:DLE:HD21	1.69	0.74
1:C:11:TRP:CZ2	1:D:4:DLE:HD11	2.22	0.74
1:A:13:TRP:CZ3	1:B:1:FVA:HG22	2.23	0.74
1:C:10:DLE:HD22	1:C:11:TRP:HZ3	1.52	0.74
1:C:9:TRP:CD1	1:D:11:TRP:HB2	2.23	0.73
1:A:16:ETA:HA1	5:A:2003:HOH:O	1.88	0.73
1:C:12:DLE:HB3	1:D:2:GLY:HA3	1.70	0.73
1:C:3:ALA:HA	1:D:16:ETA:O	1.89	0.72
1:A:9:TRP:HB2	5:B:2005:HOH:O	1.89	0.72
1:B:3:ALA:HB1	1:B:4:DLE:HD13	1.71	0.72
1:A:6:DVA:HG23	1:B:9:TRP:H	1.53	0.72
1:C:10:DLE:O	1:D:9:TRP:CA	2.36	0.72
1:A:5:ALA:HB2	1:B:15:TRP:CE3	2.23	0.71
1:A:14:DLE:O	1:B:5:ALA:HA	1.89	0.71
1:C:10:DLE:HD22	1:C:11:TRP:CZ3	2.26	0.71
1:A:11:TRP:HE1	1:B:4:DLE:CD1	1.97	0.71
1:B:11:TRP:CG	1:B:11:TRP:O	2.42	0.71
1:C:4:DLE:HA	1:D:10:DLE:CD2	2.19	0.71
1:C:13:TRP:HD1	1:D:7:VAL:HG23	1.56	0.70
1:D:1:FVA:HG22	1:D:1:FVA:CN	2.21	0.70
1:C:11:TRP:HD1	1:D:3:ALA:HB3	1.57	0.70
1:C:5:ALA:CA	1:D:14:DLE:O	2.40	0.70
1:C:4:DLE:HD22	1:D:10:DLE:HD23	1.74	0.70
1:C:4:DLE:N	1:D:16:ETA:O	2.24	0.70
1:C:14:DLE:O	1:D:5:ALA:HA	1.92	0.69
1:C:4:DLE:HA	1:D:10:DLE:HG	1.73	0.69
5:A:2003:HOH:O	3:B:117:CL:CL	2.46	0.69
1:A:9:TRP:CE3	1:A:10:DLE:CD1	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:122:MOH:C	1:D:6:DVA:HG21	2.23	0.69
1:C:11:TRP:HB3	1:D:9:TRP:CD1	2.26	0.69
1:A:10:DLE:HG	1:B:10:DLE:N	2.07	0.69
1:A:1:FVA:O	1:B:13:TRP:O	2.11	0.69
1:D:11:TRP:CG	1:D:11:TRP:O	2.46	0.68
1:C:14:DLE:HB2	1:D:6:DVA:HG12	1.75	0.68
1:C:13:TRP:O	1:D:1:FVA:O1	2.11	0.68
1:A:7:VAL:CG1	1:B:7:VAL:HG13	2.22	0.68
1:A:4:DLE:HB3	1:B:10:DLE:HG	0.87	0.68
1:A:9:TRP:C	1:A:10:DLE:HD13	2.13	0.68
1:C:10:DLE:C	1:C:11:TRP:CE3	2.78	0.67
1:C:8:DVA:CG1	1:D:6:DVA:HB	2.23	0.67
1:A:11:TRP:HA	1:B:8:DVA:O	1.93	0.67
1:A:3:ALA:HB3	1:B:11:TRP:CD1	2.29	0.67
1:A:16:ETA:CB	1:B:4:DLE:HD13	2.24	0.67
1:C:3:ALA:H	4:D:132:MOH:C	2.08	0.67
1:C:7:VAL:CG1	1:D:7:VAL:HG13	2.15	0.66
1:A:16:ETA:HB1	1:B:4:DLE:HG	1.78	0.66
1:D:11:TRP:CE3	1:D:12:DLE:HD12	2.30	0.66
1:C:13:TRP:CD1	1:D:7:VAL:HG23	2.30	0.66
1:C:16:ETA:HB2	1:D:4:DLE:HB2	1.78	0.66
3:C:118:CL:CL	4:D:132:MOH:C	2.81	0.66
1:A:6:DVA:HG11	1:B:8:DVA:HG12	1.76	0.66
1:A:11:TRP:CE2	1:B:4:DLE:HD23	2.30	0.66
1:C:11:TRP:CD1	1:D:3:ALA:HB3	2.31	0.65
1:D:15:TRP:C	1:D:15:TRP:CD1	2.70	0.65
1:A:10:DLE:CB	1:A:11:TRP:CE3	2.80	0.65
3:A:119:CL:CL	4:A:133:MOH:C	2.81	0.65
1:C:11:TRP:HZ2	1:D:4:DLE:HD11	1.60	0.65
1:C:3:ALA:CB	1:D:11:TRP:NE1	2.55	0.65
1:B:14:DLE:HD23	1:B:15:TRP:N	2.12	0.64
1:C:14:DLE:N	1:D:6:DVA:O	2.30	0.64
1:A:14:DLE:O	1:B:6:DVA:N	2.30	0.64
1:C:8:DVA:O	1:D:11:TRP:HA	1.95	0.64
1:D:15:TRP:CD1	1:D:15:TRP:O	2.50	0.64
1:C:4:DLE:CB	1:D:16:ETA:HB2	2.26	0.64
1:C:4:DLE:HA	1:D:10:DLE:HD11	1.80	0.64
5:A:2001:HOH:O	1:B:2:GLY:HA3	1.98	0.64
1:A:14:DLE:CD1	1:A:15:TRP:CE2	2.80	0.64
1:A:4:DLE:N	1:B:16:ETA:HB2	2.13	0.63
1:B:12:DLE:HG	1:B:13:TRP:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:DLE:HD11	1:A:15:TRP:CH2	2.33	0.63
1:C:6:DVA:HB	1:D:14:DLE:HB2	1.81	0.63
1:C:4:DLE:HA	1:D:10:DLE:CD1	2.28	0.63
1:A:6:DVA:CG1	1:A:7:VAL:HG12	2.12	0.62
1:C:9:TRP:CZ2	1:D:11:TRP:CE3	2.87	0.62
1:D:11:TRP:CE3	1:D:12:DLE:HB3	2.34	0.62
1:C:1:FVA:O	1:D:13:TRP:O	2.16	0.62
1:C:9:TRP:CH2	1:D:11:TRP:CE3	2.87	0.62
1:A:16:ETA:HB2	1:B:4:DLE:CB	2.29	0.62
1:B:5:ALA:CB	5:B:2005:HOH:O	2.47	0.62
1:C:6:DVA:HB	1:D:14:DLE:CB	2.30	0.62
1:A:6:DVA:HG21	1:B:8:DVA:CG1	2.29	0.62
1:C:2:GLY:HA3	1:D:12:DLE:HB2	1.82	0.62
1:D:3:ALA:C	1:D:4:DLE:HD22	2.20	0.62
1:A:7:VAL:HG13	1:B:7:VAL:CG1	2.29	0.61
1:C:9:TRP:CD2	1:D:11:TRP:HB2	2.35	0.61
1:A:14:DLE:HG	1:A:15:TRP:CE3	2.36	0.61
1:A:5:ALA:HB2	1:B:15:TRP:HE3	1.64	0.61
1:A:14:DLE:HD21	1:A:15:TRP:CZ3	2.36	0.61
1:C:7:VAL:O	1:C:8:DVA:HG12	2.01	0.60
1:C:9:TRP:NE1	1:D:11:TRP:CB	2.62	0.60
1:B:14:DLE:HD12	1:B:15:TRP:H	1.66	0.60
1:D:4:DLE:HD22	1:D:4:DLE:N	2.17	0.60
1:C:8:DVA:O	1:C:9:TRP:CE3	2.55	0.59
1:B:11:TRP:CD2	1:B:11:TRP:O	2.55	0.59
1:A:11:TRP:CB	1:B:9:TRP:CZ3	2.78	0.59
1:C:8:DVA:HG21	1:D:6:DVA:CG2	2.32	0.59
1:C:10:DLE:CD2	1:C:11:TRP:HZ3	2.16	0.58
1:C:1:FVA:HG13	1:D:13:TRP:CE3	2.38	0.58
1:A:12:DLE:HA	5:A:2001:HOH:O	2.03	0.58
1:B:11:TRP:CZ3	1:B:12:DLE:HB3	2.39	0.58
1:C:4:DLE:CB	1:D:10:DLE:HD21	2.33	0.58
1:C:13:TRP:CA	1:D:6:DVA:O	2.49	0.57
1:D:7:VAL:O	1:D:8:DVA:HB	2.04	0.57
1:A:6:DVA:CG1	1:B:8:DVA:HG12	2.35	0.57
1:B:2:GLY:N	5:B:2002:HOH:O	2.38	0.57
1:C:16:ETA:HB2	1:D:4:DLE:N	2.19	0.57
1:A:9:TRP:CE2	1:B:11:TRP:HB2	2.33	0.57
1:C:11:TRP:CZ2	1:D:4:DLE:CD1	2.87	0.57
1:A:5:ALA:CA	1:B:14:DLE:O	2.51	0.57
1:A:14:DLE:HD12	1:B:6:DVA:HG11	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:DVA:HG21	1:B:8:DVA:CB	2.34	0.56
1:B:6:DVA:O	1:B:6:DVA:HG22	2.05	0.56
1:D:12:DLE:C	5:D:2001:HOH:O	2.52	0.56
1:B:1:FVA:CN	1:B:1:FVA:CG2	2.82	0.56
1:A:13:TRP:HB3	1:B:7:VAL:HB	1.87	0.56
1:A:8:DVA:HG23	1:B:6:DVA:HA	1.87	0.56
1:A:6:DVA:HG21	1:B:8:DVA:HG12	1.87	0.56
1:C:16:ETA:HA1	4:D:131:MOH:C	2.35	0.56
1:A:5:ALA:O	1:A:6:DVA:CG2	2.42	0.56
1:A:11:TRP:CD1	1:B:3:ALA:C	2.79	0.56
1:C:6:DVA:HG23	1:D:8:DVA:HG21	1.87	0.56
1:A:8:DVA:O	1:B:11:TRP:HA	2.05	0.56
1:C:7:VAL:O	1:D:7:VAL:O	2.23	0.55
1:A:13:TRP:HZ3	1:B:1:FVA:HG22	1.69	0.55
1:C:3:ALA:C	1:D:10:DLE:HD11	2.26	0.55
1:B:11:TRP:HZ3	1:B:12:DLE:HD23	1.70	0.55
1:C:9:TRP:CD1	1:D:11:TRP:CB	2.89	0.55
1:C:8:DVA:CG2	1:D:6:DVA:HG22	2.36	0.55
1:B:5:ALA:HB3	5:B:2005:HOH:O	2.06	0.55
1:A:9:TRP:NE1	1:B:11:TRP:CB	2.43	0.55
1:C:7:VAL:HG12	1:D:7:VAL:CG1	2.17	0.55
1:C:3:ALA:O	1:D:11:TRP:O	2.25	0.55
1:A:7:VAL:HG22	1:B:7:VAL:HG13	1.88	0.54
1:A:14:DLE:HD12	1:B:6:DVA:CB	2.36	0.54
1:A:9:TRP:CB	5:B:2005:HOH:O	2.52	0.54
1:D:6:DVA:O	1:D:7:VAL:HB	2.07	0.54
3:C:118:CL:CL	4:D:132:MOH:O	2.63	0.54
1:A:8:DVA:HG22	5:B:2005:HOH:O	2.08	0.54
1:A:10:DLE:HD21	1:B:10:DLE:HD23	1.89	0.53
1:C:11:TRP:HE3	1:D:9:TRP:HD1	1.56	0.53
1:C:8:DVA:CB	1:D:6:DVA:HG22	2.37	0.53
1:C:9:TRP:CH2	1:D:11:TRP:HE3	2.26	0.53
1:D:5:ALA:O	1:D:6:DVA:HG22	2.08	0.53
1:B:9:TRP:O	1:B:10:DLE:HB2	2.06	0.53
1:A:6:DVA:O	1:B:13:TRP:CB	2.55	0.53
1:C:6:DVA:O	1:D:13:TRP:HA	2.08	0.53
1:A:14:DLE:HD12	1:B:6:DVA:HB	1.90	0.53
1:A:4:DLE:N	1:B:16:ETA:CB	2.71	0.53
1:C:4:DLE:HD13	1:D:16:ETA:CB	2.35	0.53
1:A:11:TRP:O	1:B:3:ALA:O	2.26	0.53
1:C:16:ETA:O	1:D:3:ALA:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:DVA:HB	1:D:6:DVA:HG22	1.89	0.53
1:A:1:FVA:HG12	1:A:2:GLY:N	2.23	0.53
1:C:11:TRP:CD1	1:D:3:ALA:O	2.62	0.53
1:C:16:ETA:HB2	1:D:4:DLE:CA	2.39	0.53
1:D:1:FVA:C	3:D:119:CL:CL	2.94	0.52
1:D:15:TRP:CG	1:D:16:ETA:N	2.77	0.52
1:C:4:DLE:CA	1:D:10:DLE:CD2	2.76	0.52
1:B:1:FVA:HN	1:B:1:FVA:HG23	1.88	0.52
1:A:16:ETA:CB	1:B:4:DLE:CG	2.88	0.52
1:C:4:DLE:HD22	1:D:10:DLE:HD12	1.92	0.52
1:C:14:DLE:HD13	1:D:1:FVA:O1	2.09	0.52
1:A:12:DLE:O	1:B:8:DVA:N	2.43	0.52
1:A:6:DVA:CB	1:B:8:DVA:HG12	2.40	0.52
1:C:4:DLE:HB3	1:D:16:ETA:CB	2.38	0.52
1:D:11:TRP:HE3	1:D:12:DLE:HD12	1.74	0.52
1:D:13:TRP:CA	5:D:2001:HOH:O	2.29	0.52
1:A:16:ETA:CB	1:B:4:DLE:CB	2.88	0.51
1:A:4:DLE:CG	1:B:10:DLE:HG	2.38	0.51
1:C:2:GLY:CA	4:D:132:MOH:C	2.86	0.51
1:A:13:TRP:O	1:B:1:FVA:O	2.29	0.51
1:B:9:TRP:O	1:B:10:DLE:CB	2.57	0.51
1:C:4:DLE:O	1:D:15:TRP:CB	2.58	0.51
1:A:13:TRP:N	5:A:2001:HOH:O	2.44	0.51
1:C:7:VAL:C	1:C:8:DVA:HG12	2.31	0.51
1:A:7:VAL:CA	1:B:13:TRP:HB3	2.38	0.50
1:B:14:DLE:HD23	1:B:14:DLE:C	2.41	0.50
1:A:8:DVA:HG22	1:A:9:TRP:N	2.26	0.50
1:C:11:TRP:HA	1:D:8:DVA:O	2.12	0.50
1:C:8:DVA:CG2	1:D:7:VAL:N	2.72	0.50
1:A:13:TRP:CZ3	1:B:1:FVA:CG2	2.94	0.50
1:A:7:VAL:HG13	1:B:7:VAL:O	2.12	0.50
1:C:15:TRP:C	5:C:2003:HOH:O	2.49	0.50
1:C:9:TRP:CA	1:D:10:DLE:O	2.43	0.50
1:A:14:DLE:HD12	1:B:6:DVA:HG13	1.92	0.49
1:C:4:DLE:O	1:D:15:TRP:HB2	2.12	0.49
1:C:8:DVA:HG21	1:D:6:DVA:HG22	1.92	0.49
1:A:6:DVA:O	1:B:13:TRP:CA	2.57	0.49
1:A:14:DLE:N	1:B:6:DVA:O	2.46	0.49
1:A:6:DVA:CG2	1:B:9:TRP:H	2.22	0.49
1:C:7:VAL:CG2	5:D:2001:HOH:O	2.60	0.49
1:A:16:ETA:O	1:B:4:DLE:CD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:FVA:HG23	1:D:1:FVA:CN	2.41	0.48
1:D:2:GLY:N	3:D:119:CL:CL	2.83	0.48
1:A:4:DLE:CD2	1:B:16:ETA:CB	2.81	0.48
1:C:16:ETA:HB2	1:D:4:DLE:CB	2.42	0.48
1:C:14:DLE:CD1	1:D:1:FVA:O1	2.62	0.48
1:C:4:DLE:HD22	1:D:10:DLE:CD2	2.42	0.48
1:B:8:DVA:O	1:B:8:DVA:HG22	2.12	0.48
1:A:6:DVA:CG2	1:B:8:DVA:HG12	2.44	0.48
1:A:13:TRP:HZ3	1:B:1:FVA:CG2	2.27	0.47
1:D:5:ALA:O	1:D:6:DVA:CG2	2.62	0.47
1:C:7:VAL:H	1:D:8:DVA:HB	1.79	0.47
1:A:3:ALA:O	1:B:11:TRP:O	2.32	0.47
1:C:8:DVA:CG2	1:D:6:DVA:CA	2.76	0.47
1:A:14:DLE:CD1	1:B:6:DVA:HB	2.44	0.47
1:C:11:TRP:CE3	1:D:9:TRP:HD1	2.30	0.47
1:C:8:DVA:CG2	1:D:6:DVA:HB	2.42	0.47
1:B:14:DLE:HD12	1:B:15:TRP:N	2.29	0.47
1:A:6:DVA:CG2	1:B:8:DVA:CA	2.61	0.47
5:C:2003:HOH:O	3:D:119:CL:CL	2.58	0.47
1:A:16:ETA:HB2	1:B:4:DLE:CA	2.44	0.47
1:B:2:GLY:O	1:B:3:ALA:CB	2.63	0.47
1:A:16:ETA:CB	1:B:4:DLE:HB2	2.45	0.47
1:A:13:TRP:CA	1:B:6:DVA:O	2.55	0.47
1:D:13:TRP:CB	5:D:2001:HOH:O	2.61	0.47
1:C:11:TRP:CE2	1:D:4:DLE:HG	2.51	0.47
1:A:7:VAL:HG13	1:B:7:VAL:HG22	1.97	0.46
1:A:8:DVA:N	1:B:12:DLE:O	2.48	0.46
1:C:7:VAL:HA	1:D:12:DLE:O	2.16	0.46
1:C:4:DLE:CB	1:D:10:DLE:HD11	2.45	0.46
1:C:11:TRP:O	1:D:3:ALA:O	2.32	0.46
1:D:11:TRP:CD2	1:D:11:TRP:O	2.69	0.46
1:C:1:FVA:N	1:D:13:TRP:O	2.45	0.46
1:C:10:DLE:CG	1:C:11:TRP:HZ3	2.28	0.46
1:C:1:FVA:HG13	1:D:13:TRP:CZ3	2.49	0.46
1:A:10:DLE:HG	1:B:10:DLE:C	2.44	0.46
1:A:10:DLE:CD2	1:B:10:DLE:HD23	2.45	0.46
1:A:4:DLE:N	1:B:16:ETA:O	2.49	0.46
1:C:4:DLE:N	1:D:10:DLE:HD11	2.31	0.46
1:C:6:DVA:HG22	1:C:7:VAL:N	2.31	0.46
1:A:6:DVA:HG13	1:A:7:VAL:N	2.30	0.45
1:C:4:DLE:CB	1:D:16:ETA:CB	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:TRP:CZ3	1:B:12:DLE:HD23	2.48	0.45
1:C:4:DLE:CD1	1:D:16:ETA:CB	2.91	0.45
1:C:16:ETA:CB	1:D:4:DLE:N	2.80	0.45
1:A:6:DVA:N	1:B:14:DLE:O	2.50	0.45
1:D:7:VAL:O	1:D:8:DVA:CB	2.65	0.45
1:D:9:TRP:O	1:D:10:DLE:CD2	2.59	0.45
1:A:7:VAL:CG2	1:B:7:VAL:HG13	2.46	0.45
1:B:2:GLY:CA	4:B:146:MOH:O	2.64	0.45
1:C:10:DLE:CD1	1:D:10:DLE:CB	2.95	0.45
1:C:3:ALA:O	1:D:10:DLE:CD1	2.65	0.45
1:C:6:DVA:O	1:D:14:DLE:N	2.49	0.45
3:D:119:CL:CL	4:D:131:MOH:C	3.02	0.45
1:C:11:TRP:CD1	1:D:3:ALA:CB	2.99	0.44
1:C:10:DLE:HD13	1:D:10:DLE:CA	2.47	0.44
1:D:8:DVA:HG13	1:D:9:TRP:H	1.82	0.44
1:C:4:DLE:CA	1:D:10:DLE:CD1	2.87	0.44
1:C:4:DLE:O	1:D:15:TRP:HA	2.18	0.44
1:C:11:TRP:HB3	1:D:9:TRP:CE2	2.49	0.44
1:C:7:VAL:HG22	5:D:2001:HOH:O	2.18	0.44
1:C:10:DLE:CD2	1:C:11:TRP:CZ3	2.95	0.43
1:B:10:DLE:HD13	1:B:11:TRP:H	1.84	0.43
1:C:6:DVA:HA	1:D:8:DVA:CB	2.48	0.43
1:D:15:TRP:HD1	1:D:15:TRP:O	1.96	0.43
1:A:11:TRP:CZ2	1:B:4:DLE:CD2	2.72	0.43
1:C:16:ETA:CB	1:D:4:DLE:HB2	2.47	0.43
1:A:16:ETA:HB1	1:B:4:DLE:CG	2.46	0.42
1:C:6:DVA:CA	1:D:8:DVA:HG11	2.42	0.42
1:A:3:ALA:CA	1:B:16:ETA:O	2.62	0.42
1:A:14:DLE:CD1	1:A:15:TRP:CD2	3.03	0.42
1:A:16:ETA:CB	1:B:4:DLE:CD1	2.94	0.42
1:C:3:ALA:HA	1:D:16:ETA:HO	1.80	0.42
1:C:10:DLE:N	1:D:10:DLE:O	2.52	0.42
1:A:4:DLE:CA	1:B:16:ETA:HB2	2.50	0.42
1:C:6:DVA:HB	1:D:14:DLE:HB3	2.01	0.42
1:C:10:DLE:CB	1:C:11:TRP:HZ3	2.19	0.42
1:D:10:DLE:HD13	1:D:11:TRP:H	1.85	0.42
1:C:4:DLE:HB2	1:D:16:ETA:O	2.20	0.42
1:C:11:TRP:CE3	1:D:9:TRP:CD1	3.07	0.42
1:A:9:TRP:CD2	1:A:10:DLE:HD11	2.54	0.42
3:A:119:CL:CL	1:B:7:VAL:N	2.90	0.41
1:A:8:DVA:HG21	4:A:138:MOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:C	4:A:133:MOH:C	2.89	0.41
1:C:11:TRP:HE3	1:D:9:TRP:CD1	2.36	0.41
1:D:11:TRP:CZ3	1:D:12:DLE:HD12	2.54	0.41
1:B:2:GLY:O	1:B:3:ALA:HB2	2.20	0.41
1:C:16:ETA:CA	4:D:131:MOH:O	2.61	0.41
1:D:15:TRP:O	5:D:2002:HOH:O	2.21	0.41
1:C:8:DVA:N	1:D:12:DLE:O	2.54	0.41
1:A:1:FVA:N	1:B:13:TRP:O	2.46	0.41
1:C:3:ALA:O	1:D:10:DLE:HD11	2.22	0.40
1:C:6:DVA:O	5:D:2001:HOH:O	2.22	0.40
1:A:6:DVA:HG22	1:A:7:VAL:N	2.26	0.40
1:A:12:DLE:C	1:A:13:TRP:CD1	3.04	0.40
1:A:16:ETA:HB2	1:B:4:DLE:HB2	1.99	0.40

All (2) 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:A:1:FVA:O1	1:A:16:ETA:O[3_555]	2.11	0.09
1:C:1:FVA:O1	4:D:131:MOH:O[3_655]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	8/16 (50%)	5 (62%)	2 (25%)	1 (12%)	0	0
1	B	8/16 (50%)	4 (50%)	3 (38%)	1 (12%)	0	0
1	C	8/16 (50%)	5 (62%)	2 (25%)	1 (12%)	0	0
1	D	8/16 (50%)	4 (50%)	2 (25%)	2 (25%)	0	0
All	All	32/64 (50%)	18 (56%)	9 (28%)	5 (16%)	0	0

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ALA
1	A	3	ALA
1	C	3	ALA
1	D	3	ALA
1	D	7	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	5/5 (100%)	3 (60%)	2 (40%)	0	0
1	B	5/5 (100%)	3 (60%)	2 (40%)	0	0
1	C	5/5 (100%)	2 (40%)	3 (60%)	0	0
1	D	5/5 (100%)	1 (20%)	4 (80%)	0	0
All	All	20/20 (100%)	9 (45%)	11 (55%)	0	0

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	11	TRP
1	B	11	TRP
1	B	13	TRP
1	C	7	VAL
1	C	11	TRP
1	C	13	TRP
1	D	9	TRP
1	D	11	TRP
1	D	13	TRP
1	D	15	TRP

Some 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 ⓘ

32 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	A	1	1	8,8,9	1.62	1 (12%)	8,9,11	1.89	2 (25%)
1	DLE	A	10	1	6,7,8	1.15	1 (16%)	6,8,10	1.90	3 (50%)
1	DLE	A	12	1	6,7,8	1.70	1 (16%)	6,8,10	1.18	0
1	DLE	A	14	1,2	6,7,8	0.96	0	6,8,10	1.28	1 (16%)
1	ETA	A	16	1	3,3,3	1.00	0	2,2,2	0.70	0
1	DLE	A	4	1	6,7,8	1.45	1 (16%)	6,8,10	3.31	2 (33%)
1	DVA	A	6	1	6,6,7	3.07	2 (33%)	6,7,9	5.45	2 (33%)
1	DVA	A	8	1	6,6,7	1.32	1 (16%)	6,7,9	2.89	4 (66%)
1	FVA	B	1	1	8,8,9	5.10	2 (25%)	8,9,11	2.24	5 (62%)
1	DLE	B	10	1	6,7,8	1.32	1 (16%)	6,8,10	2.08	1 (16%)
1	DLE	B	12	1	6,7,8	1.22	1 (16%)	6,8,10	0.74	0
1	DLE	B	14	1	6,7,8	2.25	1 (16%)	6,8,10	1.63	1 (16%)
1	ETA	B	16	1	3,3,3	0.63	0	2,2,2	0.83	0
1	DLE	B	4	1	6,7,8	4.01	1 (16%)	6,8,10	2.04	2 (33%)
1	DVA	B	6	1	6,6,7	1.28	1 (16%)	6,7,9	2.71	3 (50%)
1	DVA	B	8	1	6,6,7	1.88	1 (16%)	6,7,9	3.17	3 (50%)
1	FVA	C	1	1	8,8,9	2.14	2 (25%)	8,9,11	2.27	4 (50%)
1	DLE	C	10	1	6,7,8	2.91	1 (16%)	6,8,10	2.84	3 (50%)
1	DLE	C	12	1	6,7,8	2.15	1 (16%)	6,8,10	3.12	2 (33%)
1	DLE	C	14	1	6,7,8	3.59	1 (16%)	6,8,10	0.63	0
1	ETA	C	16	1	3,3,3	0.70	0	2,2,2	0.29	0
1	DLE	C	4	1	6,7,8	4.72	1 (16%)	6,8,10	3.66	3 (50%)
1	DVA	C	6	1	6,6,7	1.59	2 (33%)	6,7,9	4.56	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DVA	C	8	1	6,6,7	3.29	3 (50%)	6,7,9	4.63	1 (16%)
1	FVA	D	1	1	8,8,9	3.15	5 (62%)	8,9,11	2.09	2 (25%)
1	DLE	D	10	1	6,7,8	1.81	1 (16%)	6,8,10	2.08	2 (33%)
1	DLE	D	12	1,2	6,7,8	1.99	1 (16%)	6,8,10	1.92	4 (66%)
1	DLE	D	14	1	6,7,8	0.85	0	6,8,10	1.89	3 (50%)
1	ETA	D	16	1	3,3,3	0.45	0	2,2,2	0.88	0
1	DLE	D	4	1	6,7,8	2.01	1 (16%)	6,8,10	0.72	0
1	DVA	D	6	1	6,6,7	1.57	1 (16%)	6,7,9	3.17	2 (33%)
1	DVA	D	8	1	6,6,7	2.33	2 (33%)	6,7,9	4.42	2 (33%)

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	A	1	1	-	0/5/9/11	0/0/0/0
1	DLE	A	10	1	-	0/4/6/8	0/0/0/0
1	DLE	A	12	1	-	0/4/6/8	0/0/0/0
1	DLE	A	14	1,2	-	0/4/6/8	0/0/0/0
1	ETA	A	16	1	-	0/1/1/1	0/0/0/0
1	DLE	A	4	1	-	0/4/6/8	0/0/0/0
1	DVA	A	6	1	1/1/2/3	0/4/6/8	0/0/0/0
1	DVA	A	8	1	-	0/4/6/8	0/0/0/0
1	FVA	B	1	1	-	0/5/9/11	0/0/0/0
1	DLE	B	10	1	-	0/4/6/8	0/0/0/0
1	DLE	B	12	1	-	0/4/6/8	0/0/0/0
1	DLE	B	14	1	-	0/4/6/8	0/0/0/0
1	ETA	B	16	1	-	0/1/1/1	0/0/0/0
1	DLE	B	4	1	-	0/4/6/8	0/0/0/0
1	DVA	B	6	1	-	0/4/6/8	0/0/0/0
1	DVA	B	8	1	-	0/4/6/8	0/0/0/0
1	FVA	C	1	1	-	0/5/9/11	0/0/0/0
1	DLE	C	10	1	-	0/4/6/8	0/0/0/0
1	DLE	C	12	1	-	0/4/6/8	0/0/0/0
1	DLE	C	14	1	-	0/4/6/8	0/0/0/0
1	ETA	C	16	1	-	0/1/1/1	0/0/0/0
1	DLE	C	4	1	-	0/4/6/8	0/0/0/0
1	DVA	C	6	1	-	0/4/6/8	0/0/0/0
1	DVA	C	8	1	1/1/2/3	0/4/6/8	0/0/0/0
1	FVA	D	1	1	-	0/5/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DLE	D	10	1	-	0/4/6/8	0/0/0/0
1	DLE	D	12	1,2	-	0/4/6/8	0/0/0/0
1	DLE	D	14	1	-	0/4/6/8	0/0/0/0
1	ETA	D	16	1	-	0/1/1/1	0/0/0/0
1	DLE	D	4	1	-	0/4/6/8	0/0/0/0
1	DVA	D	6	1	-	0/4/6/8	0/0/0/0
1	DVA	D	8	1	1/1/2/3	0/4/6/8	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	DVA	CB-CA	-6.77	1.33	1.54
1	C	12	DLE	CA-C	-5.22	1.43	1.50
1	C	8	DVA	CG2-CB	-4.69	1.35	1.52
1	D	12	DLE	CA-C	-4.40	1.44	1.50
1	C	8	DVA	CB-CA	-3.89	1.42	1.54
1	A	1	FVA	CB-CA	-3.57	1.48	1.54
1	D	8	DVA	CG1-CB	-2.83	1.42	1.52
1	A	6	DVA	CG2-CB	-2.67	1.42	1.52
1	A	8	DVA	CB-CA	-2.49	1.46	1.54
1	D	1	FVA	O1-CN	-2.42	1.15	1.22
1	A	10	DLE	CD1-CG	-2.17	1.39	1.51
1	C	6	DVA	CA-N	2.03	1.54	1.47
1	B	12	DLE	CA-C	2.10	1.53	1.50
1	D	1	FVA	CB-CA	2.16	1.58	1.54
1	D	1	FVA	O-C	2.18	1.28	1.19
1	B	6	DVA	CA-C	2.28	1.53	1.50
1	C	6	DVA	CG2-CB	2.47	1.61	1.52
1	D	1	FVA	CA-N	2.72	1.50	1.46
1	D	6	DVA	CB-CA	2.90	1.63	1.54
1	B	10	DLE	CA-C	2.97	1.54	1.50
1	C	1	FVA	CA-N	3.13	1.51	1.46
1	A	4	DLE	CA-C	3.44	1.54	1.50
1	A	12	DLE	CA-C	3.90	1.55	1.50
1	D	10	DLE	CA-C	4.12	1.55	1.50
1	B	8	DVA	CA-C	4.28	1.55	1.50
1	C	1	FVA	CA-C	4.54	1.56	1.50
1	D	8	DVA	CA-C	4.66	1.56	1.50
1	D	4	DLE	CA-C	4.72	1.56	1.50
1	C	8	DVA	CA-C	5.12	1.57	1.50
1	B	14	DLE	CA-C	5.31	1.57	1.50
1	C	10	DLE	CA-C	6.57	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	FVA	CA-N	6.82	1.56	1.46
1	D	1	FVA	CA-C	7.45	1.60	1.50
1	C	14	DLE	CA-C	8.66	1.61	1.50
1	B	4	DLE	CA-C	9.34	1.62	1.50
1	C	4	DLE	CA-C	11.36	1.65	1.50
1	B	1	FVA	CA-C	12.33	1.66	1.50

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	DVA	CB-CA-C	-9.30	100.22	112.96
1	C	4	DLE	CB-CA-N	-6.24	96.52	110.43
1	A	6	DVA	CB-CA-C	-5.94	104.83	112.96
1	A	1	FVA	CB-CA-C	-4.62	107.20	113.07
1	A	4	DLE	CD1-CG-CB	-4.19	95.72	111.08
1	B	8	DVA	O-C-CA	-4.10	115.53	125.09
1	C	10	DLE	CB-CA-N	-4.08	101.32	110.43
1	C	6	DVA	O-C-CA	-3.90	116.01	125.09
1	B	6	DVA	CB-CA-C	-3.81	107.74	112.96
1	C	1	FVA	CG1-CB-CG2	-3.73	100.00	110.63
1	C	10	DLE	O-C-CA	-3.71	114.77	124.96
1	D	10	DLE	CG-CB-CA	-3.60	96.12	116.19
1	B	6	DVA	O-C-CA	-3.31	117.38	125.09
1	B	8	DVA	CB-CA-C	-3.18	108.61	112.96
1	B	14	DLE	CB-CA-N	-3.11	103.49	110.43
1	D	14	DLE	CD1-CG-CB	-3.09	99.75	111.08
1	C	1	FVA	CB-CA-C	-3.03	109.22	113.07
1	D	1	FVA	CG1-CB-CG2	-2.88	102.43	110.63
1	B	1	FVA	CB-CA-C	-2.85	109.45	113.07
1	B	1	FVA	CG1-CB-CA	-2.83	106.80	111.21
1	A	8	DVA	CB-CA-C	-2.78	109.16	112.96
1	D	10	DLE	CD1-CG-CB	-2.75	101.00	111.08
1	A	10	DLE	CB-CA-N	-2.73	104.33	110.43
1	B	1	FVA	CG2-CB-CA	-2.69	107.02	111.21
1	C	6	DVA	CG2-CB-CG1	-2.58	103.29	110.63
1	A	10	DLE	CD1-CG-CB	-2.48	101.99	111.08
1	A	8	DVA	O-C-CA	-2.47	119.34	125.09
1	C	4	DLE	CD1-CG-CB	-2.47	102.05	111.08
1	D	12	DLE	O-C-CA	-2.45	118.23	124.96
1	A	8	DVA	CG2-CB-CG1	-2.43	103.72	110.63
1	A	10	DLE	O-C-CA	-2.40	118.36	124.96
1	D	12	DLE	CD2-CG-CB	-2.25	102.84	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	DLE	O-C-CA	-2.20	118.91	124.96
1	A	14	DLE	CB-CA-N	-2.18	105.56	110.43
1	B	1	FVA	O-C-CA	-2.07	120.05	125.12
1	A	1	FVA	O-C-CA	-2.04	120.12	125.12
1	D	12	DLE	CG-CB-CA	2.05	127.62	116.19
1	D	14	DLE	CD2-CG-CB	2.08	118.70	111.08
1	B	4	DLE	CD1-CG-CB	2.12	118.85	111.08
1	C	1	FVA	CG1-CB-CA	2.49	115.08	111.21
1	D	12	DLE	CB-CA-N	2.53	116.07	110.43
1	C	1	FVA	CA-N-CN	2.65	126.90	122.42
1	D	6	DVA	CG2-CB-CG1	2.73	118.43	110.63
1	B	1	FVA	CA-N-CN	2.88	127.29	122.42
1	B	4	DLE	CG-CB-CA	3.25	134.32	116.19
1	C	10	DLE	CG-CB-CA	3.84	137.61	116.19
1	B	6	DVA	C-CA-N	4.00	117.93	109.86
1	C	6	DVA	C-CA-N	4.02	117.97	109.86
1	C	12	DLE	CG-CB-CA	4.42	140.84	116.19
1	D	1	FVA	CA-N-CN	4.67	130.32	122.42
1	B	10	DLE	CG-CB-CA	5.05	144.32	116.19
1	A	8	DVA	C-CA-N	5.47	120.91	109.86
1	B	8	DVA	C-CA-N	5.51	120.98	109.86
1	C	4	DLE	CG-CB-CA	5.52	146.96	116.19
1	C	12	DLE	CB-CA-N	5.95	123.70	110.43
1	A	4	DLE	CG-CB-CA	6.50	152.42	116.19
1	D	6	DVA	C-CA-N	6.79	123.56	109.86
1	D	8	DVA	CB-CA-C	7.10	122.68	112.96
1	D	8	DVA	C-CA-N	7.87	125.75	109.86
1	C	8	DVA	C-CA-N	11.13	132.31	109.86
1	A	6	DVA	C-CA-N	11.80	133.67	109.86

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	6	DVA	CA
1	C	8	DVA	CA
1	D	8	DVA	CA

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 303 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FVA	7	1
1	A	10	DLE	15	0
1	A	12	DLE	4	0
1	A	14	DLE	19	0
1	A	16	ETA	14	1
1	A	4	DLE	13	0
1	A	6	DVA	27	0
1	A	8	DVA	6	0
1	B	1	FVA	8	0
1	B	10	DLE	14	0
1	B	12	DLE	7	0
1	B	14	DLE	7	0
1	B	16	ETA	10	0
1	B	4	DLE	23	0
1	B	6	DVA	15	0
1	B	8	DVA	16	0
1	C	1	FVA	4	1
1	C	10	DLE	18	0
1	C	12	DLE	2	0
1	C	14	DLE	7	0
1	C	16	ETA	10	0
1	C	4	DLE	30	0
1	C	6	DVA	13	0
1	C	8	DVA	24	0
1	D	1	FVA	9	0
1	D	10	DLE	30	0
1	D	12	DLE	10	0
1	D	14	DLE	7	0
1	D	16	ETA	13	0
1	D	4	DLE	12	0
1	D	6	DVA	21	0
1	D	8	DVA	11	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	A	133	2	1,1,1	0.23	0	0,0,0	0.00	-
4	MOH	A	138	-	1,1,1	0.21	0	0,0,0	0.00	-
4	MOH	A	140	-	1,1,1	0.40	0	0,0,0	0.00	-
4	MOH	A	145	-	1,1,1	0.09	0	0,0,0	0.00	-
4	MOH	B	139	-	1,1,1	0.09	0	0,0,0	0.00	-
4	MOH	B	146	-	1,1,1	0.28	0	0,0,0	0.00	-
4	MOH	B	151	-	1,1,1	0.38	0	0,0,0	0.00	-
4	MOH	C	120	2	1,1,1	0.56	0	0,0,0	0.00	-
4	MOH	C	122	-	1,1,1	0.05	0	0,0,0	0.00	-
4	MOH	D	121	-	1,1,1	0.16	0	0,0,0	0.00	-
4	MOH	D	127	-	1,1,1	0.17	0	0,0,0	0.00	-
4	MOH	D	131	-	1,1,1	0.16	0	0,0,0	0.00	-
4	MOH	D	132	-	1,1,1	0.78	0	0,0,0	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MOH	A	133	2	-	0/0/0/0	0/0/0/0
4	MOH	A	138	-	-	0/0/0/0	0/0/0/0
4	MOH	A	140	-	-	0/0/0/0	0/0/0/0
4	MOH	A	145	-	-	0/0/0/0	0/0/0/0
4	MOH	B	139	-	-	0/0/0/0	0/0/0/0
4	MOH	B	146	-	-	0/0/0/0	0/0/0/0
4	MOH	B	151	-	-	0/0/0/0	0/0/0/0
4	MOH	C	120	2	-	0/0/0/0	0/0/0/0
4	MOH	C	122	-	-	0/0/0/0	0/0/0/0
4	MOH	D	121	-	-	0/0/0/0	0/0/0/0
4	MOH	D	127	-	-	0/0/0/0	0/0/0/0
4	MOH	D	131	-	-	0/0/0/0	0/0/0/0
4	MOH	D	132	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	133	MOH	2	0
4	A	138	MOH	1	0
4	B	146	MOH	1	0
4	C	120	MOH	1	0
4	C	122	MOH	1	0
4	D	121	MOH	1	0
4	D	131	MOH	4	1
4	D	132	MOH	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.