Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:00 am BST

PDB ID	:	6GXC
Title	:	Bacterial oligosaccharyltransferase PglB in complex with an inhibitory peptide and a reactive lipid-linked oligosaccharide analog
Authors	:	Napiorkowska, M.; Locher, K.P.; Boilevin, J.; Darbre, T.; Reymond, J.-L.
Deposited on	:	2018-06-27
Resolution	:	3.40 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:

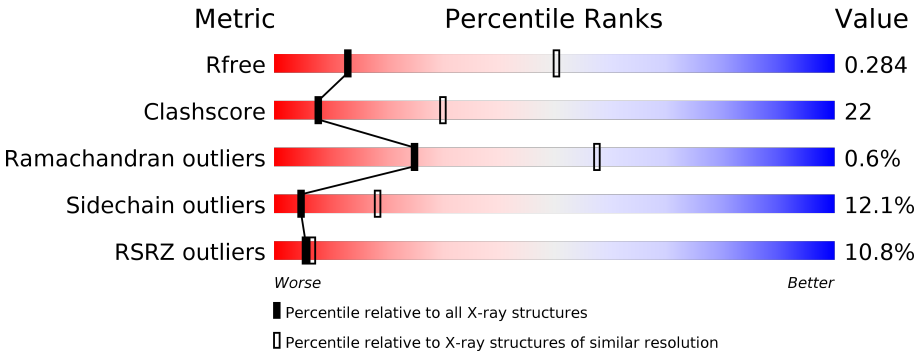
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	724	11% 59% 32% 6%
2	B	8	50% 38% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5931 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 Undecaprenyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5808	3867	885	1031	25			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP B9KDD4
A	17	ALA	CYS	engineered mutation	UNP B9KDD4
A	30	ALA	CYS	engineered mutation	UNP B9KDD4
A	108	THR	ALA	engineered mutation	UNP B9KDD4
A	350	LEU	CYS	engineered mutation	UNP B9KDD4
A	535	GLN	ASN	engineered mutation	UNP B9KDD4
A	549	PRO	LYS	engineered mutation	UNP B9KDD4
A	550	ASN	ASP	engineered mutation	UNP B9KDD4
A	553	ILE	PHE	engineered mutation	UNP B9KDD4
A	556	PRO	ASN	engineered mutation	UNP B9KDD4
A	600	PRO	ALA	engineered mutation	UNP B9KDD4
A	601	LEU	ILE	engineered mutation	UNP B9KDD4
A	602	ASP	ALA	engineered mutation	UNP B9KDD4
A	606	LYS	THR	engineered mutation	UNP B9KDD4
A	607	GLN	THR	engineered mutation	UNP B9KDD4
A	610	ILE	VAL	engineered mutation	UNP B9KDD4
A	611	THR	MET	engineered mutation	UNP B9KDD4
A	619	SER	ILE	engineered mutation	UNP B9KDD4
A	622	TYR	PHE	engineered mutation	UNP B9KDD4
A	624	SER	ALA	engineered mutation	UNP B9KDD4
A	627	ILE	VAL	engineered mutation	UNP B9KDD4
A	630	ASN	ALA	engineered mutation	UNP B9KDD4
A	663	TYR	PHE	engineered mutation	UNP B9KDD4
A	670	TYR	PHE	engineered mutation	UNP B9KDD4
A	713	GLU	-	expression tag	UNP B9KDD4
A	714	PHE	-	expression tag	UNP B9KDD4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	715	HIS	-	expression tag	UNP B9KDD4
A	716	HIS	-	expression tag	UNP B9KDD4
A	717	HIS	-	expression tag	UNP B9KDD4
A	718	HIS	-	expression tag	UNP B9KDD4
A	719	HIS	-	expression tag	UNP B9KDD4
A	720	HIS	-	expression tag	UNP B9KDD4
A	721	HIS	-	expression tag	UNP B9KDD4
A	722	HIS	-	expression tag	UNP B9KDD4
A	723	HIS	-	expression tag	UNP B9KDD4
A	724	HIS	-	expression tag	UNP B9KDD4

- Molecule 2 is a protein called GLY-ASP-GLN-DAB-ALA-THR-PPN-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	5	0	0
			58	33	11	14			

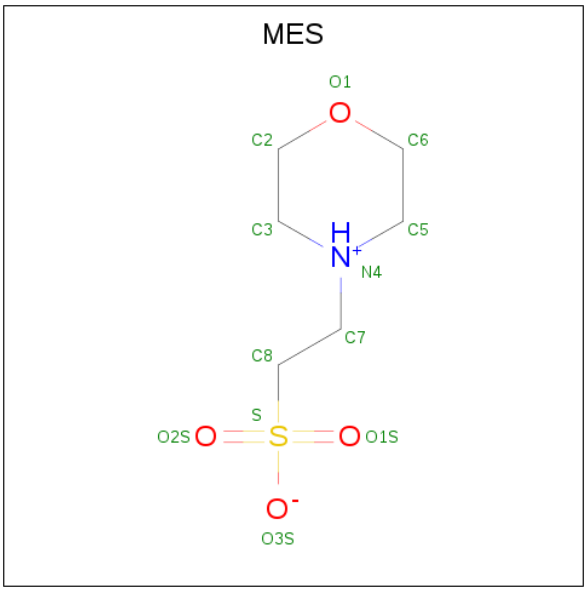
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

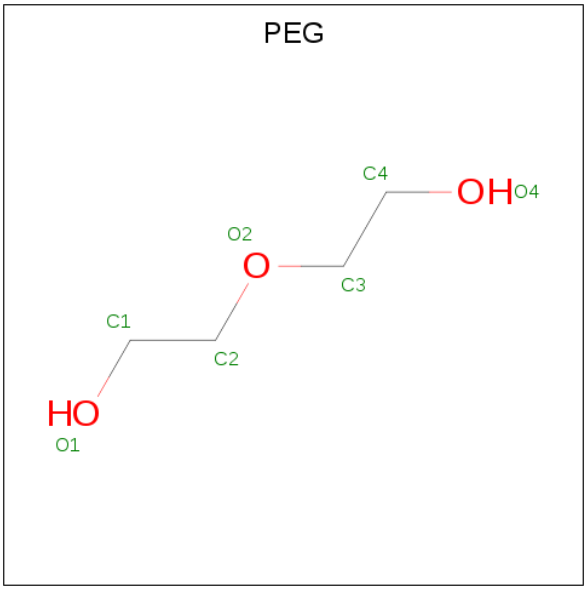
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- 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		

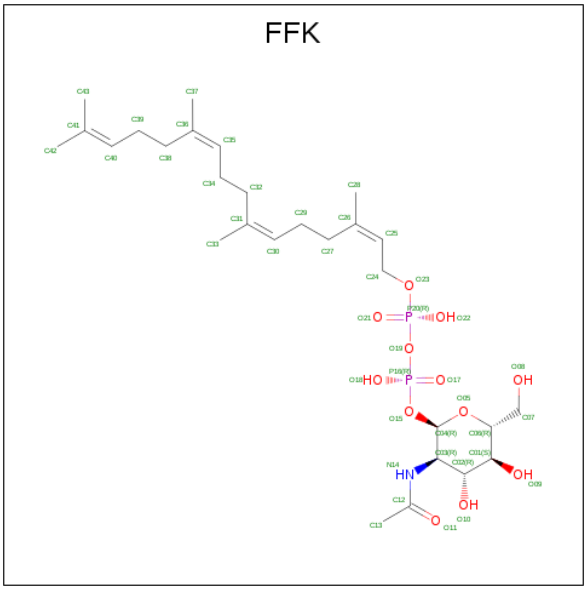
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			7	4	3			

- Molecule 7 is [(2 {R},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl] [oxidanyl-[(2 {Z},6 {Z},10 {Z})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoxy]phosphoryl] hydrogen phosphate (three-letter code: FFK) (formula:

$C_{28}H_{49}NO_{12}P_2$).



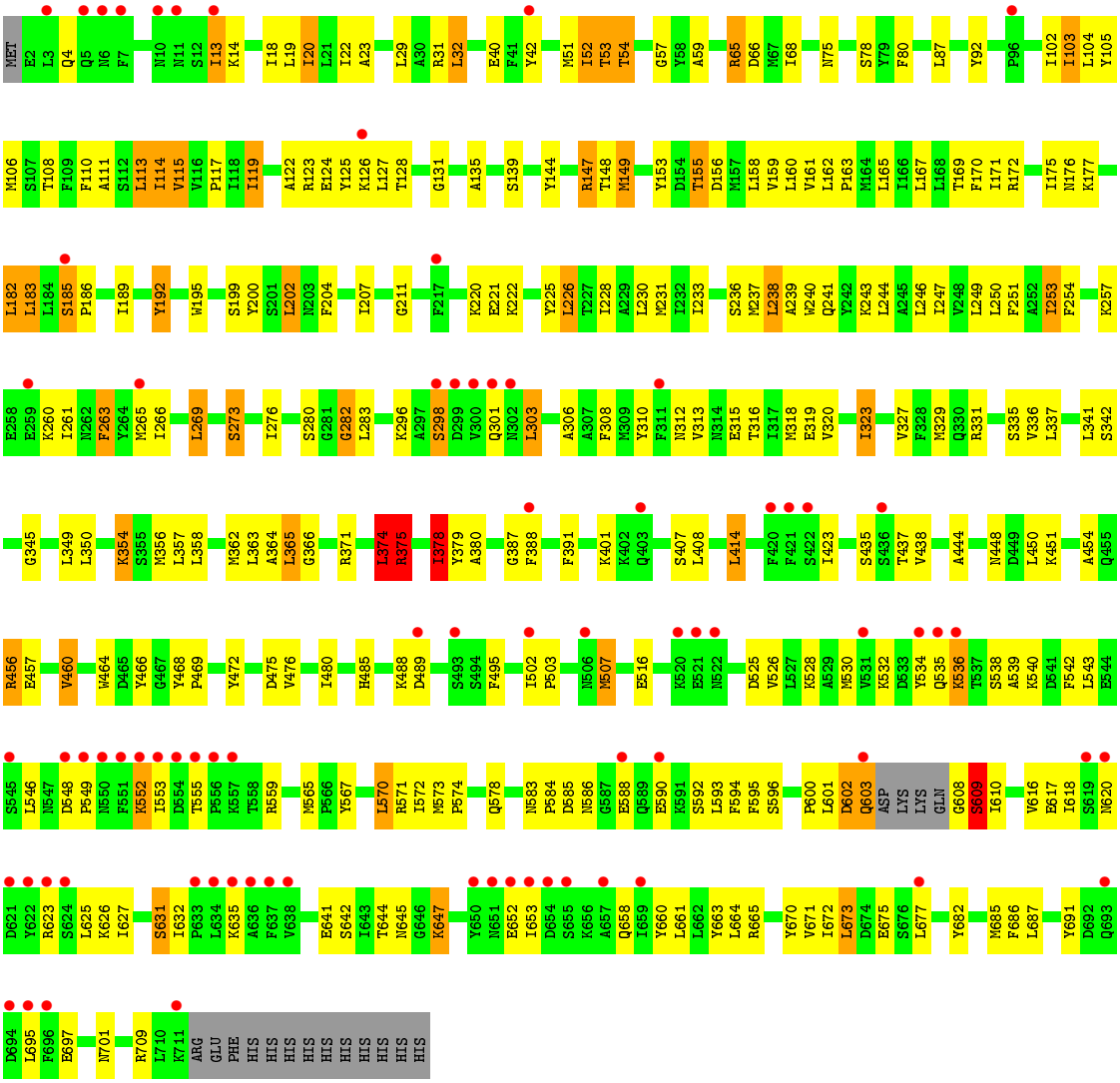
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			43	28	1	12	2		

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: Undecaprenyl-diphosphooligosaccharide--protein glycotransferase

Chain A:



- Molecule 2: GLY-ASP-GLN-DAB-ALA-THR-PPN-GLY

Chain B:


G10
D11
Q12
A13
F16
G17

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.81Å 116.54Å 173.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 3.40 47.67 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.1 (41.09-3.40) 92.2 (47.67-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.40Å)	Xtriage
Refinement program	PHENIX v1.12	Depositor
R, R_{free}	0.249 , 0.283 0.254 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (9.01%)	wwPDB-VP
Wilson B-factor (Å^2)	120.0	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	5931	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: DAB, NA, MN, PPN, FFK, MES, PEG

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	0.44	0/5962	0.64	1/8084 (0.0%)
2	B	0.46	0/34	0.57	0/41
All	All	0.44	0/5996	0.64	1/8125 (0.0%)

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	0	1

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	374	LEU	CA-CB-CG	5.97	129.02	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ASN	Peptide

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	5808	0	5843	255	1
2	B	58	0	44	6	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	12	0	12	4	0
6	A	7	0	10	0	0
7	A	43	0	0	2	0
All	All	5931	0	5909	255	1

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 22.

All (255) 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:296:LYS:HD3	1:A:371:ARG:HH21	1.21	1.05
1:A:31:ARG:HG3	1:A:108:THR:HG23	1.45	0.99
1:A:609:SER:N	1:A:620:ASN:OD1	1.97	0.97
1:A:20:ILE:HG13	1:A:119:ILE:HD11	1.43	0.96
1:A:240:TRP:HB3	5:A:804:MES:H82	1.51	0.91
1:A:115:VAL:HG22	1:A:135:ALA:HB1	1.55	0.88
1:A:31:ARG:NH2	1:A:139:SER:O	2.07	0.87
1:A:182:LEU:HD11	1:A:226:LEU:HD13	1.55	0.86
1:A:552:LYS:HD3	1:A:552:LYS:H	1.39	0.85
1:A:507:MET:O	1:A:507:MET:HE2	1.79	0.82
1:A:375:ARG:NH1	7:A:806:FFK:O17	2.14	0.81
1:A:354:LYS:O	1:A:357:LEU:HB2	1.82	0.80
1:A:586:ASN:HB3	1:A:588:GLU:H	1.46	0.79
1:A:263:PHE:O	1:A:266:ILE:HG13	1.84	0.78
1:A:13:ILE:H	1:A:13:ILE:HD13	1.51	0.76
1:A:147:ARG:NH2	1:A:319:GLU:HG2	2.01	0.75
1:A:237:MET:HG3	1:A:280:SER:HB3	1.68	0.74
1:A:51:MET:HB2	1:A:437:THR:CG2	2.18	0.74
1:A:618:ILE:HD13	1:A:661:LEU:HD21	1.69	0.74
1:A:238:LEU:HD21	1:A:276:ILE:HD13	1.67	0.74
1:A:236:SER:O	1:A:243:LYS:NZ	2.18	0.74
1:A:341:LEU:HD22	1:A:391:PHE:CZ	2.24	0.73
1:A:257:LYS:HG2	1:A:260:LYS:N	2.04	0.73
1:A:104:LEU:HD23	1:A:105:TYR:CE1	2.24	0.72
1:A:617:GLU:HB2	1:A:626:LYS:HB3	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:HD2	1:A:354:LYS:H	1.55	0.71
1:A:460:VAL:CG1	1:A:476:VAL:HG21	2.20	0.71
1:A:516:GLU:HG2	1:A:559:ARG:NH1	2.05	0.71
1:A:144:TYR:HA	1:A:378:ILE:HD11	1.73	0.70
1:A:177:LYS:HE2	1:A:221:GLU:OE2	1.92	0.70
1:A:296:LYS:HD3	1:A:371:ARG:NH2	2.02	0.69
1:A:257:LYS:HG2	1:A:260:LYS:H	1.55	0.69
1:A:608:GLY:HA2	1:A:620:ASN:HD21	1.57	0.69
1:A:578:GLN:NE2	1:A:593:LEU:HD12	2.08	0.68
1:A:600:PRO:HB3	1:A:670:TYR:HE1	1.58	0.68
1:A:14:LYS:O	1:A:18:ILE:HG13	1.94	0.67
1:A:502:ILE:H	1:A:502:ILE:HD12	1.59	0.67
1:A:147:ARG:HH22	1:A:319:GLU:HG2	1.58	0.66
1:A:448:ASN:O	1:A:451:LYS:HB3	1.95	0.66
1:A:660:TYR:HE1	1:A:675:GLU:HG2	1.61	0.66
1:A:20:ILE:HG13	1:A:119:ILE:CD1	2.22	0.65
1:A:158:LEU:HB2	1:A:195:TRP:CZ3	2.32	0.65
1:A:117:PRO:HB3	1:A:165:LEU:HD23	1.79	0.64
1:A:51:MET:HB2	1:A:437:THR:HG21	1.79	0.64
1:A:239:ALA:HA	5:A:804:MES:H31	1.79	0.64
1:A:296:LYS:CD	1:A:371:ARG:HH21	2.04	0.64
1:A:331:ARG:HH22	2:B:11:ASP:CG	2.01	0.64
1:A:644:THR:HG22	1:A:701:ASN:OD1	1.98	0.64
1:A:540:LYS:HG2	1:A:583:ASN:OD1	1.98	0.63
1:A:660:TYR:HB2	1:A:673:LEU:CD1	2.29	0.63
1:A:542:PHE:CZ	1:A:546:LEU:HD21	2.35	0.62
1:A:185:SER:HB3	1:A:186:PRO:HD3	1.81	0.62
1:A:539:ALA:CB	1:A:584:PRO:HB2	2.29	0.62
1:A:52:ILE:HG13	1:A:153:TYR:HB3	1.82	0.62
1:A:342:SER:OG	1:A:388:PHE:HB2	2.00	0.61
1:A:456:ARG:HD3	1:A:475:ASP:O	2.01	0.61
1:A:641:GLU:HB3	1:A:665:ARG:CZ	2.31	0.61
1:A:104:LEU:HD23	1:A:105:TYR:CZ	2.37	0.60
1:A:51:MET:HB2	1:A:437:THR:HG23	1.81	0.60
1:A:257:LYS:CG	1:A:260:LYS:H	2.13	0.60
1:A:354:LYS:CD	1:A:354:LYS:H	2.13	0.60
1:A:635:LYS:HE3	1:A:675:GLU:OE2	2.00	0.60
1:A:119:ILE:HG22	1:A:131:GLY:O	2.02	0.60
1:A:200:TYR:OH	1:A:282:GLY:HA2	2.02	0.60
1:A:160:LEU:HD21	1:A:379:TYR:HA	1.82	0.59
1:A:641:GLU:OE2	1:A:647:LYS:HG2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:HG3	1:A:559:ARG:HH21	1.67	0.59
1:A:318:MET:HG2	2:B:16:PPN:HB2	1.84	0.59
1:A:155:THR:O	1:A:195:TRP:CZ3	2.56	0.59
1:A:507:MET:CE	1:A:507:MET:HA	2.33	0.58
1:A:87:LEU:HD21	1:A:110:PHE:CZ	2.38	0.58
1:A:664:LEU:HD21	1:A:687:LEU:HD21	1.85	0.58
1:A:170:PHE:HE1	1:A:185:SER:OG	1.87	0.58
1:A:495:PHE:CD2	1:A:507:MET:HG3	2.38	0.58
1:A:507:MET:HG2	1:A:546:LEU:HD13	1.85	0.58
1:A:610:ILE:O	1:A:617:GLU:HA	2.03	0.57
1:A:253:ILE:HG22	1:A:261:ILE:HD11	1.85	0.57
1:A:225:TYR:HB3	1:A:266:ILE:HD13	1.85	0.57
1:A:673:LEU:HD12	1:A:673:LEU:N	2.19	0.57
1:A:301:GLN:OE1	1:A:488:LYS:HE3	2.04	0.57
1:A:160:LEU:HD11	1:A:378:ILE:O	2.03	0.57
1:A:175:ILE:HG22	1:A:176:ASN:OD1	2.05	0.56
1:A:608:GLY:HA2	1:A:620:ASN:ND2	2.20	0.56
1:A:685:MET:HG2	1:A:691:TYR:HB3	1.87	0.56
1:A:226:LEU:HD12	1:A:254:PHE:CD1	2.41	0.56
1:A:341:LEU:HD22	1:A:391:PHE:CE2	2.40	0.56
1:A:240:TRP:CB	5:A:804:MES:H82	2.32	0.56
1:A:160:LEU:HA	1:A:163:PRO:HG2	1.87	0.55
1:A:673:LEU:HD12	1:A:673:LEU:H	1.71	0.55
1:A:162:LEU:HD13	1:A:192:TYR:HA	1.89	0.55
1:A:222:LYS:HZ3	1:A:260:LYS:CB	2.20	0.55
1:A:68:ILE:HD13	1:A:92:TYR:CD2	2.41	0.55
1:A:204:PHE:CZ	1:A:283:LEU:HD13	2.42	0.54
1:A:623:ARG:NH1	1:A:653:ILE:HG23	2.23	0.54
1:A:182:LEU:HD22	1:A:230:LEU:HD12	1.88	0.54
1:A:53:THR:HG21	1:A:149:MET:CE	2.38	0.54
1:A:573:MET:N	1:A:574:PRO:HD2	2.23	0.54
1:A:230:LEU:HD13	1:A:247:ILE:HG23	1.89	0.54
1:A:123:ARG:HG3	1:A:128:THR:OG1	2.08	0.53
1:A:552:LYS:N	1:A:552:LYS:HD3	2.18	0.53
1:A:182:LEU:HB3	1:A:251:PHE:HD1	1.73	0.53
1:A:238:LEU:HD22	1:A:276:ILE:HG21	1.89	0.53
1:A:53:THR:O	1:A:53:THR:HG23	2.06	0.53
1:A:331:ARG:NH2	2:B:11:ASP:OD2	2.42	0.53
1:A:543:LEU:O	1:A:546:LEU:HB2	2.10	0.52
1:A:583:ASN:HB3	1:A:586:ASN:HB2	1.91	0.52
1:A:320:VAL:HG12	1:A:320:VAL:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:VAL:HG11	1:A:672:ILE:CD1	2.40	0.52
1:A:202:LEU:HG	1:A:365:LEU:HD12	1.90	0.52
1:A:583:ASN:CG	1:A:586:ASN:HB2	2.30	0.52
1:A:616:VAL:HG22	1:A:627:ILE:HG13	1.91	0.52
1:A:160:LEU:HD22	1:A:362:MET:CE	2.40	0.52
1:A:211:GLY:HA2	1:A:228:ILE:CD1	2.39	0.52
1:A:158:LEU:HB2	1:A:195:TRP:CH2	2.45	0.52
1:A:528:LYS:O	1:A:532:LYS:HG2	2.09	0.52
1:A:23:ALA:HB1	1:A:115:VAL:HG21	1.92	0.51
1:A:466:TYR:C	1:A:469:PRO:HD2	2.31	0.51
1:A:608:GLY:O	1:A:609:SER:O	2.28	0.51
1:A:233:ILE:HG13	1:A:273:SER:OG	2.10	0.51
1:A:102:ILE:O	1:A:106:MET:HG3	2.10	0.51
1:A:301:GLN:HB2	1:A:303:LEU:HD11	1.91	0.51
1:A:507:MET:HG2	1:A:546:LEU:CD1	2.41	0.51
1:A:57:GLY:HA2	1:A:153:TYR:O	2.11	0.51
1:A:19:LEU:HD23	1:A:22:ILE:HD12	1.93	0.51
1:A:54:THR:HG23	2:B:12:GLN:OE1	2.11	0.50
1:A:238:LEU:CD2	1:A:276:ILE:HG21	2.42	0.50
1:A:642:SER:HB3	1:A:645:ASN:HB2	1.94	0.50
1:A:502:ILE:HB	1:A:503:PRO:HD3	1.93	0.50
1:A:189:ILE:HD13	1:A:207:ILE:HD11	1.93	0.50
1:A:59:ALA:HB2	1:A:468:TYR:CG	2.47	0.50
1:A:623:ARG:CZ	1:A:653:ILE:HG23	2.41	0.50
1:A:660:TYR:HB2	1:A:673:LEU:HD13	1.93	0.50
1:A:594:PHE:HE2	1:A:672:ILE:HG22	1.77	0.50
1:A:211:GLY:HA2	1:A:228:ILE:HD11	1.94	0.49
1:A:51:MET:HE3	1:A:444:ALA:HB2	1.92	0.49
1:A:313:VAL:O	1:A:316:THR:HB	2.13	0.49
1:A:327:VAL:O	1:A:331:ARG:HG3	2.13	0.49
1:A:52:ILE:O	1:A:438:VAL:HG23	2.12	0.49
1:A:625:LEU:O	1:A:631:SER:HA	2.12	0.49
1:A:642:SER:CB	1:A:645:ASN:HB2	2.43	0.49
1:A:697:GLU:OE2	1:A:709:ARG:NH1	2.44	0.49
1:A:374:LEU:HD13	1:A:374:LEU:H	1.78	0.49
1:A:52:ILE:HD11	1:A:103:ILE:HG23	1.94	0.49
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.54	0.49
1:A:110:PHE:HA	1:A:113:LEU:HD22	1.94	0.49
1:A:183:LEU:O	1:A:186:PRO:HD2	2.12	0.49
1:A:53:THR:HG21	1:A:149:MET:HE1	1.95	0.48
1:A:329:MET:HE3	1:A:336:VAL:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:MET:HE1	1:A:685:MET:HB2	1.95	0.48
1:A:567:TYR:HB2	1:A:686:PHE:HZ	1.78	0.48
1:A:204:PHE:CE2	1:A:283:LEU:HD13	2.49	0.48
1:A:610:ILE:HB	1:A:618:ILE:HB	1.96	0.48
1:A:257:LYS:HG2	1:A:260:LYS:CA	2.44	0.48
1:A:464:TRP:HZ3	2:B:13:DAB:O	1.97	0.48
1:A:163:PRO:HD3	1:A:192:TYR:CZ	2.49	0.48
1:A:125:TYR:CE1	1:A:356:MET:HE3	2.49	0.48
1:A:573:MET:HE3	1:A:677:LEU:HD22	1.95	0.48
1:A:65:ARG:HG2	1:A:66:ASP:N	2.28	0.47
1:A:401:LYS:HE3	1:A:401:LYS:HB2	1.63	0.47
1:A:548:ASP:OD1	1:A:549:PRO:HD2	2.14	0.47
1:A:437:THR:HG22	1:A:438:VAL:N	2.29	0.47
1:A:170:PHE:HB3	1:A:358:LEU:HD13	1.97	0.47
1:A:226:LEU:CD1	1:A:254:PHE:HB2	2.45	0.47
1:A:222:LYS:HZ3	1:A:260:LYS:HB2	1.79	0.47
1:A:595:PHE:CD2	1:A:596:SER:N	2.83	0.47
1:A:323:ILE:CD1	1:A:327:VAL:HG11	2.46	0.46
1:A:163:PRO:HD3	1:A:192:TYR:CE2	2.51	0.46
1:A:51:MET:SD	1:A:437:THR:HG21	2.56	0.46
1:A:160:LEU:HA	1:A:163:PRO:CG	2.46	0.46
1:A:663:TYR:CD1	1:A:670:TYR:CE2	3.03	0.46
1:A:114:ILE:HA	1:A:161:VAL:HG22	1.97	0.46
1:A:534:TYR:O	1:A:536:LYS:HD3	2.16	0.45
1:A:570:LEU:HD23	1:A:682:TYR:HE2	1.81	0.45
1:A:257:LYS:O	1:A:260:LYS:HG2	2.16	0.45
1:A:507:MET:HE2	1:A:507:MET:CA	2.47	0.45
1:A:155:THR:O	1:A:195:TRP:CH2	2.70	0.45
1:A:345:GLY:HA3	1:A:387:GLY:O	2.17	0.45
1:A:480:ILE:HG22	1:A:489:ASP:HB3	1.99	0.45
1:A:53:THR:CG2	1:A:53:THR:O	2.65	0.45
1:A:608:GLY:HA2	1:A:620:ASN:OD1	2.17	0.45
1:A:32:LEU:HA	1:A:32:LEU:HD12	1.52	0.45
1:A:113:LEU:HA	1:A:113:LEU:HD12	1.57	0.45
1:A:525:ASP:HB3	1:A:528:LYS:HB2	1.99	0.45
1:A:572:ILE:C	1:A:574:PRO:HD2	2.38	0.44
1:A:594:PHE:HE2	1:A:672:ILE:CG2	2.31	0.44
1:A:225:TYR:CB	1:A:266:ILE:HD13	2.48	0.44
1:A:583:ASN:CB	1:A:586:ASN:HB2	2.47	0.44
1:A:237:MET:HG3	1:A:280:SER:CB	2.42	0.44
1:A:526:VAL:O	1:A:530:MET:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:HB3	1:A:131:GLY:HA3	2.00	0.44
1:A:567:TYR:HB2	1:A:686:PHE:CZ	2.53	0.44
1:A:144:TYR:HA	1:A:378:ILE:CD1	2.45	0.44
1:A:125:TYR:OH	1:A:356:MET:CE	2.65	0.44
1:A:456:ARG:HD3	1:A:456:ARG:HA	1.71	0.44
1:A:507:MET:HA	1:A:507:MET:HE3	1.98	0.44
1:A:661:LEU:HD12	1:A:671:VAL:O	2.18	0.44
1:A:349:LEU:HG	1:A:356:MET:HG2	1.99	0.44
1:A:303:LEU:HB3	1:A:306:ALA:HB3	1.99	0.43
1:A:167:LEU:O	1:A:171:ILE:HG12	2.18	0.43
1:A:454:ALA:O	1:A:456:ARG:NH2	2.51	0.43
1:A:466:TYR:O	1:A:469:PRO:HD2	2.18	0.43
1:A:147:ARG:HD3	1:A:156:ASP:OD2	2.18	0.43
1:A:240:TRP:HB3	5:A:804:MES:C8	2.37	0.43
1:A:507:MET:CE	1:A:507:MET:CA	2.96	0.43
1:A:600:PRO:HD3	1:A:670:TYR:CD1	2.53	0.43
1:A:65:ARG:NH1	1:A:472:TYR:O	2.51	0.43
1:A:4:GLN:O	1:A:4:GLN:HG3	2.17	0.43
1:A:185:SER:CB	1:A:186:PRO:HD3	2.46	0.43
1:A:354:LYS:HD2	1:A:354:LYS:N	2.30	0.43
1:A:583:ASN:HB3	1:A:586:ASN:CB	2.48	0.43
1:A:329:MET:HE1	1:A:336:VAL:HG13	2.01	0.43
1:A:595:PHE:HA	1:A:672:ILE:O	2.18	0.42
1:A:538:SER:HB2	1:A:585:ASP:CG	2.40	0.42
1:A:87:LEU:HA	1:A:87:LEU:HD12	1.78	0.42
1:A:365:LEU:HD13	1:A:379:TYR:CD2	2.54	0.42
1:A:111:ALA:CB	1:A:148:THR:HB	2.48	0.42
1:A:207:ILE:HG23	1:A:231:MET:HE3	2.01	0.42
1:A:236:SER:HB2	1:A:276:ILE:HG22	2.01	0.42
1:A:147:ARG:HH22	1:A:319:GLU:CG	2.30	0.42
1:A:250:LEU:HD21	1:A:269:LEU:HD11	2.02	0.42
1:A:507:MET:HE2	1:A:507:MET:C	2.40	0.42
1:A:110:PHE:O	1:A:113:LEU:HB2	2.20	0.42
1:A:124:GLU:OE2	1:A:172:ARG:NE	2.50	0.42
1:A:13:ILE:H	1:A:13:ILE:CD1	2.24	0.42
1:A:308:PHE:CE1	1:A:528:LYS:HA	2.55	0.42
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.72	0.42
1:A:540:LYS:NZ	1:A:590:GLU:OE2	2.52	0.42
1:A:602:ASP:C	1:A:603:GLN:HG2	2.39	0.42
1:A:119:ILE:CG2	1:A:135:ALA:HB2	2.49	0.41
1:A:162:LEU:N	1:A:163:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TRP:CZ3	2:B:13:DAB:O	2.73	0.41
1:A:103:ILE:HG12	1:A:153:TYR:CE1	2.55	0.41
1:A:59:ALA:HB2	1:A:468:TYR:CD1	2.55	0.41
1:A:374:LEU:HD22	1:A:375:ARG:N	2.36	0.41
1:A:378:ILE:HA	1:A:378:ILE:HD12	1.77	0.41
1:A:59:ALA:HB2	1:A:468:TYR:CD2	2.56	0.41
1:A:126:LYS:O	1:A:127:LEU:HD23	2.20	0.41
1:A:78:SER:C	1:A:80:PHE:H	2.24	0.41
1:A:147:ARG:NH1	1:A:156:ASP:OD2	2.40	0.41
1:A:192:TYR:CZ	1:A:199:SER:HB2	2.56	0.41
1:A:23:ALA:HB1	1:A:115:VAL:CG2	2.51	0.41
1:A:594:PHE:CE2	1:A:672:ILE:HG22	2.56	0.41
1:A:52:ILE:CD1	1:A:103:ILE:HG23	2.51	0.40
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.80	0.40
1:A:125:TYR:HE1	1:A:356:MET:HE3	1.85	0.40
1:A:366:GLY:HA3	1:A:380:ALA:HB2	2.03	0.40
1:A:625:LEU:HD13	1:A:672:ILE:HD13	2.03	0.40
1:A:695:LEU:HD23	1:A:695:LEU:HA	1.91	0.40
1:A:298:SER:OG	1:A:312:ASN:HB2	2.21	0.40
1:A:310:TYR:CE2	1:A:488:LYS:HA	2.56	0.40
1:A:623:ARG:HA	1:A:653:ILE:HD13	2.03	0.40
1:A:671:VAL:HG12	1:A:673:LEU:HG	2.03	0.40
1:A:364:ALA:CB	7:A:806:FFK:C42	2.99	0.40
1:A:53:THR:CG2	1:A:149:MET:HE1	2.52	0.40
1:A:350:LEU:HA	1:A:350:LEU:HD12	1.94	0.40

All (1) 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:42:TYR:OH	1:A:586:ASN:ND2[4_557]	2.19	0.01

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	702/724 (97%)	653 (93%)	45 (6%)	4 (1%)	25 57
2	B	4/8 (50%)	4 (100%)	0	0	100 100
All	All	706/732 (96%)	657 (93%)	45 (6%)	4 (1%)	25 57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	609	SER
1	A	282	GLY
1	A	375	ARG
1	A	378	ILE

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	632/650 (97%)	556 (88%)	76 (12%)	5 19
2	B	3/3 (100%)	2 (67%)	1 (33%)	0 1
All	All	635/653 (97%)	558 (88%)	77 (12%)	5 18

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	20	ILE
1	A	29	LEU
1	A	32	LEU
1	A	40	GLU
1	A	52	ILE
1	A	53	THR
1	A	54	THR
1	A	65	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	103	ILE
1	A	113	LEU
1	A	114	ILE
1	A	115	VAL
1	A	119	ILE
1	A	147	ARG
1	A	149	MET
1	A	155	THR
1	A	159	VAL
1	A	169	THR
1	A	182	LEU
1	A	183	LEU
1	A	185	SER
1	A	192	TYR
1	A	202	LEU
1	A	220	LYS
1	A	226	LEU
1	A	238	LEU
1	A	241	GLN
1	A	244	LEU
1	A	246	LEU
1	A	249	LEU
1	A	253	ILE
1	A	263	PHE
1	A	265	MET
1	A	269	LEU
1	A	273	SER
1	A	298	SER
1	A	303	LEU
1	A	315	GLU
1	A	323	ILE
1	A	335	SER
1	A	337	LEU
1	A	354	LYS
1	A	363	LEU
1	A	365	LEU
1	A	374	LEU
1	A	375	ARG
1	A	378	ILE
1	A	407	SER
1	A	408	LEU
1	A	414	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	423	ILE
1	A	435	SER
1	A	450	LEU
1	A	456	ARG
1	A	460	VAL
1	A	485	HIS
1	A	507	MET
1	A	535	GLN
1	A	536	LYS
1	A	552	LYS
1	A	553	ILE
1	A	555	THR
1	A	570	LEU
1	A	571	ARG
1	A	592	SER
1	A	601	LEU
1	A	602	ASP
1	A	603	GLN
1	A	609	SER
1	A	631	SER
1	A	632	ILE
1	A	647	LYS
1	A	652	GLU
1	A	658	GLN
1	A	673	LEU
2	B	12	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	586	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	DAB	B	13	2	5,6,7	0.87	0	1,6,8	0.50	0
2	PPN	B	16	2	12,14,15	1.02	0	13,18,20	1.13	2 (15%)

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	DAB	B	13	2	-	1/4/5/7	-
2	PPN	B	16	2	-	1/7/10/12	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	16	PPN	CB-CA-C	-2.34	107.08	111.47
2	B	16	PPN	CG-CB-CA	-2.01	110.04	114.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	13	DAB	N-CA-CB-CG
2	B	16	PPN	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	13	DAB	2	0
2	B	16	PPN	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\|>2$
7	FFK	A	806	-	40,43,43	2.30	19 (47%)	53,59,59	1.89	17 (32%)
6	PEG	A	805	-	6,6,6	0.67	0	5,5,5	0.62	0
5	MES	A	804	-	12,12,12	2.07	1 (8%)	14,16,16	2.37	6 (42%)

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
7	FFK	A	806	-	-	6/41/62/62	0/1/1/1
6	PEG	A	805	-	-	3/4/4/4	-
5	MES	A	804	-	-	4/6/14/14	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	MES	C8-S	-6.72	1.68	1.77
7	A	806	FFK	O05-C04	6.17	1.57	1.41
7	A	806	FFK	C12-N14	4.53	1.49	1.34
7	A	806	FFK	C13-C12	3.63	1.58	1.50
7	A	806	FFK	C38-C36	3.50	1.58	1.51
7	A	806	FFK	C03-N14	3.46	1.51	1.45
7	A	806	FFK	P16-O15	3.08	1.68	1.60
7	A	806	FFK	C25-C26	2.87	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	806	FFK	C04-C03	2.78	1.57	1.53
7	A	806	FFK	C02-C03	-2.60	1.48	1.53
7	A	806	FFK	C43-C41	2.58	1.57	1.50
7	A	806	FFK	O10-C02	2.53	1.48	1.43
7	A	806	FFK	C27-C26	2.48	1.56	1.51
7	A	806	FFK	C24-C25	2.30	1.56	1.49
7	A	806	FFK	O05-C06	2.29	1.49	1.44
7	A	806	FFK	P16-O18	-2.26	1.44	1.55
7	A	806	FFK	C29-C30	2.24	1.57	1.50
7	A	806	FFK	O09-C01	2.15	1.48	1.43
7	A	806	FFK	O11-C12	-2.15	1.18	1.23
7	A	806	FFK	C34-C35	2.08	1.57	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	804	MES	C5-N4-C3	5.12	120.36	108.83
7	A	806	FFK	O05-C06-C01	4.79	118.40	109.69
7	A	806	FFK	O19-P16-O15	4.62	111.79	102.48
7	A	806	FFK	P20-O19-P16	-4.19	118.43	132.83
7	A	806	FFK	O05-C04-O15	3.89	116.46	111.36
5	A	804	MES	C7-N4-C3	3.54	120.28	111.23
5	A	804	MES	O3S-S-C8	3.51	111.44	105.77
7	A	806	FFK	C07-C06-C01	-2.97	106.04	113.00
5	A	804	MES	O1S-S-C8	2.97	110.49	106.92
7	A	806	FFK	C03-N14-C12	-2.74	116.52	123.18
7	A	806	FFK	O18-P16-O17	-2.72	98.80	112.24
7	A	806	FFK	C04-O05-C06	2.72	119.02	113.69
7	A	806	FFK	C43-C41-C42	2.66	120.47	114.60
7	A	806	FFK	C37-C36-C35	-2.51	117.25	123.68
7	A	806	FFK	C38-C36-C35	2.41	126.00	121.12
5	A	804	MES	C7-N4-C5	2.38	117.31	111.23
7	A	806	FFK	C13-C12-N14	2.30	119.98	116.10
5	A	804	MES	C6-C5-N4	-2.27	106.66	110.10
7	A	806	FFK	C24-C25-C26	-2.20	122.25	126.04
7	A	806	FFK	C02-C03-N14	-2.17	106.52	110.62
7	A	806	FFK	C39-C40-C41	-2.16	120.38	127.75
7	A	806	FFK	C27-C29-C30	2.04	118.58	111.88
7	A	806	FFK	O22-P20-O21	-2.02	102.25	112.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	806	FFK	O05-C04-O15-P16
5	A	804	MES	N4-C7-C8-S
6	A	805	PEG	O2-C3-C4-O4
6	A	805	PEG	O1-C1-C2-O2
7	A	806	FFK	C26-C27-C29-C30
7	A	806	FFK	O05-C06-C07-O08
7	A	806	FFK	P20-O19-P16-O17
5	A	804	MES	C7-C8-S-O3S
5	A	804	MES	C7-C8-S-O1S
6	A	805	PEG	C4-C3-O2-C2
7	A	806	FFK	C04-C03-N14-C12
5	A	804	MES	C8-C7-N4-C3
7	A	806	FFK	C28-C26-C27-C29

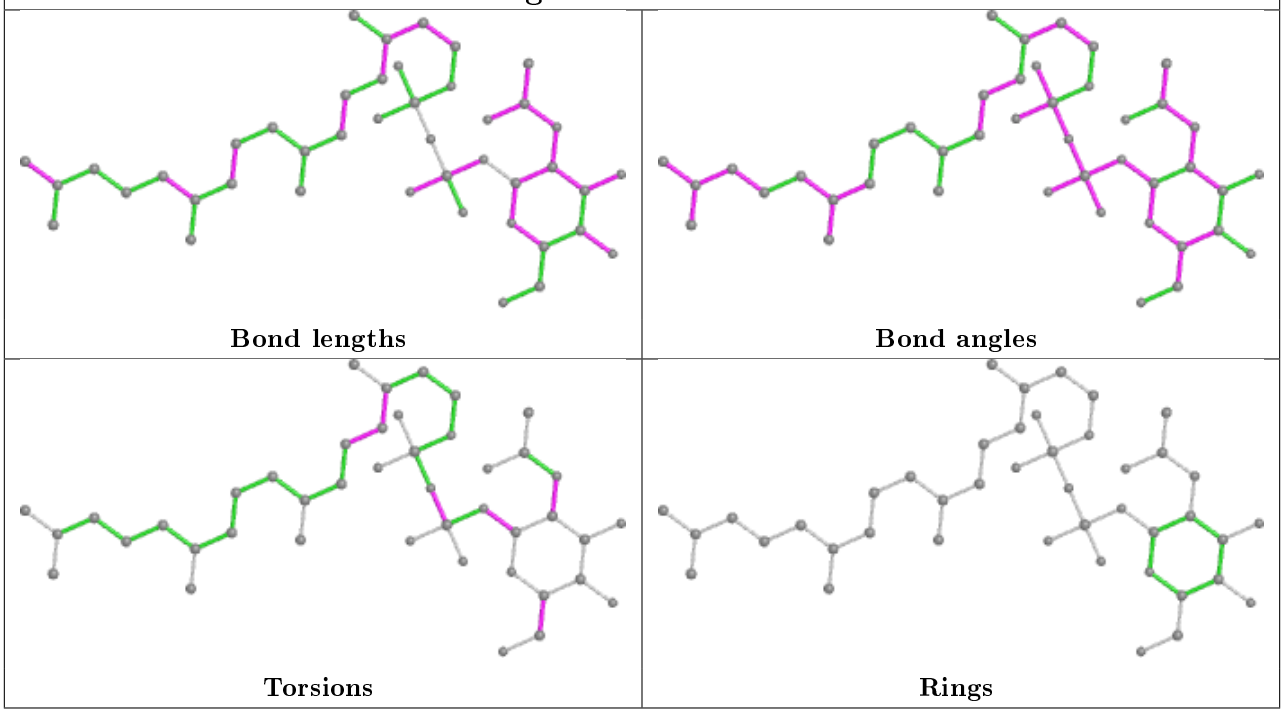
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	806	FFK	2	0
5	A	804	MES	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FFK A 806



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	706/724 (97%)	0.42	77 (10%) 5 6	84, 107, 142, 174	0
2	B	6/8 (75%)	0.04	0 100 100	86, 87, 89, 93	2 (33%)
All	All	712/732 (97%)	0.42	77 (10%) 5 7	84, 107, 142, 174	2 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	LYS	11.7
1	A	554	ASP	10.3
1	A	653	ILE	9.7
1	A	623	ARG	8.8
1	A	551	PHE	8.5
1	A	553	ILE	7.9
1	A	652	GLU	7.5
1	A	299	ASP	6.5
1	A	621	ASP	6.1
1	A	622	TYR	6.0
1	A	301	GLN	5.9
1	A	550	ASN	5.7
1	A	651	ASN	5.5
1	A	535	GLN	5.4
1	A	534	TYR	5.4
1	A	555	THR	5.4
1	A	650	TYR	5.3
1	A	300	VAL	4.9
1	A	654	ASP	4.9
1	A	521	GLU	4.8
1	A	655	SER	4.8
1	A	635	LYS	4.3
1	A	636	ALA	4.3
1	A	695	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	520	LYS	4.2
1	A	302	ASN	4.1
1	A	590	GLU	4.0
1	A	557	LYS	3.9
1	A	388	PHE	3.9
1	A	506	ASN	3.8
1	A	421	PHE	3.8
1	A	657	ALA	3.7
1	A	298	SER	3.7
1	A	694	ASP	3.7
1	A	502	ILE	3.6
1	A	556	PRO	3.4
1	A	522	ASN	3.4
1	A	634	LEU	3.3
1	A	549	PRO	3.2
1	A	265	MET	3.1
1	A	637	PHE	3.1
1	A	693	GLN	3.1
1	A	531	VAL	3.0
1	A	711	LYS	3.0
1	A	3	LEU	3.0
1	A	624	SER	2.9
1	A	126	LYS	2.9
1	A	96	PRO	2.8
1	A	620	ASN	2.8
1	A	42	TYR	2.8
1	A	659	ILE	2.7
1	A	6	ASN	2.7
1	A	10	ASN	2.7
1	A	420	PHE	2.7
1	A	696	PHE	2.7
1	A	548	ASP	2.6
1	A	536	LYS	2.6
1	A	545	SER	2.5
1	A	5	GLN	2.5
1	A	11	ASN	2.4
1	A	13	ILE	2.4
1	A	603	GLN	2.4
1	A	311	PHE	2.4
1	A	403	GLN	2.3
1	A	633	PRO	2.3
1	A	7	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	217	PHE	2.2
1	A	422	SER	2.2
1	A	489	ASP	2.2
1	A	259	GLU	2.2
1	A	677	LEU	2.1
1	A	638	VAL	2.1
1	A	493	SER	2.1
1	A	619	SER	2.1
1	A	185	SER	2.1
1	A	588	GLU	2.1
1	A	436	SER	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	DAB	B	13	7/8	0.91	0.36	85,89,94,94	0
2	PPN	B	16	14/15	0.93	0.18	92,99,101,102	0

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	A	805	7/7	0.74	0.24	114,114,114,114	0
4	NA	A	803	1/1	0.79	0.30	75,75,75,75	0
7	FFK	A	806	43/43	0.85	0.34	85,105,105,105	43
5	MES	A	804	12/12	0.89	0.20	127,127,127,127	0
3	MN	A	802	1/1	0.91	0.28	108,108,108,108	1

Continued on next page...

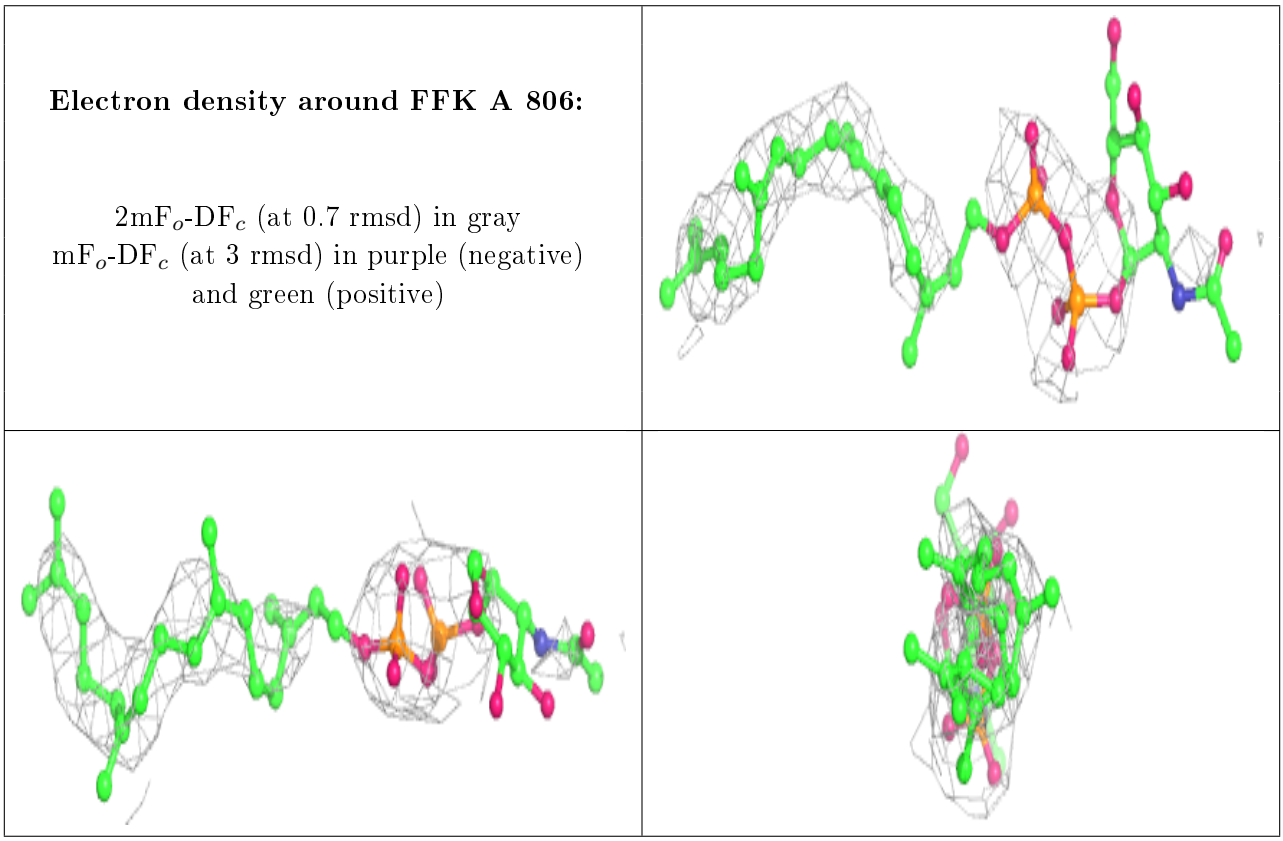
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	A	801	1/1	0.96	0.31	92,92,92,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FFK A 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.