



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 19, 2018 – 05:31 PM EST

PDB ID : 6BE1  
EMDB ID: : EMD-7088  
Title : Cryo-EM structure of serotonin receptor  
Authors : Basak, S.; Chakrapani, S.  
Deposited on : 2017-10-24  
Resolution : 4.31 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

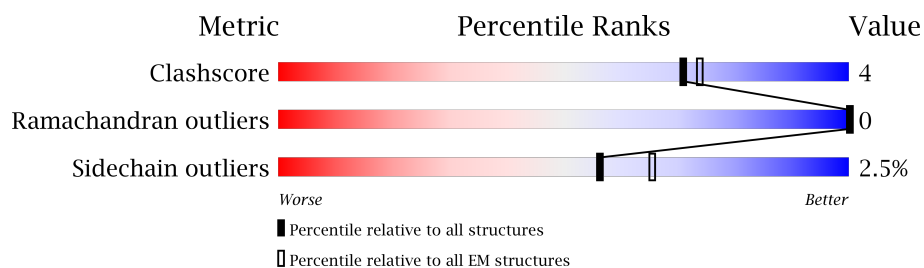
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.31 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	457	
1	B	457	
1	C	457	
1	D	457	
1	E	457	

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	NAG	A	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	506	X	-	-	-
2	NAG	C	502	X	-	-	-
2	NAG	C	507	X	-	-	-
2	NAG	E	504	X	-	-	-
2	NAG	E	506	X	-	-	-
3	BMA	E	503	X	-	-	-

## 2 Entry composition [i](#)

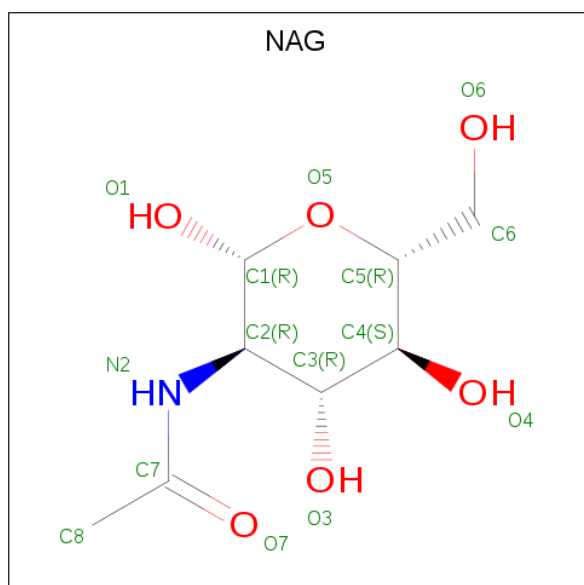
There are 7 unique types of molecules in this entry. The entry contains 16910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5-hydroxytryptamine receptor 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	399	Total	C	N	O	S	0	0
			3277	2155	536	576	10		
1	B	399	Total	C	N	O	S	0	0
			3265	2145	534	576	10		
1	C	399	Total	C	N	O	S	0	0
			3272	2150	534	578	10		
1	D	399	Total	C	N	O	S	0	0
			3266	2146	534	576	10		
1	E	399	Total	C	N	O	S	0	0
			3269	2147	534	578	10		

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	

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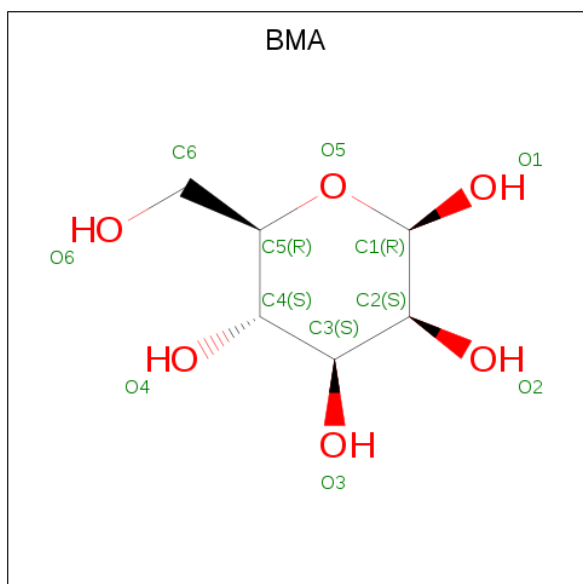
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	A	1	Total	C	N	O	0
			84	48	6	30	
2	B	1	Total	C	N	O	0
			83	48	6	29	
2	B	1	Total	C	N	O	0
			83	48	6	29	
2	B	1	Total	C	N	O	0
			83	48	6	29	
2	B	1	Total	C	N	O	0
			83	48	6	29	
2	B	1	Total	C	N	O	0
			83	48	6	29	
2	B	1	Total	C	N	O	0
			83	48	6	29	
2	C	1	Total	C	N	O	0
			83	48	6	29	
2	C	1	Total	C	N	O	0
			83	48	6	29	
2	C	1	Total	C	N	O	0
			83	48	6	29	
2	C	1	Total	C	N	O	0
			83	48	6	29	
2	C	1	Total	C	N	O	0
			83	48	6	29	
2	C	1	Total	C	N	O	0
			83	48	6	29	
2	D	1	Total	C	N	O	0
			69	40	5	24	
2	D	1	Total	C	N	O	0
			69	40	5	24	
2	D	1	Total	C	N	O	0
			69	40	5	24	
2	D	1	Total	C	N	O	0
			69	40	5	24	
2	D	1	Total	C	N	O	0
			69	40	5	24	

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Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	N	O	0
			84	48	6	30	
2	E	1	Total	C	N	O	0
			84	48	6	30	
2	E	1	Total	C	N	O	0
			84	48	6	30	
2	E	1	Total	C	N	O	0
			84	48	6	30	
2	E	1	Total	C	N	O	0
			84	48	6	30	

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

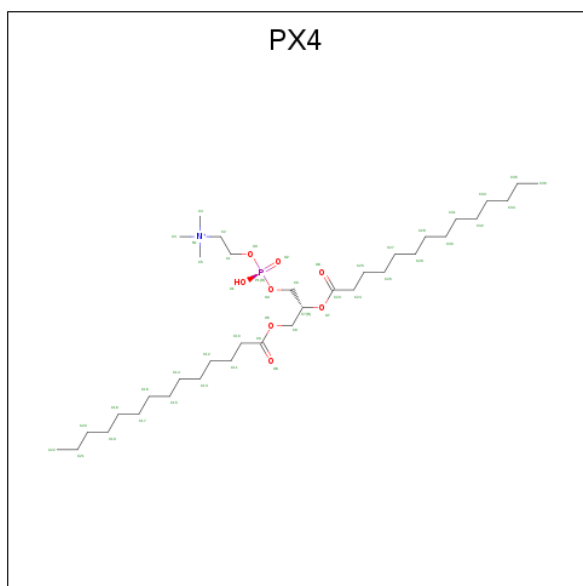


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			11	6	5	
3	B	1	Total	C	O	0
			12	6	6	
3	C	1	Total	C	O	0
			12	6	6	
3	D	1	Total	C	O	0
			12	6	6	
3	E	1	Total	C	O	0
			11	6	5	

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

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

- Molecule 5 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			35	19	14	2	
5	A	1	Total	C	O	P	0
			35	19	14	2	
5	C	1	Total	C	O	P	0
			18	10	7	1	
5	D	1	Total	C	O	P	0
			17	9	7	1	
5	E	1	Total	C	O	P	0
			17	9	7	1	

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

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Cl	0
			1	1	

- Molecule 7 is water.

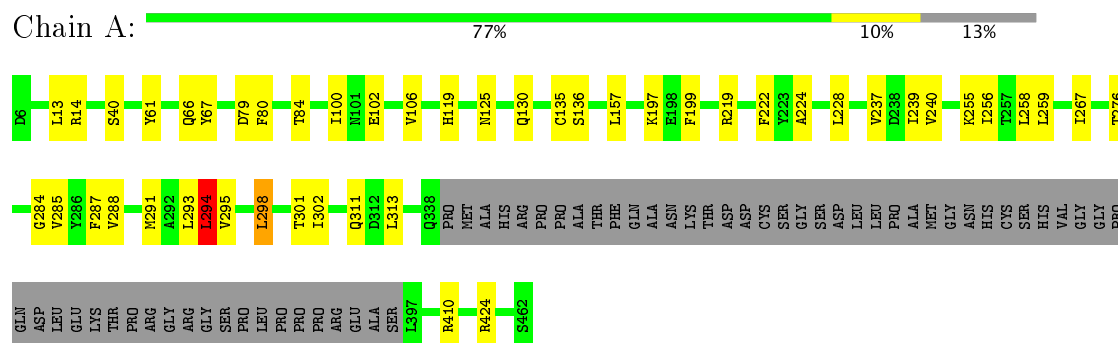
Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total 3	O 3	0
7	B	1	Total 1	O 1	0
7	C	3	Total 3	O 3	0
7	D	2	Total 2	O 2	0
7	E	2	Total 2	O 2	0



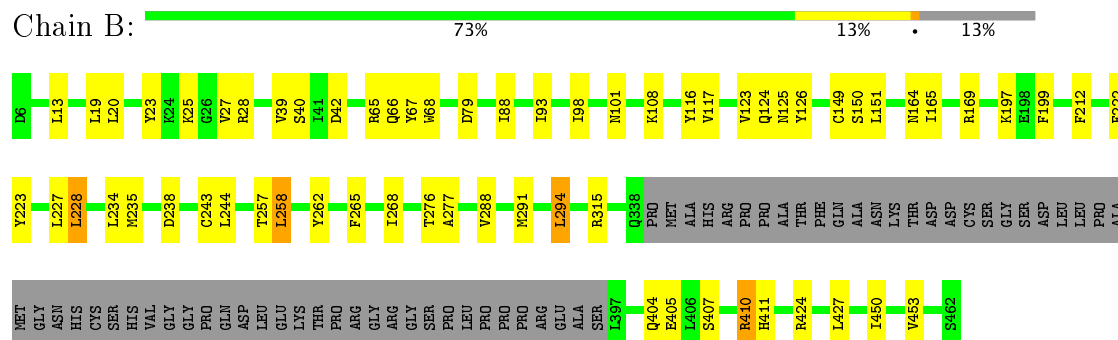
### 3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

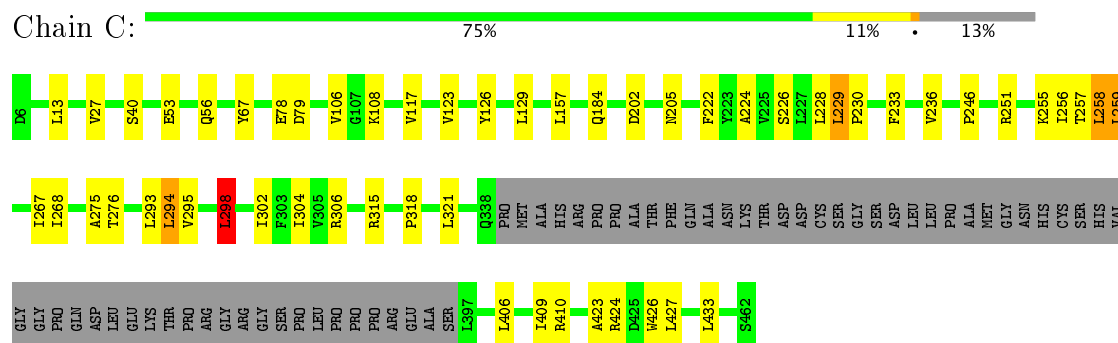
#### • Molecule 1: 5-hydroxytryptamine receptor 3A



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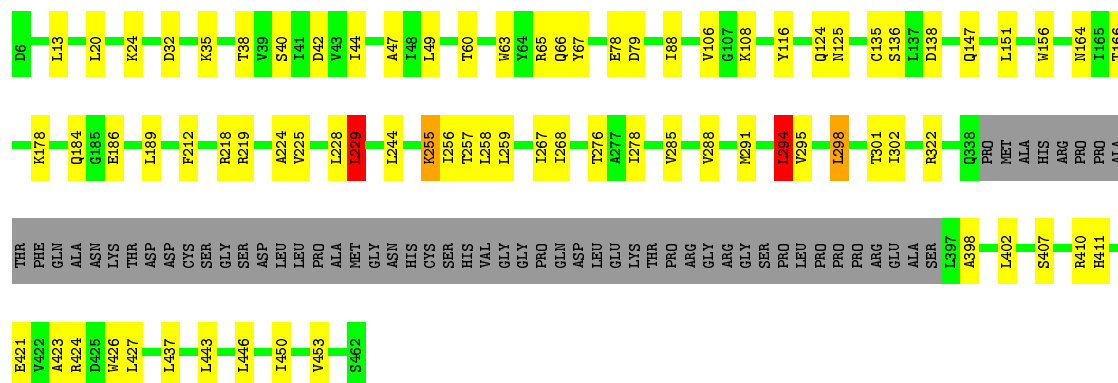


#### • Molecule 1: 5-hydroxytryptamine receptor 3A




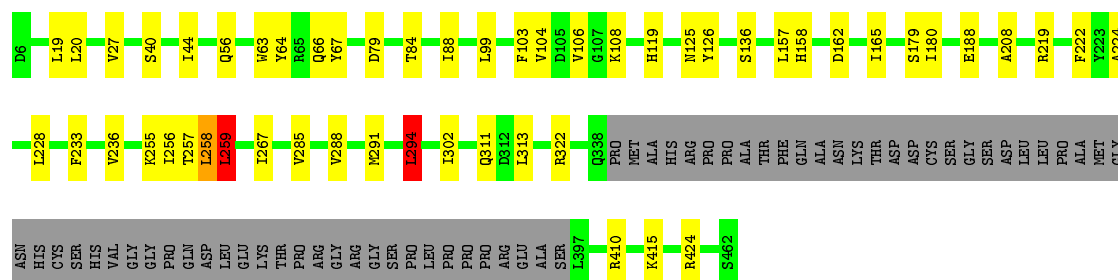
#### • Molecule 1: 5-hydroxytryptamine receptor 3A

Chain D:  70% 16% 13%



- Molecule 1: 5-hydroxytryptamine receptor 3A

Chain E:  76% 11% 13%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	3D CRYSTAL, $a$ =Not provided Å, $b$ =Not provided Å, $c$ =Not provided Å, $\alpha$ =Not provided°, $\beta$ =Not provided°, $\gamma$ =Not provided°, space group=Not provided	Depositor
Number of particles used	108727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, BMA, NAG, PX4, CL

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  >2	RMSZ	# Z  >2
1	A	0.27	0/3367	0.62	4/4600 (0.1%)
1	B	0.27	0/3354	0.62	3/4583 (0.1%)
1	C	0.27	0/3361	0.65	8/4592 (0.2%)
1	D	0.27	0/3355	0.63	5/4584 (0.1%)
1	E	0.28	0/3358	0.61	3/4588 (0.1%)
All	All	0.27	0/16795	0.63	23/22947 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	229	LEU	CA-CB-CG	7.34	132.19	115.30
1	C	129	LEU	CA-CB-CG	7.28	132.03	115.30
1	D	79	ASP	CB-CG-OD1	7.16	124.74	118.30
1	B	294	LEU	CA-CB-CG	7.01	131.43	115.30
1	D	229	LEU	CA-CB-CG	6.51	130.27	115.30
1	C	298	LEU	CA-CB-CG	6.28	129.74	115.30
1	E	294	LEU	CA-CB-CG	6.27	129.72	115.30
1	C	294	LEU	CA-CB-CG	6.07	129.26	115.30
1	D	294	LEU	CA-CB-CG	5.86	128.78	115.30
1	C	293	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	228	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	259	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	79	ASP	CB-CG-OD1	5.63	123.36	118.30
1	E	79	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	78	GLU	C-N-CA	5.57	135.62	121.70
1	D	259	LEU	CA-CB-CG	5.51	127.96	115.30
1	C	259	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	79	ASP	CB-CG-OD1	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	259	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	78	GLU	C-N-CA	5.22	134.75	121.70
1	A	293	LEU	CA-CB-CG	5.12	127.07	115.30

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	3277	0	3278	24	0
1	B	3265	0	3254	35	0
1	C	3272	0	3266	34	0
1	D	3266	0	3255	43	0
1	E	3269	0	3257	32	0
2	A	84	0	74	0	0
2	B	83	0	73	0	0
2	C	83	0	73	0	0
2	D	69	0	61	1	0
2	E	84	0	73	0	0
3	A	11	0	10	0	0
3	B	12	0	11	0	0
3	C	12	0	11	0	0
3	D	12	0	11	0	0
3	E	11	0	10	0	0
4	A	1	0	0	0	0
5	A	35	0	28	0	0
5	C	18	0	15	0	0
5	D	17	0	13	0	0
5	E	17	0	13	0	0
6	C	1	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	2	0	0	0	0
All	All	16910	0	16786	137	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 4.

All (137) 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:D:66:GLN:HB2	1:D:125:ASN:HB3	1.76	0.66
1:D:224:ALA:O	1:D:228:LEU:HB2	1.99	0.62
1:A:157:LEU:HD12	1:E:126:TYR:HB2	1.82	0.61
1:B:238:ASP:HB3	1:B:258:LEU:HD11	1.82	0.61
1:B:40:SER:HB2	1:B:67:TYR:HB2	1.81	0.60
1:A:61:TYR:HD1	1:A:130:GLN:HB3	1.67	0.60
1:A:106:VAL:HB	1:E:108:LYS:HE2	1.85	0.59
1:C:40:SER:HB2	1:C:67:TYR:HB2	1.85	0.58
1:E:311:GLN:HB3	1:E:313:LEU:HD13	1.86	0.57
1:B:126:TYR:HB2	1:C:157:LEU:HD12	1.85	0.57
1:C:268:ILE:HG21	1:D:267:ILE:HD12	1.87	0.57
1:C:257:THR:HG21	1:D:256:ILE:HB	1.87	0.56
1:C:108:LYS:HE2	1:D:106:VAL:HB	1.87	0.56
1:D:255:LYS:NZ	1:D:301:THR:OG1	2.38	0.56
1:B:257:THR:HG21	1:C:256:ILE:HB	1.88	0.56
1:A:224:ALA:HA	1:A:228:LEU:HD23	1.87	0.55
1:A:219:ARG:NH1	1:B:277:ALA:O	2.39	0.55
1:C:202:ASP:HB2	1:C:205:ASN:HB2	1.87	0.55
1:A:311:GLN:HB3	1:A:313:LEU:HD13	1.87	0.55
1:D:40:SER:HB2	1:D:67:TYR:HB2	1.88	0.55
1:D:108:LYS:HE2	1:E:106:VAL:HB	1.88	0.54
1:A:255:LYS:NZ	1:A:301:THR:OG1	2.41	0.54
1:D:268:ILE:HG21	1:E:267:ILE:HD12	1.89	0.54
1:D:178:LYS:NZ	1:D:189:LEU:O	2.40	0.54
1:D:116:TYR:HB2	1:D:124:GLN:HB3	1.90	0.54
1:D:407:SER:O	1:D:411:HIS:ND1	2.37	0.54
1:D:38:THR:HG22	1:D:164:ASN:HB3	1.90	0.53
1:D:166:THR:HG22	2:D:501:NAG:H61	1.90	0.53
1:B:66:GLN:HB2	1:B:125:ASN:HB3	1.90	0.53
1:B:42:ASP:OD1	1:B:169:ARG:NH1	2.41	0.53
1:E:158:HIS:HB3	1:E:162:ASP:HB3	1.90	0.52
1:D:257:THR:HG21	1:E:256:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:HB3	1:B:65:ARG:HB2	1.91	0.51
1:B:108:LYS:HE2	1:C:106:VAL:HB	1.92	0.51
1:E:20:LEU:HD11	1:E:88:ILE:HD11	1.93	0.51
1:E:40:SER:HB2	1:E:67:TYR:HB2	1.93	0.51
1:B:13:LEU:HD12	1:C:27:VAL:HG11	1.93	0.51
1:E:165:ILE:HG12	1:E:208:ALA:HB1	1.93	0.51
1:D:244:LEU:HD22	1:E:302:ILE:HD11	1.92	0.50
1:C:304:ILE:HD13	1:C:433:LEU:HD12	1.92	0.50
1:B:222:PHE:HB2	1:C:276:THR:HB	1.93	0.50
1:C:233:PHE:HA	1:C:236:VAL:HG22	1.92	0.50
1:E:66:GLN:HB2	1:E:125:ASN:HB3	1.93	0.50
1:A:66:GLN:HB2	1:A:125:ASN:HB3	1.93	0.50
1:D:295:VAL:HA	1:D:298:LEU:HD23	1.94	0.49
1:B:149:CYS:SG	1:B:150:SER:N	2.86	0.49
1:E:255:LYS:HA	1:E:258:LEU:HD23	1.95	0.49
1:D:225:VAL:HG23	1:D:229:LEU:HD21	1.94	0.48
1:B:244:LEU:HD22	1:C:302:ILE:HD11	1.96	0.48
1:C:222:PHE:HB2	1:D:276:THR:HA	1.95	0.48
1:D:44:ILE:HB	1:D:63:TRP:HB2	1.95	0.48
1:A:256:ILE:HB	1:E:257:THR:HG21	1.95	0.48
1:C:224:ALA:O	1:C:228:LEU:HB2	2.13	0.48
1:B:291:MET:HA	1:B:294:LEU:HD23	1.95	0.48
1:E:256:ILE:HA	1:E:259:LEU:HD23	1.95	0.48
1:D:151:LEU:HB2	1:D:212:PHE:HB2	1.96	0.47
1:B:151:LEU:HB2	1:B:212:PHE:HB2	1.96	0.47
1:A:100:ILE:HD12	1:A:102:GLU:H	1.78	0.47
1:C:117:VAL:HA	1:C:123:VAL:HG12	1.96	0.47
1:C:229:LEU:HD23	1:C:230:PRO:HD3	1.97	0.47
1:D:47:ALA:O	1:D:60:THR:OG1	2.30	0.47
1:B:222:PHE:HD1	1:C:275:ALA:HB3	1.80	0.47
1:D:288:VAL:HA	1:D:291:MET:HG3	1.96	0.47
1:B:407:SER:O	1:B:411:HIS:ND1	2.36	0.46
1:E:84:THR:HG23	1:E:119:HIS:HD2	1.80	0.46
1:D:285:VAL:HA	1:D:288:VAL:HG12	1.95	0.46
1:D:42:ASP:HB3	1:D:65:ARG:HB2	1.97	0.46
1:B:410:ARG:HE	1:B:411:HIS:CE1	2.34	0.46
1:D:116:TYR:OH	1:E:157:LEU:O	2.34	0.46
1:D:20:LEU:HD21	1:D:88:ILE:HD11	1.98	0.46
1:A:295:VAL:HA	1:A:298:LEU:HD23	1.97	0.46
1:D:291:MET:HA	1:D:294:LEU:HD23	1.97	0.46
1:D:398:ALA:HA	1:D:402:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:LEU:HB2	1:E:103:PHE:HE2	1.81	0.46
1:E:179:SER:OG	1:E:180:ILE:N	2.48	0.46
1:A:284:GLY:HA2	1:A:287:PHE:HD2	1.81	0.45
1:E:224:ALA:HA	1:E:228:LEU:HD23	1.98	0.45
1:A:222:PHE:HB3	1:B:276:THR:HG22	1.98	0.45
1:E:188:GLU:OE2	1:E:219:ARG:NE	2.49	0.45
1:A:13:LEU:HB3	1:B:27:VAL:HG11	1.98	0.45
1:A:197:LYS:HE2	1:A:199:PHE:HB2	1.98	0.45
1:B:288:VAL:HA	1:B:291:MET:HG3	1.99	0.45
1:B:116:TYR:HB2	1:B:124:GLN:HB2	1.97	0.44
1:C:184:GLN:HG2	1:D:278:ILE:HD13	2.00	0.44
1:C:267:ILE:HA	1:C:267:ILE:HD12	1.88	0.44
1:B:262:TYR:HE2	1:B:291:MET:HB3	1.82	0.44
1:A:40:SER:HB2	1:A:67:TYR:HB2	1.98	0.44
1:B:404:GLN:NE2	1:B:405:GLU:OE2	2.51	0.44
1:E:291:MET:HA	1:E:294:LEU:HD23	1.99	0.43
1:A:276:THR:HA	1:E:222:PHE:HB2	2.00	0.43
1:C:295:VAL:HA	1:C:298:LEU:HD23	2.01	0.43
1:D:184:GLN:H	1:D:219:ARG:HH22	1.67	0.43
1:D:423:ALA:HA	1:D:426:TRP:HD1	1.84	0.43
1:C:255:LYS:HA	1:C:258:LEU:HD23	2.00	0.43
1:D:32:ASP:HB3	1:D:35:LYS:HD3	2.00	0.43
1:A:84:THR:HG23	1:A:119:HIS:HD2	1.82	0.43
1:D:443:LEU:HD23	1:D:446:LEU:HD21	2.00	0.43
1:A:291:MET:HA	1:A:294:LEU:HD23	2.01	0.43
1:B:98:ILE:HG21	1:B:165:ILE:HD11	2.00	0.43
1:C:13:LEU:HD11	1:D:24:LYS:HD3	2.01	0.43
1:B:243:CYS:O	1:C:306:ARG:NH1	2.49	0.42
1:B:39:VAL:HG12	1:B:68:TRP:HB3	2.01	0.42
1:C:222:PHE:O	1:C:226:SER:OG	2.34	0.42
1:B:450:ILE:HA	1:B:453:VAL:HG22	2.02	0.42
1:E:233:PHE:HA	1:E:236:VAL:HG22	2.00	0.42
1:A:285:VAL:HA	1:A:288:VAL:HG12	2.00	0.42
1:C:126:TYR:O	1:D:156:TRP:NE1	2.36	0.42
1:C:246:PRO:HB3	1:C:251:ARG:HD3	2.02	0.42
1:C:423:ALA:HA	1:C:426:TRP:HD1	1.85	0.42
1:E:44:ILE:HB	1:E:63:TRP:HB2	2.02	0.42
1:B:117:VAL:HA	1:B:123:VAL:HG12	2.02	0.41
1:A:237:VAL:HA	1:A:240:VAL:HG22	2.02	0.41
1:C:406:LEU:HA	1:C:409:ILE:HD12	2.02	0.41
1:A:14:ARG:HH22	1:A:80:PHE:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LYS:HE2	1:B:199:PHE:HB2	2.02	0.41
1:D:13:LEU:HD12	1:E:27:VAL:HG11	2.01	0.41
1:B:20:LEU:HD21	1:B:88:ILE:HD11	2.02	0.41
1:E:285:VAL:HA	1:E:288:VAL:HG12	2.03	0.41
1:B:223:TYR:O	1:B:227:LEU:HB2	2.21	0.41
1:B:23:TYR:HE2	1:B:93:ILE:HA	1.84	0.41
1:B:268:ILE:HG21	1:C:267:ILE:HG12	2.03	0.41
1:D:450:ILE:HA	1:D:453:VAL:HG22	2.02	0.41
1:E:64:TYR:HE2	1:E:66:GLN:HE21	1.69	0.41
1:C:53:GLU:O	1:C:56:GLN:NE2	2.54	0.41
1:E:56:GLN:HE21	1:E:136:SER:HA	1.85	0.41
1:A:239:ILE:HA	1:A:239:ILE:HD13	1.97	0.41
1:D:421:GLU:OE2	1:E:415:LYS:NZ	2.45	0.41
1:C:255:LYS:HA	1:C:255:LYS:HD3	1.91	0.40
1:E:255:LYS:HD3	1:E:255:LYS:HA	1.91	0.40
1:C:256:ILE:HA	1:C:259:LEU:HG	2.04	0.40
1:D:186:GLU:OE2	1:D:218:ARG:NH1	2.54	0.40
1:D:49:LEU:HD21	1:E:104:VAL:HB	2.04	0.40
1:A:135:CYS:SG	1:A:136:SER:N	2.94	0.40
1:B:265:PHE:HA	1:B:268:ILE:HG22	2.03	0.40
1:C:318:PRO:HA	1:C:321:LEU:HG	2.04	0.40
1:D:135:CYS:SG	1:D:136:SER:N	2.94	0.40
1:D:138:ASP:O	1:D:147:GLN:NE2	2.44	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 PDB entries followed by that with respect to all EM entries.

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	395/457 (86%)	367 (93%)	28 (7%)	0	100	100
1	B	395/457 (86%)	366 (93%)	29 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	395/457 (86%)	366 (93%)	29 (7%)	0	100	100
1	D	395/457 (86%)	363 (92%)	32 (8%)	0	100	100
1	E	395/457 (86%)	373 (94%)	22 (6%)	0	100	100
All	All	1975/2285 (86%)	1835 (93%)	140 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	364/419 (87%)	357 (98%)	7 (2%)	62	83
1	B	361/419 (86%)	348 (96%)	13 (4%)	40	70
1	C	363/419 (87%)	356 (98%)	7 (2%)	62	83
1	D	361/419 (86%)	350 (97%)	11 (3%)	46	73
1	E	362/419 (86%)	355 (98%)	7 (2%)	62	83
All	All	1811/2095 (86%)	1766 (98%)	45 (2%)	56	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	LEU
1	A	267	ILE
1	A	294	LEU
1	A	298	LEU
1	A	302	ILE
1	A	410	ARG
1	A	424	ARG
1	B	19	LEU
1	B	25	LYS
1	B	28	ARG
1	B	101	ASN
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	228	LEU
1	B	234	LEU
1	B	235	MET
1	B	258	LEU
1	B	315	ARG
1	B	410	ARG
1	B	424	ARG
1	B	427	LEU
1	C	258	LEU
1	C	294	LEU
1	C	298	LEU
1	C	315	ARG
1	C	410	ARG
1	C	424	ARG
1	C	427	LEU
1	D	229	LEU
1	D	255	LYS
1	D	258	LEU
1	D	294	LEU
1	D	298	LEU
1	D	302	ILE
1	D	322	ARG
1	D	410	ARG
1	D	424	ARG
1	D	427	LEU
1	D	437	LEU
1	E	19	LEU
1	E	258	LEU
1	E	259	LEU
1	E	294	LEU
1	E	322	ARG
1	E	410	ARG
1	E	424	ARG

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

Mol	Chain	Res	Type
1	A	119	HIS
1	B	101	ASN
1	B	164	ASN
1	D	119	HIS
1	D	124	GLN

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Mol	Chain	Res	Type
1	E	9	GLN
1	E	56	GLN
1	E	119	HIS

### 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 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 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	$\# Z  > 2$
2	NAG	A	501	1,2	13,13,15	0.56	0	13,17,21	1.08	1 (7%)
2	NAG	A	502	2	15,15,15	0.38	0	21,21,21	0.22	0
2	NAG	A	503	1,2	13,13,15	0.41	0	13,17,21	0.45	0
2	NAG	A	504	3,2	15,15,15	0.20	0	21,21,21	0.27	0
3	BMA	A	505	2	11,11,12	0.80	0	13,15,17	0.85	0
2	NAG	A	506	1,2	13,13,15	0.39	0	13,17,21	0.46	0
2	NAG	A	507	2	15,15,15	0.25	0	21,21,21	0.17	0
5	PX4	A	509	-	17,17,45	1.99	5 (29%)	20,21,53	1.15	1 (5%)
5	PX4	A	510	-	16,16,45	1.71	4 (25%)	19,20,53	1.25	2 (10%)
2	NAG	B	500	3,2	13,13,15	0.51	0	13,17,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	501	2	14,14,15	0.73	0	15,19,21	1.67	5 (33%)
3	BMA	B	502	2	12,12,12	0.96	1 (8%)	17,17,17	1.03	1 (5%)
2	NAG	B	503	1,2	14,14,15	0.67	0	15,19,21	1.28	3 (20%)
2	NAG	B	504	2	14,14,15	0.36	0	15,19,21	0.59	0
2	NAG	B	505	1,2	14,14,15	0.22	0	15,19,21	0.62	0
2	NAG	B	506	2	14,14,15	0.46	0	15,19,21	0.61	0
2	NAG	C	501	1,2	14,14,15	0.58	0	15,19,21	0.80	1 (6%)
2	NAG	C	502	3,2	13,13,15	0.43	0	13,17,21	0.52	0
3	BMA	C	503	2	12,12,12	0.65	0	17,17,17	0.70	0
2	NAG	C	504	1,2	14,14,15	0.32	0	15,19,21	0.57	0
2	NAG	C	505	2	14,14,15	0.32	0	15,19,21	0.56	0
2	NAG	C	506	1,2	14,14,15	0.33	0	15,19,21	0.56	0
2	NAG	C	507	2	14,14,15	0.34	0	16,19,21	0.22	0
5	PX4	C	509	-	17,17,45	1.67	4 (23%)	20,21,53	1.24	2 (10%)
2	NAG	D	501	1,2	14,14,15	0.41	0	15,19,21	0.63	0
2	NAG	D	502	3,2	13,13,15	0.69	1 (7%)	15,17,21	0.63	0
3	BMA	D	503	2	12,12,12	0.61	0	17,17,17	0.78	0
2	NAG	D	504	1	14,14,15	0.38	0	15,19,21	0.55	0
2	NAG	D	505	1,2	14,14,15	0.31	0	15,19,21	0.57	0
2	NAG	D	506	2	14,14,15	0.53	0	15,19,21	0.53	0
5	PX4	D	507	-	16,16,45	1.71	4 (25%)	19,20,53	1.24	2 (10%)
2	NAG	E	501	1,2	13,13,15	0.44	0	13,17,21	0.45	0
2	NAG	E	502	3,2	15,15,15	0.24	0	21,21,21	0.18	0
3	BMA	E	503	2	11,11,12	0.86	0	15,15,17	0.99	0
2	NAG	E	504	1,2	13,13,15	0.47	0	13,17,21	0.46	0
2	NAG	E	505	2	15,15,15	0.25	0	21,21,21	0.18	0
2	NAG	E	506	1,2	13,13,15	1.33	1 (7%)	13,17,21	1.78	3 (23%)
2	NAG	E	507	2	15,15,15	0.35	0	21,21,21	0.23	0
5	PX4	E	508	-	16,16,45	2.05	5 (31%)	19,20,53	1.17	1 (5%)

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	NAG	A	501	1,2	-	0/6/19/26	0/1/1/1
2	NAG	A	502	2	-	0/6/26/26	0/1/1/1
2	NAG	A	503	1,2	1/1/4/7	0/6/19/26	0/1/1/1
2	NAG	A	504	3,2	-	0/6/26/26	0/1/1/1
3	BMA	A	505	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	506	1,2	1/1/4/7	0/6/19/26	0/1/1/1
2	NAG	A	507	2	-	0/6/26/26	0/1/1/1
5	PX4	A	509	-	-	0/17/17/49	0/0/0/0
5	PX4	A	510	-	-	0/16/16/49	0/0/0/0
2	NAG	B	500	3,2	-	0/6/19/26	1/1/1/1
2	NAG	B	501	2	-	0/6/23/26	0/1/1/1
3	BMA	B	502	2	-	0/2/22/22	0/1/1/1
2	NAG	B	503	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	504	2	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	506	2	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	502	3,2	1/1/4/7	0/6/19/26	0/1/1/1
3	BMA	C	503	2	-	0/2/22/22	0/1/1/1
2	NAG	C	504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	505	2	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	507	2	1/1/5/7	0/6/22/26	0/1/1/1
5	PX4	C	509	-	-	0/17/17/49	0/0/0/0
2	NAG	D	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	502	3,2	-	0/6/19/26	0/1/1/1
3	BMA	D	503	2	-	0/2/22/22	0/1/1/1
2	NAG	D	504	1	-	0/6/23/26	0/1/1/1
2	NAG	D	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	506	2	-	0/6/23/26	0/1/1/1
5	PX4	D	507	-	-	0/16/16/49	0/0/0/0
2	NAG	E	501	1,2	-	0/6/19/26	0/1/1/1
2	NAG	E	502	3,2	-	0/6/26/26	0/1/1/1
3	BMA	E	503	2	1/1/4/5	0/2/18/22	0/1/1/1
2	NAG	E	504	1,2	1/1/4/7	0/6/19/26	0/1/1/1
2	NAG	E	505	2	-	0/6/26/26	0/1/1/1
2	NAG	E	506	1,2	1/1/4/7	0/6/19/26	0/1/1/1
2	NAG	E	507	2	-	0/6/26/26	0/1/1/1
5	PX4	E	508	-	-	0/16/16/49	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	508	PX4	P1-O1	-2.19	1.45	1.54
5	A	509	PX4	P1-O1	-2.19	1.45	1.54
2	D	502	NAG	C1-C2	2.00	1.53	1.51
3	B	502	BMA	C4-C3	2.13	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	509	PX4	P1-O4	2.18	1.67	1.60
5	D	507	PX4	P1-O4	2.18	1.67	1.60
5	A	509	PX4	P1-O4	2.19	1.67	1.60
5	A	510	PX4	P1-O4	2.20	1.67	1.60
5	E	508	PX4	P1-O4	2.20	1.67	1.60
5	C	509	PX4	C10-C9	2.30	1.57	1.50
5	E	508	PX4	C10-C9	2.31	1.57	1.50
5	D	507	PX4	C10-C9	2.32	1.57	1.50
5	A	509	PX4	C10-C9	2.32	1.57	1.50
5	A	510	PX4	C10-C9	2.33	1.57	1.50
5	E	508	PX4	O5-C9	3.44	1.43	1.33
5	D	507	PX4	O5-C9	3.44	1.43	1.33
5	A	510	PX4	O5-C9	3.46	1.43	1.33
5	C	509	PX4	O5-C9	3.46	1.43	1.33
5	A	509	PX4	O5-C9	3.48	1.43	1.33
5	C	509	PX4	P1-O3	3.61	1.69	1.54
5	D	507	PX4	P1-O3	3.62	1.69	1.54
5	A	510	PX4	P1-O3	3.62	1.69	1.54
2	E	506	NAG	O5-C1	3.90	1.50	1.43
5	A	509	PX4	P1-O2	5.52	1.69	1.50
5	E	508	PX4	P1-O2	5.53	1.69	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	509	PX4	O1-P1-O2	-2.37	101.22	110.50
5	A	510	PX4	O1-P1-O2	-2.37	101.22	110.50
5	D	507	PX4	O1-P1-O2	-2.36	101.28	110.50
2	E	506	NAG	C4-C5-C6	-2.19	108.64	112.53
2	B	503	NAG	C3-C4-C5	2.05	113.83	110.22
2	C	501	NAG	C1-O5-C5	2.05	114.99	112.17
2	B	503	NAG	C4-C3-C2	2.18	114.21	111.02
2	B	501	NAG	C3-C4-C5	2.52	114.65	110.22
2	B	501	NAG	C1-C2-N2	2.58	114.90	110.49
2	B	501	NAG	C1-O5-C5	2.67	115.84	112.17
5	A	509	PX4	O5-C9-C10	2.70	119.76	111.90
5	D	507	PX4	O5-C9-C10	2.71	119.78	111.90
5	A	510	PX4	O5-C9-C10	2.72	119.80	111.90
5	C	509	PX4	O5-C9-C10	2.73	119.85	111.90
3	B	502	BMA	C4-C3-C2	2.76	115.70	110.84
5	E	508	PX4	O5-C9-C10	2.76	119.93	111.90
2	B	501	NAG	C4-C3-C2	2.87	115.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAG	C2-N2-C7	2.95	127.25	122.94
2	B	503	NAG	C2-N2-C7	2.98	127.29	122.94
2	E	506	NAG	C3-C4-C5	3.08	116.41	111.26
2	B	501	NAG	C2-N2-C7	3.33	127.81	122.94
2	E	506	NAG	C1-O5-C5	4.67	123.61	113.47

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	502	NAG	C4
2	E	506	NAG	C4
2	E	504	NAG	C4
2	A	503	NAG	C4
2	C	507	NAG	C3
2	A	506	NAG	C4
3	E	503	BMA	C4

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	NAG	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NAG	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.