Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:05 pm BST

PDB ID	:	6QEP
Title	:	EngBF DARPin Fusion 4b H14
Authors	:	Ernst, P.; Pluckthun, A.; Mittl, P.R.E.
Deposited on	:	2019-01-08
Resolution	:	2.60 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:

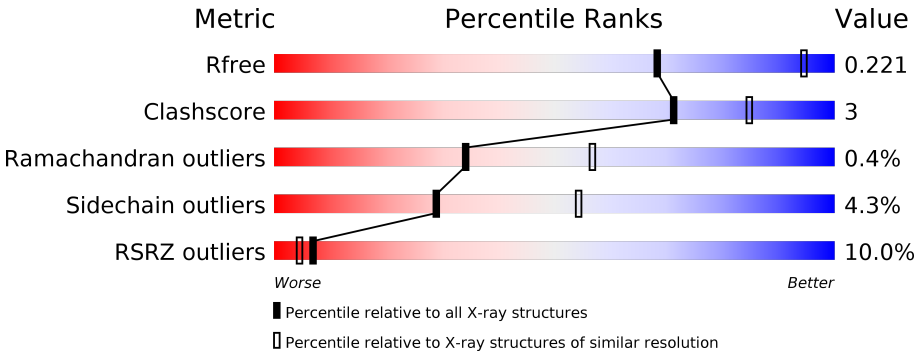
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	1354	10% 87% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10896 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.

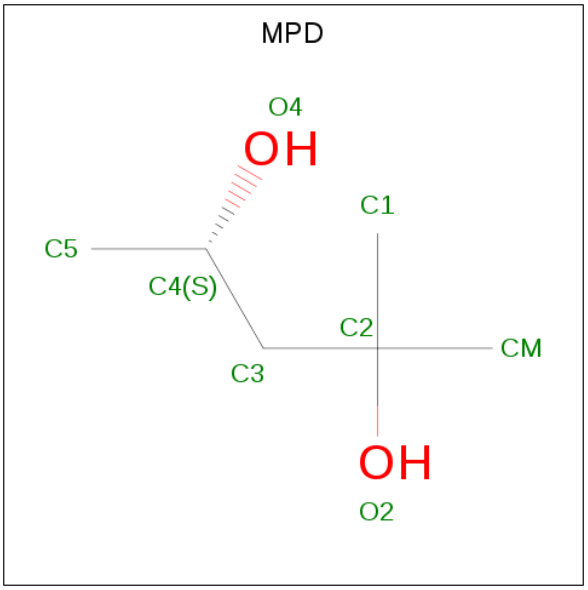
- Molecule 1 is a protein called PEGA domain-containing protein,EngBF-DARPin Fusion 4b H14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1341	10299	6412	1770	2091	26	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

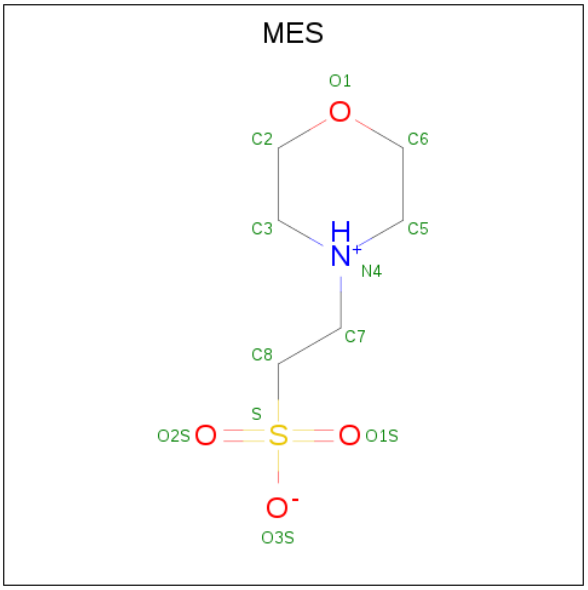
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP A0A374RF80
A	335	PRO	-	expression tag	UNP A0A374RF80
A	336	LEU	-	expression tag	UNP A0A374RF80
A	337	GLY	-	expression tag	UNP A0A374RF80
A	338	SER	-	expression tag	UNP A0A374RF80
A	339	MET	-	expression tag	UNP A0A374RF80
A	1309	ARG	GLN	conflict	UNP A0A374RF80

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



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

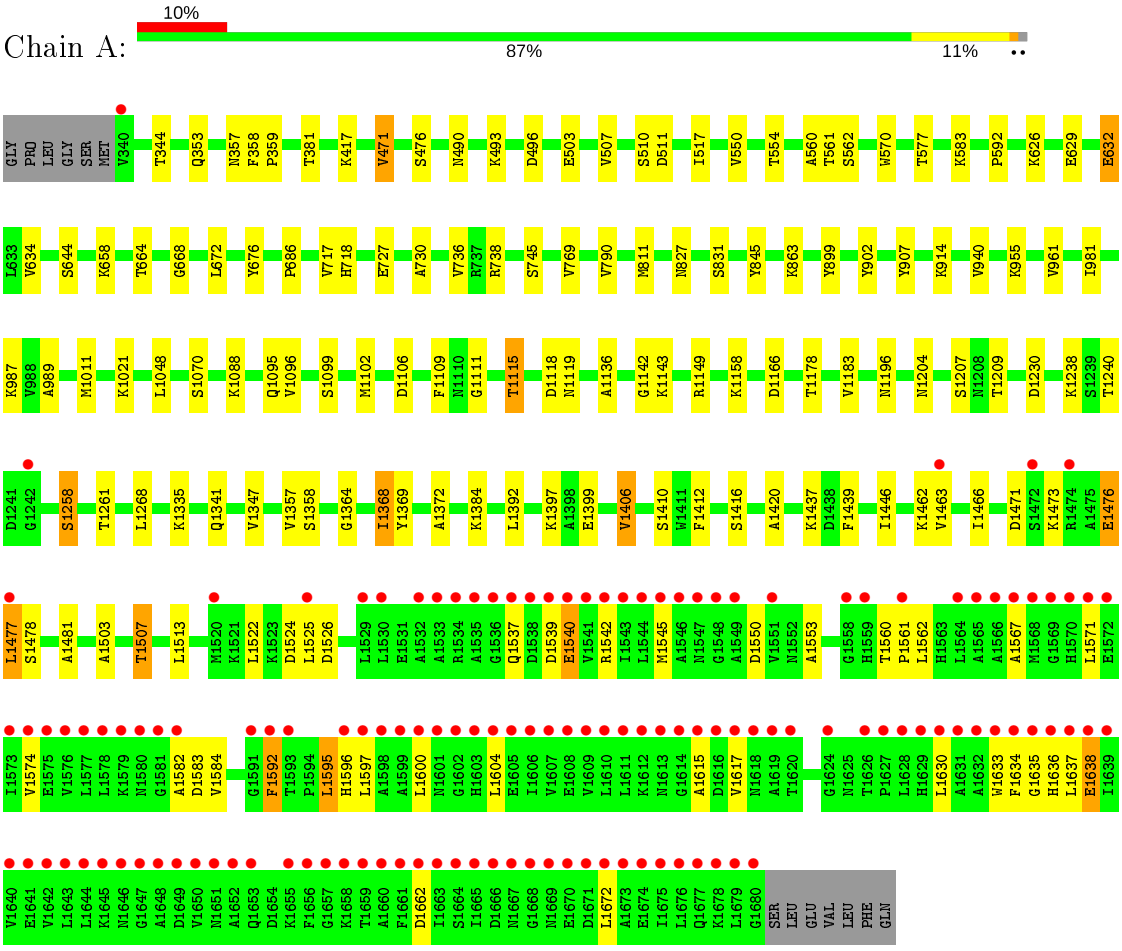
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	573	Total O 573 573	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.

- Molecule 1: PEGA domain-containing protein,EngBF-DARPin Fusion 4b H14



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	192.69Å 192.69Å 123.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.28 – 2.60 48.17 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.28-2.60) 99.9 (48.17-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.177 , 0.215 0.181 , 0.221	Depositor DCC
R_{free} test set	4017 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10896	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: MPD, MN, MES

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	0.51	0/10498	0.74	1/14239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	727	GLU	CB-CA-C	-5.46	99.49	110.40

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	10299	0	9868	70	0
2	A	8	0	14	0	0
3	A	12	0	13	0	0
4	A	4	0	0	0	0
5	A	573	0	0	0	0
All	All	10896	0	9895	70	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 3.

All (70) 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:471:VAL:HG13	1:A:517:ILE:HD11	1.55	0.89
1:A:1149:ARG:HH12	1:A:1230:ASP:HA	1.49	0.78
1:A:1142:GLY:HA2	1:A:1240:THR:HA	1.71	0.71
1:A:1571:LEU:HA	1:A:1574:VAL:HG22	1.74	0.68
1:A:1115:THR:HG22	1:A:1119:ASN:OD1	1.92	0.68
1:A:1462:LYS:O	1:A:1466:ILE:HG12	1.93	0.68
1:A:1364:GLY:HA2	1:A:1392:LEU:HD13	1.76	0.65
1:A:507:VAL:HG22	1:A:510:SER:HB2	1.78	0.65
1:A:1178:THR:HG22	1:A:1183:VAL:HA	1.80	0.63
1:A:1143:LYS:HG2	1:A:1238:LYS:O	1.99	0.62
1:A:1550:ASP:HB3	1:A:1553:ALA:HB2	1.81	0.62
1:A:1595:LEU:HD11	1:A:1615:ALA:HB1	1.83	0.59
1:A:1106:ASP:OD2	1:A:1115:THR:HG21	2.01	0.59
1:A:570:TRP:CD2	1:A:592:PRO:HB3	2.39	0.57
1:A:507:VAL:CG2	1:A:510:SER:HB2	2.35	0.57
1:A:1567:ALA:HB2	1:A:1597:LEU:HB3	1.88	0.54
1:A:955:LYS:HG2	1:A:961:VAL:HG22	1.89	0.54
1:A:1600:LEU:HG	1:A:1630:LEU:HB3	1.90	0.53
1:A:1473:LYS:HB3	1:A:1476:GLU:HG2	1.91	0.53
1:A:1335:LYS:HB2	1:A:1416:SER:HB3	1.92	0.52
1:A:1503:ALA:O	1:A:1507:THR:HG22	2.08	0.51
1:A:1463:VAL:HG22	1:A:1513:LEU:HD11	1.94	0.50
1:A:1478:SER:HB3	1:A:1481:ALA:HB3	1.93	0.50
1:A:1111:GLY:HA3	1:A:1115:THR:HG23	1.94	0.49
1:A:344:THR:HG22	1:A:353:GLN:HG3	1.95	0.49
1:A:1109:PHE:O	1:A:1136:ALA:HB3	2.12	0.49
1:A:554:THR:HA	1:A:562:SER:O	2.13	0.49
1:A:1166:ASP:OD2	1:A:1209:THR:HG21	2.12	0.49
1:A:476:SER:HB3	1:A:560:ALA:HB2	1.95	0.48
1:A:1503:ALA:O	1:A:1507:THR:CG2	2.61	0.48
1:A:1637:LEU:HD12	1:A:1672:LEU:HA	1.96	0.48
1:A:1537:GLN:HB3	1:A:1540:GLU:HB2	1.96	0.47
1:A:1143:LYS:HG3	1:A:1240:THR:HB	1.96	0.47
1:A:1149:ARG:HH12	1:A:1230:ASP:CA	2.23	0.47
1:A:1347:VAL:HG11	1:A:1446:ILE:HD13	1.95	0.47
1:A:632:GLU:O	1:A:668:GLY:HA3	2.15	0.47
1:A:626:LYS:O	1:A:629:GLU:HG2	2.14	0.47
1:A:1477:LEU:HD22	1:A:1522:LEU:HD13	1.97	0.46
1:A:1562:LEU:HD11	1:A:1582:ALA:HB1	1.97	0.46
1:A:658:LYS:HD3	1:A:1096:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:ASN:HB3	1:A:831:SER:HB2	1.97	0.46
1:A:634:VAL:HA	1:A:914:LYS:HG3	1.97	0.45
1:A:1539:ASP:HA	1:A:1542:ARG:HE	1.82	0.45
1:A:1604:LEU:HD22	1:A:1638:GLU:HB2	1.97	0.45
1:A:736:VAL:HG12	1:A:738:ARG:HG3	1.99	0.45
1:A:1592:PHE:HB2	1:A:1596:HIS:CG	2.52	0.44
1:A:664:THR:HA	1:A:907:TYR:OH	2.18	0.44
1:A:1368:ILE:HD11	1:A:1420:ALA:C	2.38	0.44
1:A:899:TYR:O	1:A:902:TYR:HB3	2.18	0.44
1:A:1149:ARG:NH1	1:A:1230:ASP:HA	2.26	0.43
1:A:1357:VAL:O	1:A:1399:GLU:HA	2.17	0.43
1:A:769:VAL:HG23	1:A:811:MET:HG2	2.00	0.43
1:A:1048:LEU:HD11	1:A:1088:LYS:HG2	2.01	0.43
1:A:981:ILE:HD12	1:A:989:ALA:HB3	2.01	0.43
1:A:1560:THR:HB	1:A:1561:PRO:HD2	2.00	0.43
1:A:358:PHE:CG	1:A:359:PRO:HD2	2.54	0.43
1:A:1369:TYR:CD2	1:A:1439:PHE:HB2	2.53	0.43
1:A:831:SER:O	1:A:863:LYS:HE2	2.19	0.42
1:A:577:THR:OG1	1:A:583:LYS:HG2	2.20	0.41
1:A:676:TYR:CD1	1:A:717:VAL:HB	2.55	0.41
1:A:490:ASN:HA	1:A:845:TYR:O	2.21	0.41
1:A:1099:SER:HB3	1:A:1102:MET:HB2	2.02	0.41
1:A:1372:ALA:O	1:A:1412:PHE:HA	2.21	0.41
1:A:1158:LYS:NZ	1:A:1258:SER:HB3	2.35	0.41
1:A:1635:GLY:HA2	1:A:1672:LEU:HD11	2.03	0.41
1:A:686:PRO:HD2	1:A:730:ALA:HB3	2.01	0.41
1:A:490:ASN:ND2	1:A:493:LYS:HD2	2.36	0.40
1:A:1600:LEU:HD11	1:A:1630:LEU:HD22	2.03	0.40
1:A:511:ASP:HA	1:A:550:VAL:O	2.22	0.40
1:A:1196:ASN:HB3	1:A:1204:ASN:HA	2.03	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	1339/1354 (99%)	1271 (95%)	62 (5%)	6 (0%)	34 57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	790	VAL
1	A	940	VAL
1	A	1524	ASP
1	A	1583	ASP
1	A	1638	GLU
1	A	1406	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	1093/1104 (99%)	1046 (96%)	47 (4%)	29 54

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	A	381	THR
1	A	417	LYS
1	A	471	VAL
1	A	496	ASP
1	A	503	GLU
1	A	561	THR
1	A	632	GLU
1	A	644	SER
1	A	672	LEU
1	A	718	HIS
1	A	745	SER
1	A	987	LYS

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Mol	Chain	Res	Type
1	A	1011	MET
1	A	1021	LYS
1	A	1070	SER
1	A	1095	GLN
1	A	1115	THR
1	A	1118	ASP
1	A	1207	SER
1	A	1258	SER
1	A	1261	THR
1	A	1268	LEU
1	A	1341	GLN
1	A	1358	SER
1	A	1368	ILE
1	A	1384	LYS
1	A	1397	LYS
1	A	1406	VAL
1	A	1410	SER
1	A	1437	LYS
1	A	1471	ASP
1	A	1476	GLU
1	A	1477	LEU
1	A	1507	THR
1	A	1525	LEU
1	A	1526	ASP
1	A	1540	GLU
1	A	1545	MET
1	A	1584	VAL
1	A	1592	PHE
1	A	1595	LEU
1	A	1617	VAL
1	A	1633	TRP
1	A	1634	PHE
1	A	1636	HIS
1	A	1662	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	905	ASN
1	A	1277	ASN
1	A	1280	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	MES	A	1702	-	12,12,12	0.69	0	14,16,16	0.44	0
2	MPD	A	1701	-	7,7,7	0.67	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
3	MES	A	1702	-	-	2/6/14/14	0/1/1/1
2	MPD	A	1701	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1702	MES	C8-C7-N4-C5
2	A	1701	MPD	O2-C2-C3-C4
3	A	1702	MES	C8-C7-N4-C3

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	A	1341/1354 (99%)	0.15	134 (9%) 7 4	43, 74, 213, 255	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1661	PHE	9.7
1	A	1676	LEU	8.7
1	A	1678	LYS	8.5
1	A	1672	LEU	8.3
1	A	1633	TRP	8.3
1	A	1668	GLY	8.1
1	A	1544	LEU	8.1
1	A	1637	LEU	8.0
1	A	1665	ILE	7.7
1	A	1628	LEU	7.2
1	A	1674	GLU	7.0
1	A	1647	GLY	7.0
1	A	1667	ASN	6.8
1	A	1675	ILE	6.8
1	A	1617	VAL	6.5
1	A	1618	ASN	6.3
1	A	1634	PHE	6.3
1	A	1648	ALA	6.3
1	A	1630	LEU	6.2
1	A	1655	LYS	6.2
1	A	1635	GLY	6.2
1	A	1651	ASN	6.1
1	A	1670	GLU	6.1
1	A	1673	ALA	6.1
1	A	1598	ALA	6.0
1	A	1578	LEU	6.0
1	A	1571	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	1677	GLN	5.9
1	A	1565	ALA	5.9
1	A	1602	GLY	5.9
1	A	1660	ALA	5.9
1	A	1592	PHE	5.9
1	A	1581	GLY	5.8
1	A	1671	ASP	5.8
1	A	1615	ALA	5.7
1	A	1541	VAL	5.7
1	A	1645	LYS	5.6
1	A	1548	GLY	5.6
1	A	1546	ALA	5.5
1	A	1600	LEU	5.5
1	A	1679	LEU	5.5
1	A	1669	ASN	5.5
1	A	1666	ASP	5.5
1	A	1614	GLY	5.4
1	A	1646	ASN	5.4
1	A	1619	ALA	5.4
1	A	1577	LEU	5.3
1	A	1539	ASP	5.3
1	A	1639	ILE	5.2
1	A	1532	ALA	5.2
1	A	1627	PRO	5.2
1	A	1636	HIS	5.1
1	A	1656	PHE	5.0
1	A	1542	ARG	5.0
1	A	1640	VAL	5.0
1	A	1662	ASP	4.9
1	A	1543	ILE	4.9
1	A	1610	LEU	4.9
1	A	1680	GLY	4.9
1	A	1664	SER	4.9
1	A	1547	ASN	4.8
1	A	1658	LYS	4.8
1	A	1564	LEU	4.8
1	A	1535	ALA	4.8
1	A	1580	ASN	4.7
1	A	1612	LYS	4.7
1	A	1663	ILE	4.7
1	A	1652	ALA	4.6
1	A	1534	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1573	ILE	4.6
1	A	1659	THR	4.5
1	A	1620	THR	4.5
1	A	1569	GLY	4.5
1	A	1611	LEU	4.4
1	A	1607	VAL	4.3
1	A	1597	LEU	4.2
1	A	1538	ASP	4.2
1	A	1545	MET	4.2
1	A	1650	VAL	4.1
1	A	1604	LEU	4.0
1	A	1644	LEU	4.0
1	A	1609	VAL	4.0
1	A	1643	LEU	3.9
1	A	1649	ASP	3.9
1	A	1540	GLU	3.9
1	A	1631	ALA	3.9
1	A	1572	GLU	3.8
1	A	1525	LEU	3.8
1	A	1549	ALA	3.8
1	A	1608	GLU	3.8
1	A	1574	VAL	3.7
1	A	1629	HIS	3.6
1	A	1576	VAL	3.6
1	A	1606	ILE	3.6
1	A	1638	GLU	3.5
1	A	340	VAL	3.5
1	A	1566	ALA	3.5
1	A	1603	HIS	3.5
1	A	1653	GLN	3.4
1	A	1533	ALA	3.4
1	A	1632	ALA	3.4
1	A	1567	ALA	3.3
1	A	1537	GLN	3.3
1	A	1561	PRO	3.3
1	A	1642	VAL	3.2
1	A	1530	LEU	3.1
1	A	1536	GLY	3.1
1	A	1601	ASN	3.1
1	A	1477	LEU	3.1
1	A	1641	GLU	3.0
1	A	1616	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1568	MET	3.0
1	A	1626	THR	3.0
1	A	1529	LEU	2.9
1	A	1624	GLY	2.7
1	A	1474	ARG	2.7
1	A	1599	ALA	2.7
1	A	1575	GLU	2.6
1	A	1463	VAL	2.6
1	A	1613	ASN	2.6
1	A	1551	VAL	2.5
1	A	1520	MET	2.4
1	A	1579	LYS	2.4
1	A	1657	GLY	2.4
1	A	1242	GLY	2.3
1	A	1472	SER	2.3
1	A	1593	THR	2.3
1	A	1582	ALA	2.3
1	A	1570	HIS	2.3
1	A	1591	GLY	2.2
1	A	1559	HIS	2.2
1	A	1596	HIS	2.2
1	A	1605	GLU	2.0
1	A	1558	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	A	1701	8/8	0.93	0.26	101,103,105,106	0
3	MES	A	1702	12/12	0.96	0.15	88,100,108,109	0
4	MN	A	1703	1/1	0.97	0.09	91,91,91,91	0
4	MN	A	1705	1/1	0.98	0.09	78,78,78,78	0
4	MN	A	1706	1/1	0.99	0.14	83,83,83,83	0
4	MN	A	1704	1/1	0.99	0.14	72,72,72,72	0

6.5 Other polymers

There are no such residues in this entry.