Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 12:14 am GMT

PDB ID	:	8A19
Title	:	Structure of a leucinostatin derivative determined by host lattice display : L1E4V1 construct
Authors	:	Mittl, P.R.E.
Deposited on	:	2022-06-01
Resolution	:	2.36 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:

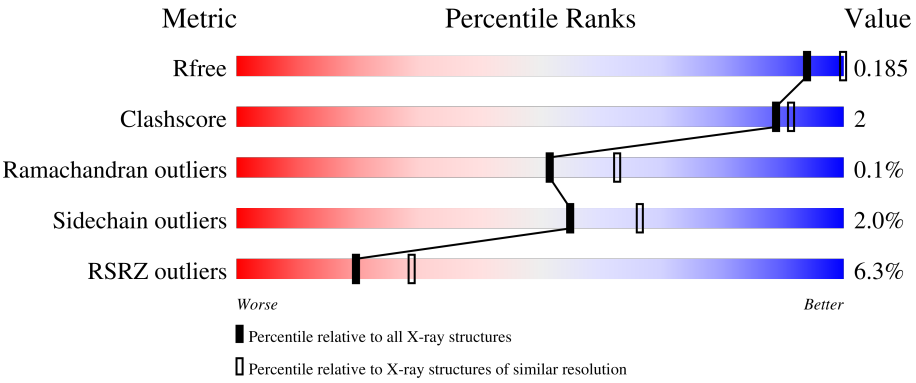
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	1347	6% 94% 6%
2	B	11	36% 73% 27%

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	HPE	B	3	-	X	-	-
6	CL	A	1711	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11807 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 L1E4v1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1345	Total	C	N	O	S	0	10	0
			10419	6491	1792	2107	29			

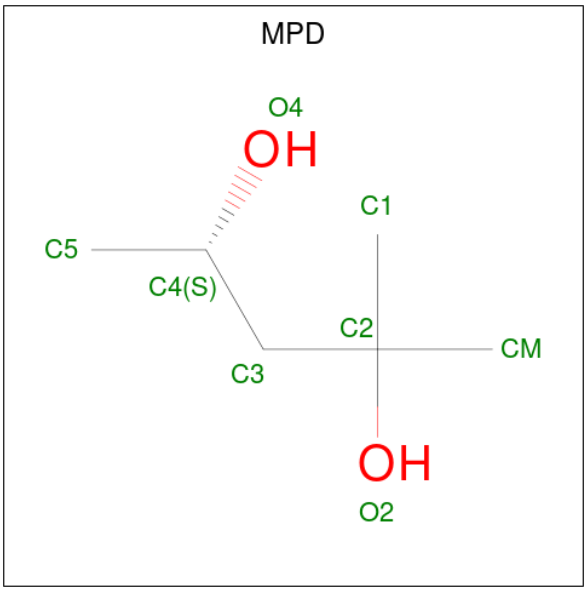
- Molecule 2 is a protein called 6-(2-methoxyethoxy)-11,15-dimethyl-8-oxa-2,11,15,19,21,23-hexazatetracyclo[15.6.1.13,7.020,24]pentacosa-1(23),3(25),4,6,17,20(24),21-heptaen-10-one.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	F	N	O	12	0	0
			84	62	1	11	10			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

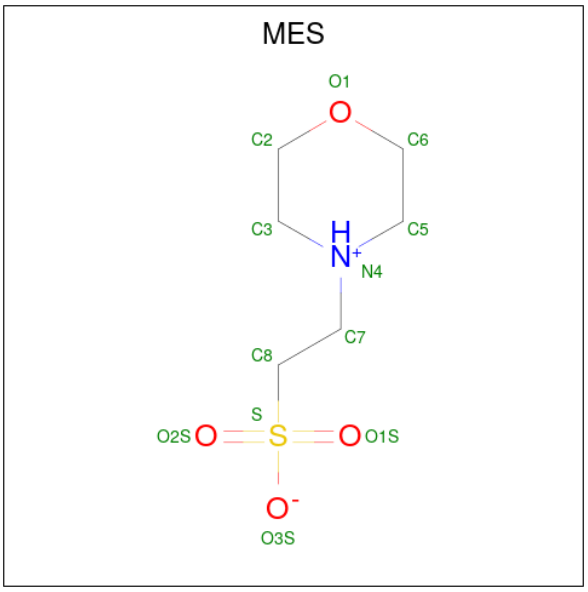
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mn	0	0
			4	4		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	Cl	0	0
			5	5		

- Molecule 7 is water.

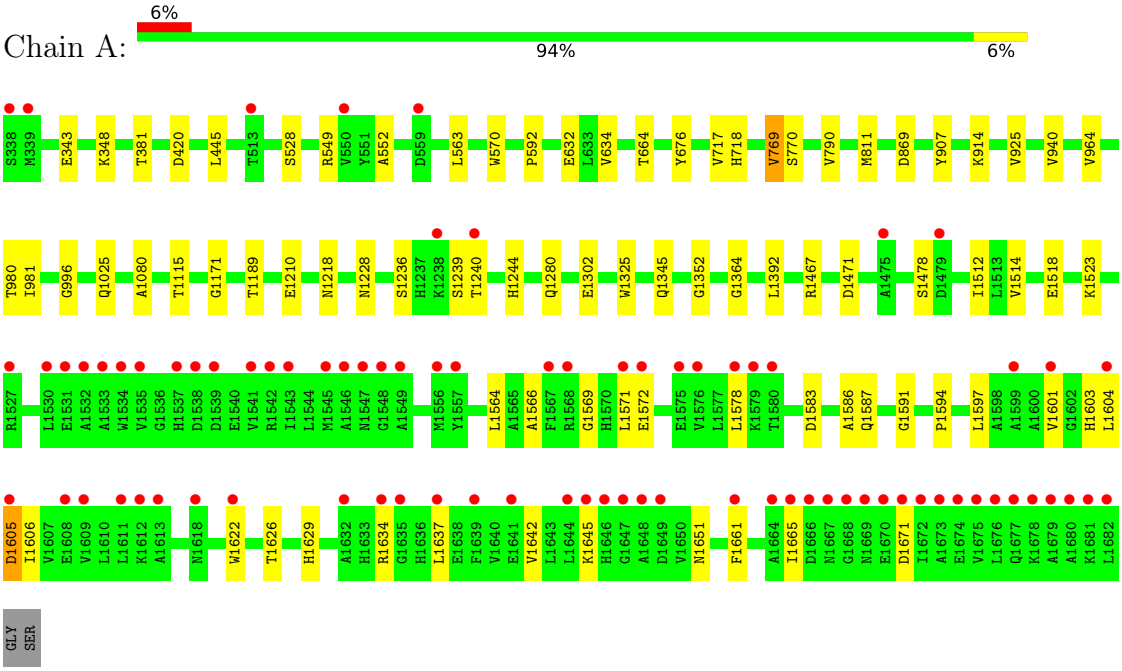
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1250	Total	O	0	0
			1250	1250		
7	B	1	Total	O	0	0
			1	1		

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.

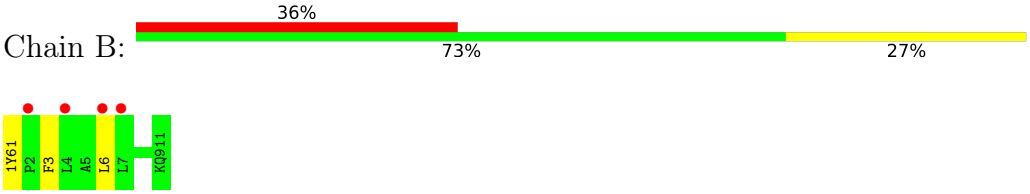
• Molecule 1: L1E4v1

Chain A:



• Molecule 2: 6-(2-methoxyethoxy)-11,15-dimethyl-8-oxa-2,11,15,19,21,23-hexazatetracyclo[15.6.1.13,7.020,24]pentacosa-1(23),3(25),4,6,17,20(24),21-heptaen-10-one

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	192.76Å 192.76Å 122.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.52 – 2.36 34.52 – 2.36	Depositor EDS
% Data completeness (in resolution range)	90.6 (34.52-2.36) 90.6 (34.52-2.36)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.36Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.163 , 0.193 0.157 , 0.185	Depositor DCC
R_{free} test set	4853 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11807	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: MES, AIB, KQ9, MPD, BAL, MN, CL, HPE, 1Y6

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	0.42	0/10624	0.62	0/14412
2	B	0.17	0/30	0.47	0/38
All	All	0.42	0/10654	0.62	0/14450

There are no bond length outliers.

There are no bond angle outliers.

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	A	10419	0	9977	40	0
2	B	84	0	79	1	0
3	A	4	0	0	0	0
4	A	32	0	56	1	0
5	A	12	0	13	0	0
6	A	5	0	0	0	0
7	A	1250	0	0	1	0
7	B	1	0	0	0	0
All	All	11807	0	10125	40	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 2.

All (40) 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:1569:GLY:HA2	1:A:1606:ILE:HD11	1.77	0.67
1:A:1171:GLY:HA3	1:A:1239:SER:HB2	1.77	0.67
1:A:925:VAL:HG12	1:A:940:VAL:HG12	1.78	0.65
1:A:1218:ASN:HD22	1:A:1280:GLN:NE2	1.97	0.62
1:A:1189:THR:HB	1:A:1345:GLN:HB3	1.82	0.62
1:A:1594:PRO:HA	1:A:1597:LEU:HD12	1.84	0.59
1:A:552:ALA:HB1	1:A:563:LEU:HD11	1.84	0.59
1:A:769[A]:VAL:HG23	1:A:811:MET:HB2	1.83	0.59
1:A:1364:GLY:HA2	1:A:1392:LEU:HD13	1.90	0.53
1:A:570:TRP:CD2	1:A:592:PRO:HB3	2.44	0.53
1:A:769[B]:VAL:HG23	1:A:811:MET:HB2	1.96	0.48
1:A:1302:GLU:HB2	1:A:1325:TRP:CZ3	2.49	0.47
1:A:1467:ARG:O	1:A:1471:ASP:HB2	2.16	0.46
1:A:634:VAL:HA	1:A:914:LYS:HG3	1.98	0.46
1:A:964[B]:VAL:HG12	1:A:981:ILE:HG12	1.98	0.46
1:A:1171:GLY:HA3	1:A:1239:SER:CB	2.45	0.46
1:A:1601:VAL:CG1	1:A:1603:HIS:CE1	2.99	0.45
1:A:1210:GLU:OE1	1:A:1244:HIS:HD2	1.99	0.45
1:A:1583:ASP:HB3	1:A:1586:ALA:HB2	1.98	0.45
1:A:1604:LEU:HD11	1:A:1642:VAL:HG21	2.00	0.44
1:A:348:LYS:HE3	1:A:348:LYS:HB2	1.85	0.44
1:A:420:ASP:HB3	1:A:445:LEU:HG	1.98	0.44
1:A:1571:LEU:HD13	1:A:1605:ASP:HB2	1.99	0.44
1:A:1514:VAL:O	1:A:1518:GLU:HG2	2.19	0.43
1:A:1352:GLY:HA2	1:A:1512:ILE:HG13	2.01	0.43
1:A:1626:THR:OG1	1:A:1629:HIS:HD2	2.00	0.43
1:A:676:TYR:CD1	1:A:717:VAL:HB	2.54	0.43
1:A:528:SER:O	1:A:549:ARG:HD2	2.19	0.43
1:A:1564:LEU:HD13	2:B:1:1Y6:H27	2.00	0.42
1:A:1569:GLY:HA2	1:A:1606:ILE:CD1	2.48	0.41
1:A:1566:ALA:HA	1:A:1606:ILE:HD13	2.02	0.41
1:A:1661:PHE:CZ	1:A:1665:ILE:HD11	2.55	0.41
1:A:980:THR:HG23	7:A:2793:HOH:O	2.21	0.41
1:A:718:HIS:CD2	1:A:718:HIS:C	2.94	0.41
1:A:869:ASP:O	1:A:996:GLY:HA3	2.20	0.41
1:A:664:THR:HA	1:A:907:TYR:OH	2.21	0.40
1:A:1587:GLN:HB3	1:A:1591:GLY:HA2	2.03	0.40
1:A:1601:VAL:CG1	1:A:1603:HIS:HE1	2.34	0.40
1:A:1080:ALA:HB2	4:A:1707:MPD:H32	2.04	0.40
1:A:1601:VAL:HG11	1:A:1603:HIS:HE1	1.87	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	1353/1347 (100%)	1304 (96%)	48 (4%)	1 (0%)	51 63
2	B	3/11 (27%)	3 (100%)	0	0	100 100
All	All	1356/1358 (100%)	1307 (96%)	48 (4%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	790	VAL

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	1107/1098 (101%)	1085 (98%)	22 (2%)	55 66
2	B	4/4 (100%)	3 (75%)	1 (25%)	0 0
All	All	1111/1102 (101%)	1088 (98%)	23 (2%)	55 65

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

Mol	Chain	Res	Type
1	A	343	GLU
1	A	381	THR

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Mol	Chain	Res	Type
1	A	632	GLU
1	A	769[A]	VAL
1	A	769[B]	VAL
1	A	770	SER
1	A	1025	GLN
1	A	1115	THR
1	A	1228	ASN
1	A	1236	SER
1	A	1240	THR
1	A	1478	SER
1	A	1523	LYS
1	A	1572	GLU
1	A	1578	LEU
1	A	1605	ASP
1	A	1622	TRP
1	A	1634	ARG
1	A	1637	LEU
1	A	1645	LYS
1	A	1651	ASN
1	A	1671	ASP
2	B	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	663	ASN
1	A	897	ASN
1	A	1055	GLN
1	A	1244	HIS
1	A	1280	GLN
1	A	1603	HIS
1	A	1629	HIS
1	A	1633	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 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	$\#\|Z\| > 2$
2	AIB	B	9	2	1,5,6	0.89	0	2,7,9	0.11	0
2	HPE	B	3	2	11,12,13	4.80	6 (54%)	9,14,16	4.56	8 (88%)
2	AIB	B	8	2	1,5,6	0.88	0	2,7,9	0.38	0
2	AIB	B	5	2	1,5,6	0.92	0	2,7,9	0.23	0
2	BAL	B	10	2	4,4,5	0.40	0	3,3,5	0.72	0

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	AIB	B	9	2	-	1/2/3/6	-
2	HPE	B	3	2	-	4/6/7/9	0/1/1/1
2	AIB	B	8	2	-	0/2/3/6	-
2	AIB	B	5	2	-	0/2/3/6	-
2	BAL	B	10	2	-	0/1/2/3	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	HPE	CZ1-CE1	6.91	1.53	1.38
2	B	3	HPE	CZ2-CE2	6.90	1.53	1.38
2	B	3	HPE	CE1-CD	6.86	1.53	1.38
2	B	3	HPE	CE2-CD	6.73	1.53	1.38
2	B	3	HPE	CH-CZ2	5.75	1.53	1.38
2	B	3	HPE	CH-CZ1	5.55	1.52	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	HPE	CH-CZ1-CE1	-5.55	111.73	120.19
2	B	3	HPE	CE2-CD-CE1	-5.42	109.65	118.17
2	B	3	HPE	CH-CZ2-CE2	-5.31	112.10	120.19
2	B	3	HPE	CZ2-CE2-CD	-5.28	112.53	120.63
2	B	3	HPE	CZ1-CE1-CD	-4.70	113.43	120.63
2	B	3	HPE	CZ2-CH-CZ1	-4.68	111.23	119.93
2	B	3	HPE	CG-CD-CE1	-3.98	111.17	121.23
2	B	3	HPE	CG-CD-CE2	-3.31	112.86	121.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	HPE	N-CA-CB-CG
2	B	3	HPE	CA-CB-CG-CD
2	B	9	AIB	O-C-CA-CB2
2	B	3	HPE	C-CA-CB-CG
2	B	3	HPE	CE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	MES	A	1709	-	12,12,12	0.84	0	14,16,16	0.47	0
4	MPD	A	1705	-	7,7,7	0.58	0	9,10,10	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MPD	A	1707	-	7,7,7	0.68	0	9,10,10	0.49	0
4	MPD	A	1706	-	7,7,7	0.84	1 (14%)	9,10,10	0.56	0
4	MPD	A	1708	-	7,7,7	0.71	0	9,10,10	0.29	0

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
5	MES	A	1709	-	-	4/6/14/14	0/1/1/1
4	MPD	A	1705	-	-	0/5/5/5	-
4	MPD	A	1707	-	-	3/5/5/5	-
4	MPD	A	1706	-	-	3/5/5/5	-
4	MPD	A	1708	-	-	2/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1706	MPD	C3-C2	2.02	1.59	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1706	MPD	C1-C2-C3-C4
4	A	1706	MPD	O2-C2-C3-C4
5	A	1709	MES	C8-C7-N4-C5
5	A	1709	MES	C7-C8-S-O2S
4	A	1708	MPD	C2-C3-C4-C5
5	A	1709	MES	C7-C8-S-O1S
4	A	1706	MPD	CM-C2-C3-C4
4	A	1707	MPD	CM-C2-C3-C4
5	A	1709	MES	N4-C7-C8-S
4	A	1707	MPD	O2-C2-C3-C4
4	A	1707	MPD	C2-C3-C4-C5
4	A	1708	MPD	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1707	MPD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	1345/1347 (99%)	-0.15	81 (6%) 21 32	29, 43, 110, 148	0
2	B	4/11 (36%)	3.87	4 (100%) 0 0	116, 117, 117, 119	0
All	All	1349/1358 (99%)	-0.14	85 (6%) 20 29	29, 43, 110, 148	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1682	LEU	8.7
1	A	1639	PHE	7.9
1	A	1534	TRP	7.0
1	A	1676	LEU	6.6
1	A	1667	ASN	6.0
1	A	1681	LYS	5.7
1	A	1579	LYS	5.7
2	B	7	LEU	5.6
1	A	1677	GLN	5.5
1	A	1661	PHE	5.5
1	A	1576	VAL	5.4
1	A	1671	ASP	5.3
1	A	1668	GLY	4.9
1	A	1539	ASP	4.8
1	A	1680	ALA	4.7
1	A	1533	ALA	4.6
1	A	1674	GLU	4.5
1	A	1670	GLU	4.5
1	A	1679	ALA	4.5
1	A	338	SER	4.4
1	A	1580	THR	4.4
1	A	1557	TYR	4.3
1	A	1664	ALA	4.2
1	A	1672	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1612	LYS	3.9
1	A	1675	VAL	3.9
1	A	1546	ALA	3.9
1	A	1669	ASN	3.9
1	A	1535	VAL	3.9
1	A	1548	GLY	3.8
1	A	1541	VAL	3.8
1	A	1572	GLU	3.7
1	A	1532	ALA	3.7
1	A	1644	LEU	3.6
1	A	1622	TRP	3.6
1	A	1556	MET	3.5
1	A	1611	LEU	3.5
1	A	1678	LYS	3.5
2	B	4	LEU	3.4
1	A	1567	PHE	3.4
1	A	1542	ARG	3.3
2	B	6	LEU	3.3
1	A	339	MET	3.2
1	A	1543	ILE	3.2
1	A	1646	HIS	3.2
2	B	2	PRO	3.2
1	A	1601	VAL	3.2
1	A	1571	LEU	3.1
1	A	1568	ARG	3.1
1	A	1575	GLU	3.0
1	A	559	ASP	3.0
1	A	1613	ALA	3.0
1	A	1665	ILE	2.9
1	A	1547	ASN	2.8
1	A	1632	ALA	2.8
1	A	1238	LYS	2.8
1	A	1538	ASP	2.7
1	A	1666	ASP	2.7
1	A	1545	MET	2.7
1	A	1531	GLU	2.7
1	A	1641	GLU	2.7
1	A	1578	LEU	2.7
1	A	1605	ASP	2.6
1	A	1637	LEU	2.6
1	A	1527	ARG	2.5
1	A	1609	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1530	LEU	2.5
1	A	1240	THR	2.5
1	A	1634	ARG	2.5
1	A	1647	GLY	2.4
1	A	1648	ALA	2.4
1	A	1604	LEU	2.4
1	A	1475	ALA	2.4
1	A	513	THR	2.3
1	A	1618	ASN	2.3
1	A	1673	ALA	2.3
1	A	1599	ALA	2.2
1	A	1608	GLU	2.2
1	A	1635	GLY	2.2
1	A	1537	HIS	2.2
1	A	1549	ALA	2.2
1	A	1649	ASP	2.1
1	A	1645	LYS	2.1
1	A	1479	ASP	2.0
1	A	550	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	BAL	B	10	5/6	0.42	0.34	121,121,137,137	3
2	AIB	B	9	6/7	0.89	0.48	121,121,121,122	0
2	HPE	B	3	12/13	0.90	0.36	115,116,116,116	0
2	AIB	B	5	6/7	0.90	0.26	117,117,117,117	0
2	AIB	B	8	6/7	0.96	0.38	120,120,120,120	0

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
6	CL	A	1711	1/1	0.55	0.45	113,113,113,113	0
4	MPD	A	1705	8/8	0.71	0.25	98,99,99,99	0
6	CL	A	1712	1/1	0.76	0.36	99,99,99,99	0
4	MPD	A	1706	8/8	0.77	0.35	87,87,88,88	0
4	MPD	A	1707	8/8	0.79	0.37	83,84,85,86	0
4	MPD	A	1708	8/8	0.89	0.23	83,84,85,85	0
5	MES	A	1709	12/12	0.93	0.21	60,65,69,69	0
6	CL	A	1714	1/1	0.97	0.12	72,72,72,72	0
6	CL	A	1710	1/1	0.98	0.47	85,85,85,85	0
6	CL	A	1713	1/1	0.99	0.30	56,56,56,56	0
3	MN	A	1703	1/1	0.99	0.07	52,52,52,52	0
3	MN	A	1701	1/1	1.00	0.03	48,48,48,48	0
3	MN	A	1704	1/1	1.00	0.03	56,56,56,56	0
3	MN	A	1702	1/1	1.00	0.09	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.