Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 07:06 PM EDT

PDB ID	:	3EUQ
Title	:	X-ray structural of a type III pentaketide synthase from Neurospora crassa
Authors	:	Zhang, H.; Brunzelle, J.S.; Nair, S.K.
Deposited on	:	2008-10-10
Resolution	:	2.10 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:

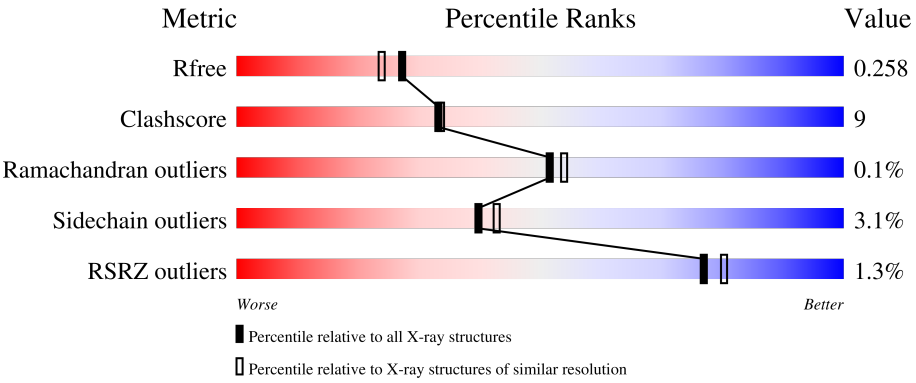
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	379	81% 18%
1	B	379	2% 85% 13%
1	C	379	% 87% 12%
1	D	379	2% 84% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSD	A	152	-	-	X	-
1	CSD	B	152	-	-	X	-
1	CSD	C	152	-	-	X	-
1	CSD	D	152	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12262 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.

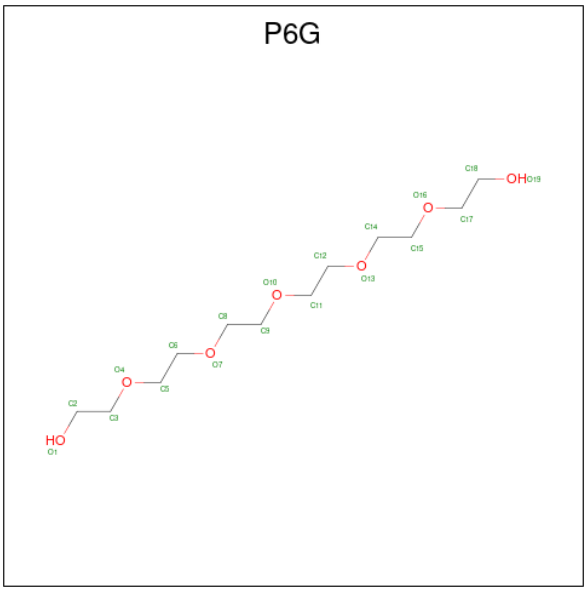
- Molecule 1 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2850	1791	498	543	18			
1	B	379	Total	C	N	O	S	0	0	0
			2850	1791	498	543	18			
1	C	379	Total	C	N	O	S	0	0	0
			2850	1791	498	543	18			
1	D	379	Total	C	N	O	S	0	0	0
			2850	1791	498	543	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	GLY	PHE	engineered mutation	UNP Q7S6N4
B	252	GLY	PHE	engineered mutation	UNP Q7S6N4
C	252	GLY	PHE	engineered mutation	UNP Q7S6N4
D	252	GLY	PHE	engineered mutation	UNP Q7S6N4

- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 19 12 7	0	0
2	C	1	Total C O 19 12 7	0	0

- Molecule 3 is water.

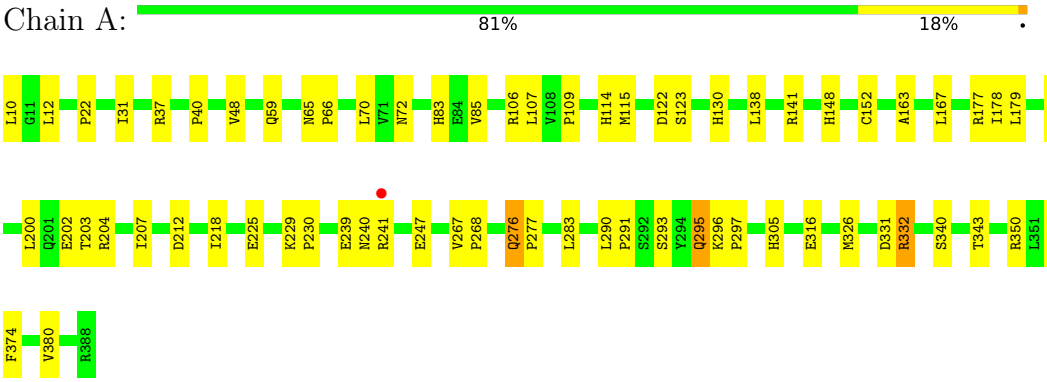
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	219	Total O 219 219	0	0
3	B	203	Total O 203 203	0	0
3	C	190	Total O 190 190	0	0
3	D	212	Total O 212 212	0	0

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.

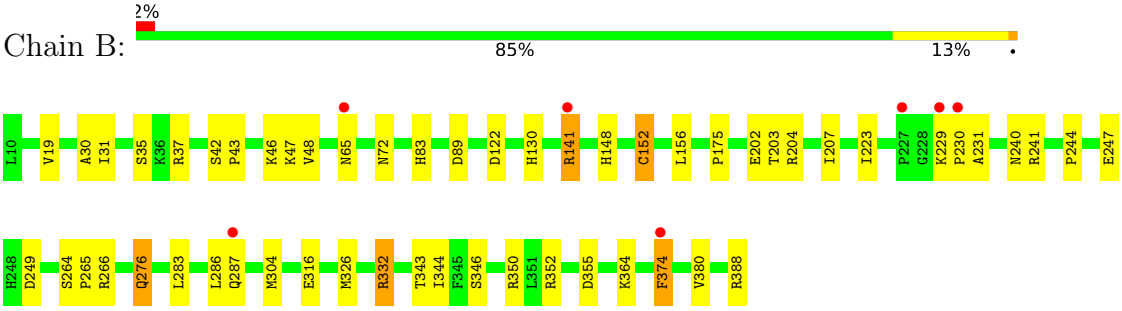
• Molecule 1: Putative uncharacterized protein

Chain A:



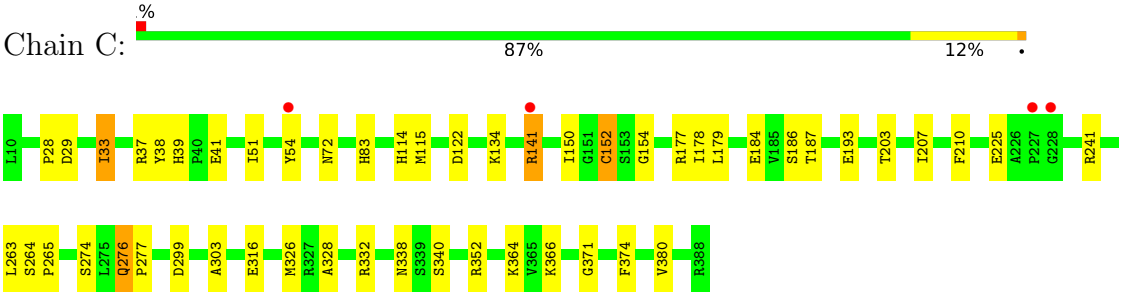
• Molecule 1: Putative uncharacterized protein

Chain B:



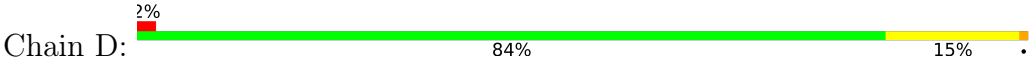
• Molecule 1: Putative uncharacterized protein

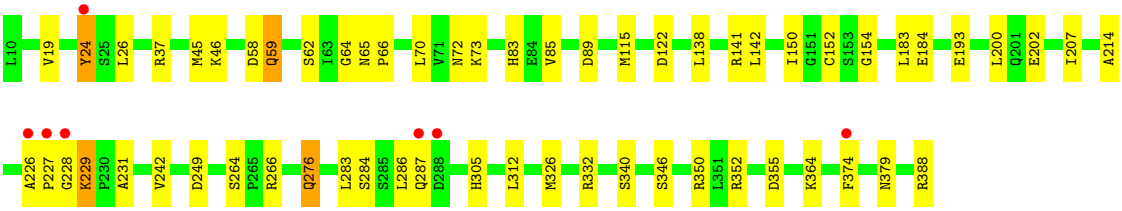
Chain C:



• Molecule 1: Putative uncharacterized protein

Chain D:




L10
V19
Y24
S25
L26
R37
M45
K46
D58
Q59
S62
I63
G64
N65
P66
L70
V71
N72
K73
H83
E84
V85
D89
M115
D122
L138
R141
L142
I150
G151
C152
S153
G154
L183
E184
E193
L200
Q201
E202
I207
A214
A226
P227
G228
K229
P230
A231
V242
D249
S264
P265
R266
Q276
L283
S284
S285
L286
Q287
D288
H305
L312
M326
R332
S340
S346
R350
L351
R352
D355
K364
F374
M379
R388

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.69Å 105.12Å 105.08Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 41.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.00-2.10) 94.4 (41.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.256 0.200 , 0.258	Depositor DCC
R_{free} test set	4264 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.035 for -h,-l,-k 0.035 for -h,l,k 0.358 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12262	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: CSD, P6G

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	0.47	0/2902	0.61	0/3944
1	B	0.48	0/2902	0.63	0/3944
1	C	0.49	0/2902	0.61	0/3944
1	D	0.48	0/2902	0.63	0/3944
All	All	0.48	0/11608	0.62	0/15776

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	2850	0	2864	69	0
1	B	2850	0	2864	54	0
1	C	2850	0	2864	45	0
1	D	2850	0	2864	44	0
2	A	19	0	26	2	0
2	C	19	0	26	2	0
3	A	219	0	0	10	0
3	B	203	0	0	7	0
3	C	190	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	212	0	0	5	0
All	All	12262	0	11508	197	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 9.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:CSD:OD2	1:C:152:CSD:SG	1.95	1.25
1:B:152:CSD:SG	1:B:152:CSD:OD2	1.95	1.25
1:D:152:CSD:SG	1:D:152:CSD:OD2	1.95	1.24
1:A:152:CSD:SG	1:A:152:CSD:OD2	1.95	1.22
1:B:152:CSD:SG	1:B:152:CSD:OD1	1.98	1.22
1:D:152:CSD:SG	1:D:152:CSD:OD1	1.99	1.21
1:C:152:CSD:SG	1:C:152:CSD:OD1	1.99	1.20
1:A:152:CSD:SG	1:A:152:CSD:OD1	1.99	1.19
1:A:167:LEU:HG	3:A:991:HOH:O	1.45	1.15
1:D:58:ASP:HB2	3:D:712:HOH:O	1.54	1.07
1:B:276:GLN:HE21	1:B:276:GLN:H	1.14	0.91
1:C:276:GLN:HE21	1:C:276:GLN:H	1.13	0.91
1:C:177:ARG:NH2	1:C:225:GLU:HG2	1.87	0.89
1:D:115:MET:HE3	1:D:142:LEU:HD21	1.54	0.88
1:C:29:ASP:O	1:C:33:ILE:HD13	1.72	0.88
1:C:28:PRO:HA	3:C:782:HOH:O	1.74	0.88
1:D:364:LYS:HA	1:D:364:LYS:CE	2.06	0.86
1:A:276:GLN:H	1:A:276:GLN:HE21	1.27	0.81
1:B:152:CSD:OD2	1:B:152:CSD:N	2.16	0.78
1:B:65:ASN:HB3	3:B:703:HOH:O	1.85	0.75
1:D:364:LYS:HA	1:D:364:LYS:HE2	1.67	0.74
1:A:115:MET:HE3	1:A:138:LEU:HD12	1.68	0.74
1:C:134:LYS:HD3	3:C:691:HOH:O	1.88	0.74
1:D:276:GLN:HE21	1:D:276:GLN:H	1.36	0.74
1:A:141:ARG:HH21	1:B:240:ASN:H	1.33	0.73
1:C:141:ARG:HH11	1:C:141:ARG:HB3	1.54	0.73
1:A:374:PHE:CD1	1:A:380:VAL:HG22	2.23	0.73
1:A:152:CSD:OD2	1:A:152:CSD:CB	2.37	0.73
1:B:316:GLU:HG3	1:B:326:MET:CE	2.19	0.73
1:A:240:ASN:H	1:B:141:ARG:NH2	1.87	0.73
1:B:83:HIS:HD2	1:B:122:ASP:OD1	1.71	0.73
1:C:152:CSD:OD2	1:C:152:CSD:CB	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:987:HOH:O	1:D:65:ASN:HB3	1.89	0.70
1:B:304:MET:SD	1:B:374:PHE:HZ	2.16	0.69
1:C:115:MET:CE	1:C:179:LEU:HD23	2.24	0.68
1:A:163:ALA:O	3:A:991:HOH:O	2.11	0.68
1:D:287:GLN:HA	3:D:668:HOH:O	1.93	0.67
1:D:364:LYS:HA	1:D:364:LYS:HE3	1.77	0.66
1:D:37:ARG:HH11	1:D:72:ASN:HD21	1.43	0.65
1:C:364:LYS:HE2	3:C:729:HOH:O	1.96	0.65
1:B:276:GLN:H	1:B:276:GLN:NE2	1.90	0.65
1:C:115:MET:HE3	1:C:179:LEU:HD23	1.79	0.64
1:C:83:HIS:HD2	1:C:122:ASP:OD1	1.81	0.63
1:B:207:ILE:HG12	3:B:604:HOH:O	1.98	0.63
1:D:115:MET:CE	1:D:142:LEU:HD21	2.28	0.62
1:B:264:SER:HB2	1:B:265:PRO:HD2	1.82	0.61
1:D:115:MET:CE	1:D:138:LEU:HD12	2.30	0.61
1:A:12:LEU:HD21	3:A:991:HOH:O	2.01	0.61
1:A:83:HIS:HD2	1:A:122:ASP:OD1	1.84	0.61
1:A:152:CSD:OD2	1:A:152:CSD:HB3	2.00	0.61
1:A:37:ARG:HH11	1:A:72:ASN:HD21	1.49	0.61
1:D:152:CSD:OD2	1:D:152:CSD:CB	2.48	0.60
1:C:187:THR:HA	2:C:600:P6G:H111	1.83	0.60
1:B:316:GLU:HG3	1:B:326:MET:HE3	1.83	0.60
1:D:115:MET:HE3	1:D:142:LEU:CD2	2.28	0.60
1:C:152:CSD:OD2	1:C:152:CSD:HB3	2.00	0.60
1:A:229:LYS:HD2	1:A:230:PRO:HD2	1.83	0.59
1:B:152:CSD:OD2	1:B:152:CSD:CB	2.50	0.59
1:B:380:VAL:HG13	3:B:677:HOH:O	2.02	0.59
1:D:115:MET:HE1	1:D:138:LEU:HD12	1.84	0.57
1:A:374:PHE:HD1	1:A:380:VAL:HG22	1.70	0.57
1:C:241:ARG:HG3	3:C:696:HOH:O	2.03	0.57
1:B:276:GLN:HE21	1:B:276:GLN:N	1.94	0.57
1:B:316:GLU:HG3	1:B:326:MET:HE1	1.86	0.57
1:D:226:ALA:H	1:D:229:LYS:HE3	1.69	0.57
1:C:316:GLU:HG3	1:C:326:MET:CE	2.35	0.56
1:D:305:HIS:HB3	3:D:578:HOH:O	2.06	0.56
1:D:350:ARG:NH1	1:D:355:ASP:OD1	2.39	0.56
1:B:240:ASN:HB2	3:B:548:HOH:O	2.06	0.56
1:D:65:ASN:HB2	1:D:66:PRO:HD2	1.87	0.56
1:D:65:ASN:HB3	3:D:528:HOH:O	2.06	0.55
1:C:37:ARG:HH11	1:C:72:ASN:HD21	1.54	0.55
1:C:374:PHE:HD1	1:C:380:VAL:HG22	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HH11	1:A:332:ARG:HA	1.72	0.55
1:A:276:GLN:HB2	1:A:277:PRO:HD3	1.88	0.55
1:B:37:ARG:HH11	1:B:72:ASN:HD21	1.55	0.54
1:A:283:LEU:HD21	1:A:295:GLN:O	2.08	0.54
1:C:177:ARG:HH21	1:C:225:GLU:HG2	1.72	0.54
1:A:48:VAL:HG11	1:A:207:ILE:HD11	1.90	0.54
1:A:10:LEU:N	3:A:978:HOH:O	2.40	0.53
1:A:186:SER:HB2	2:A:500:P6G:H52	1.89	0.53
1:A:109:PRO:HB3	1:A:138:LEU:HD23	1.89	0.53
1:A:240:ASN:H	1:B:141:ARG:HH21	1.54	0.53
1:B:229:LYS:HD2	1:B:230:PRO:HD2	1.89	0.53
1:C:141:ARG:HB3	1:C:141:ARG:NH1	2.22	0.53
1:B:19:VAL:HG21	1:B:346:SER:HA	1.89	0.53
1:D:24:TYR:CE1	1:D:64:GLY:HA2	2.44	0.53
1:B:141:ARG:HH11	1:B:141:ARG:HB3	1.73	0.52
1:A:247:GLU:OE2	1:B:130:HIS:HE1	1.91	0.52
1:C:374:PHE:CD1	1:C:380:VAL:HG22	2.44	0.52
1:D:184:GLU:HG3	1:D:340:SER:HB3	1.92	0.52
1:A:241:ARG:HH21	1:B:141:ARG:HD2	1.75	0.52
1:B:244:PRO:HD2	1:C:54:TYR:CZ	2.46	0.52
1:A:202:GLU:OE2	1:A:204:ARG:HD2	2.11	0.51
1:B:374:PHE:CD2	1:B:374:PHE:N	2.78	0.51
1:B:231:ALA:O	1:B:388:ARG:HG3	2.11	0.51
1:B:350:ARG:NH1	1:B:355:ASP:OD1	2.44	0.51
1:B:43:PRO:O	1:B:47:LYS:HG2	2.11	0.51
1:B:276:GLN:OE1	3:B:705:HOH:O	2.19	0.51
1:C:186:SER:HB2	2:C:600:P6G:H52	1.92	0.51
1:A:12:LEU:HD11	3:A:991:HOH:O	2.10	0.51
1:D:83:HIS:HD2	1:D:122:ASP:OD1	1.94	0.51
1:A:239:GLU:HA	1:B:141:ARG:HH21	1.76	0.50
1:D:242:VAL:HG22	1:D:379:ASN:OD1	2.12	0.50
1:A:115:MET:CE	1:A:138:LEU:HD12	2.41	0.50
1:A:203:THR:HG23	3:A:771:HOH:O	2.11	0.50
1:B:31:ILE:O	1:B:35:SER:HB2	2.11	0.50
1:C:276:GLN:H	1:C:276:GLN:NE2	1.94	0.50
1:A:202:GLU:OE2	1:A:204:ARG:NH1	2.42	0.49
1:A:107:LEU:HD11	1:A:218:ILE:HG21	1.92	0.49
1:C:83:HIS:HE1	3:C:657:HOH:O	1.94	0.49
1:C:203:THR:HG21	3:C:662:HOH:O	2.10	0.49
1:C:115:MET:HE2	1:C:179:LEU:CD2	2.43	0.49
1:C:274:SER:O	1:C:277:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:HIS:HB2	1:B:148:HIS:HB2	1.94	0.49
1:B:42:SER:O	1:B:46:LYS:HG3	2.12	0.49
1:C:264:SER:HB2	1:C:265:PRO:HD2	1.95	0.49
1:A:200:LEU:HB2	1:A:202:GLU:HG2	1.95	0.48
1:A:141:ARG:HD2	1:B:241:ARG:HE	1.78	0.48
1:B:249:ASP:OD1	1:B:266:ARG:HD3	2.13	0.48
1:C:39:HIS:HE1	3:C:607:HOH:O	1.95	0.48
1:C:115:MET:CE	1:C:179:LEU:CD2	2.92	0.48
1:C:150:ILE:HD12	1:C:154:GLY:HA2	1.96	0.48
1:A:123:SER:OG	1:B:148:HIS:HE1	1.97	0.47
1:D:312:LEU:O	1:D:326:MET:HE1	2.14	0.47
1:C:115:MET:HE2	1:C:179:LEU:HD23	1.94	0.47
1:B:229:LYS:HG3	1:B:230:PRO:O	2.14	0.47
1:A:10:LEU:HA	3:A:978:HOH:O	2.15	0.47
1:A:332:ARG:N	1:A:332:ARG:HD2	2.30	0.47
1:A:10:LEU:CA	3:A:978:HOH:O	2.63	0.47
1:A:331:ASP:OD2	1:A:332:ARG:NH1	2.48	0.46
1:A:187:THR:HA	2:A:500:P6G:H111	1.97	0.46
1:A:267:VAL:HB	1:A:268:PRO:HD3	1.97	0.46
1:D:45:MET:HB3	3:D:593:HOH:O	2.16	0.46
1:A:70:LEU:HD22	1:A:85:VAL:HG21	1.98	0.46
1:C:276:GLN:HB2	1:C:277:PRO:HD3	1.97	0.45
1:B:83:HIS:HE1	3:B:558:HOH:O	1.98	0.45
1:D:152:CSD:OD2	1:D:152:CSD:HB3	2.16	0.45
1:A:141:ARG:NH2	1:B:240:ASN:H	2.09	0.45
1:D:193:GLU:CB	1:D:207:ILE:HG23	2.46	0.45
1:A:31:ILE:HD12	1:A:207:ILE:HD12	1.99	0.45
1:A:152:CSD:HB3	1:A:152:CSD:HD2	1.82	0.45
1:A:10:LEU:N	3:A:970:HOH:O	2.49	0.44
1:D:70:LEU:HD22	1:D:85:VAL:HG21	1.99	0.44
1:A:130:HIS:CE1	1:B:247:GLU:CG	3.00	0.44
1:A:114:HIS:HB2	1:A:178:ILE:HG23	1.99	0.44
1:A:296:LYS:HB2	1:A:297:PRO:HD2	1.99	0.44
1:A:22:PRO:HG3	1:A:212:ASP:HB2	2.00	0.44
1:A:332:ARG:HA	1:A:332:ARG:NH1	2.32	0.44
1:D:150:ILE:HD12	1:D:154:GLY:HA2	1.99	0.44
1:D:19:VAL:HG21	1:D:346:SER:HA	2.00	0.44
1:D:24:TYR:CD2	1:D:24:TYR:N	2.85	0.44
1:D:183:LEU:HD13	1:D:214:ALA:HB2	2.00	0.44
1:A:115:MET:CE	1:A:179:LEU:HD23	2.48	0.44
1:D:59:GLN:HE21	1:D:59:GLN:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HG3	1:B:204:ARG:HG3	1.99	0.43
1:C:210:PHE:HA	1:C:338:ASN:O	2.17	0.43
1:A:184:GLU:HG3	1:A:340:SER:HB3	1.99	0.43
1:C:328:ALA:HB3	3:C:644:HOH:O	2.17	0.43
1:B:202:GLU:HG3	1:B:204:ARG:CG	2.49	0.43
1:B:332:ARG:HA	1:B:332:ARG:HD2	1.72	0.43
1:A:152:CSD:OD1	1:A:305:HIS:HE1	2.02	0.42
1:C:184:GLU:HG3	1:C:340:SER:HB3	1.99	0.42
1:C:299:ASP:O	1:C:366:LYS:HD2	2.19	0.42
1:A:316:GLU:HG3	1:A:326:MET:CE	2.49	0.42
1:A:40:PRO:HG2	1:D:24:TYR:OH	2.18	0.42
1:B:156:LEU:HD21	1:B:344:ILE:HG12	2.01	0.42
1:B:30:ALA:HB3	3:B:586:HOH:O	2.19	0.42
1:D:115:MET:CE	1:D:138:LEU:CD1	2.97	0.42
1:D:249:ASP:HA	1:D:264:SER:HB3	2.02	0.42
1:B:48:VAL:HG11	1:B:207:ILE:HD11	2.01	0.42
1:B:283:LEU:O	1:B:287:GLN:N	2.51	0.42
1:C:316:GLU:HG3	1:C:326:MET:HE1	2.01	0.42
1:D:200:LEU:HB2	1:D:202:GLU:HG2	2.01	0.42
1:B:175:PRO:HB3	1:B:223:ILE:O	2.20	0.42
1:C:51:ILE:HA	1:C:54:TYR:CD2	2.54	0.42
1:A:239:GLU:HA	1:B:141:ARG:NH2	2.35	0.42
1:A:115:MET:CE	1:A:138:LEU:CD1	2.98	0.41
1:A:177:ARG:NH2	1:A:225:GLU:HG2	2.36	0.41
1:A:290:LEU:HA	1:A:291:PRO:HD3	1.95	0.41
1:C:303:ALA:O	1:C:371:GLY:HA2	2.19	0.41
1:A:350:ARG:NH1	1:A:355:ASP:OD1	2.53	0.41
1:D:231:ALA:O	1:D:388:ARG:HG3	2.20	0.41
1:C:193:GLU:CB	1:C:207:ILE:HG23	2.51	0.41
1:D:24:TYR:CD1	1:D:64:GLY:HA2	2.56	0.41
1:A:65:ASN:HB2	1:A:66:PRO:CD	2.51	0.41
1:A:115:MET:HE3	1:A:138:LEU:CD1	2.47	0.41
1:A:130:HIS:CE1	1:B:247:GLU:HG3	2.56	0.41
1:A:305:HIS:HD2	1:A:343:THR:HB	1.85	0.41
1:A:316:GLU:HG3	1:A:326:MET:HE1	2.02	0.41
1:B:304:MET:SD	1:B:374:PHE:CZ	3.06	0.41
1:D:26:LEU:HG	1:D:62:SER:HB2	2.03	0.41
1:C:38:TYR:OH	1:C:72:ASN:HA	2.22	0.40
1:D:249:ASP:OD1	1:D:266:ARG:HD3	2.20	0.40
1:A:295:GLN:HE21	1:A:295:GLN:HB3	1.70	0.40
1:C:114:HIS:HB2	1:C:178:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LYS:CE	1:D:364:LYS:CA	2.83	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	376/379 (99%)	367 (98%)	9 (2%)	0	100	100
1	B	376/379 (99%)	367 (98%)	9 (2%)	0	100	100
1	C	376/379 (99%)	367 (98%)	9 (2%)	0	100	100
1	D	376/379 (99%)	364 (97%)	10 (3%)	2 (0%)	29	26
All	All	1504/1516 (99%)	1465 (97%)	37 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	227	PRO
1	D	228	GLY

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	308/308 (100%)	301 (98%)	7 (2%)	50	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	308/308 (100%)	298 (97%)	10 (3%)	39 41
1	C	308/308 (100%)	301 (98%)	7 (2%)	50 55
1	D	308/308 (100%)	294 (96%)	14 (4%)	27 27
All	All	1232/1232 (100%)	1194 (97%)	38 (3%)	40 43

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	106	ARG
1	A	276	GLN
1	A	293	SER
1	A	295	GLN
1	A	332	ARG
1	A	352	ARG
1	B	89	ASP
1	B	141	ARG
1	B	203	THR
1	B	276	GLN
1	B	286	LEU
1	B	332	ARG
1	B	343	THR
1	B	352	ARG
1	B	364	LYS
1	B	374	PHE
1	C	33	ILE
1	C	41	GLU
1	C	141	ARG
1	C	263	LEU
1	C	276	GLN
1	C	332	ARG
1	C	352	ARG
1	D	24	TYR
1	D	46	LYS
1	D	59	GLN
1	D	73	LYS
1	D	89	ASP
1	D	141	ARG
1	D	229	LYS
1	D	276	GLN
1	D	283	LEU

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Mol	Chain	Res	Type
1	D	284	SER
1	D	286	LEU
1	D	332	ARG
1	D	352	ARG
1	D	374	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	72	ASN
1	A	83	HIS
1	A	125	ASN
1	A	130	HIS
1	A	148	HIS
1	A	169	HIS
1	A	276	GLN
1	A	295	GLN
1	A	305	HIS
1	B	39	HIS
1	B	72	ASN
1	B	83	HIS
1	B	130	HIS
1	B	148	HIS
1	B	169	HIS
1	B	276	GLN
1	B	305	HIS
1	B	335	ASN
1	C	39	HIS
1	C	72	ASN
1	C	83	HIS
1	C	130	HIS
1	C	148	HIS
1	C	169	HIS
1	C	276	GLN
1	C	305	HIS
1	D	39	HIS
1	D	59	GLN
1	D	72	ASN
1	D	83	HIS
1	D	130	HIS
1	D	148	HIS

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Mol	Chain	Res	Type
1	D	169	HIS
1	D	276	GLN
1	D	305	HIS
1	D	335	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSD	A	152	1	3,7,8	0.49	0	1,8,10	1.04	0
1	CSD	B	152	1	3,7,8	0.72	0	1,8,10	3.64	1 (100%)
1	CSD	C	152	1	3,7,8	0.62	0	1,8,10	3.65	1 (100%)
1	CSD	D	152	1	3,7,8	0.63	0	1,8,10	0.74	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
1	CSD	A	152	1	-	1/2/6/8	-
1	CSD	B	152	1	-	1/2/6/8	-
1	CSD	C	152	1	-	1/2/6/8	-
1	CSD	D	152	1	-	1/2/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	152	CSD	OD1-SG-CB	-3.65	98.58	105.54
1	B	152	CSD	OD1-SG-CB	-3.64	98.61	105.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152	CSD	CA-CB-SG-OD1
1	B	152	CSD	CA-CB-SG-OD1
1	C	152	CSD	CA-CB-SG-OD1
1	D	152	CSD	CA-CB-SG-OD1

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	152	CSD	6	0
1	B	152	CSD	4	0
1	C	152	CSD	4	0
1	D	152	CSD	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	P6G	C	600	-	18,18,18	0.49	0	17,17,17	0.25	0
2	P6G	A	500	-	18,18,18	0.52	0	17,17,17	0.27	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	P6G	C	600	-	-	6/16/16/16	-
2	P6G	A	500	-	-	9/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	P6G	O7-C8-C9-O10
2	A	500	P6G	O10-C11-C12-O13
2	A	500	P6G	O16-C17-C18-O19
2	C	600	P6G	O16-C17-C18-O19
2	C	600	P6G	O1-C2-C3-O4
2	C	600	P6G	O7-C8-C9-O10
2	C	600	P6G	O4-C5-C6-O7
2	A	500	P6G	C15-C14-O13-C12
2	C	600	P6G	C8-C9-O10-C11
2	C	600	P6G	C15-C14-O13-C12
2	A	500	P6G	C9-C8-O7-C6
2	A	500	P6G	C5-C6-O7-C8
2	A	500	P6G	C6-C5-O4-C3
2	A	500	P6G	C14-C15-O16-C17
2	A	500	P6G	O4-C5-C6-O7

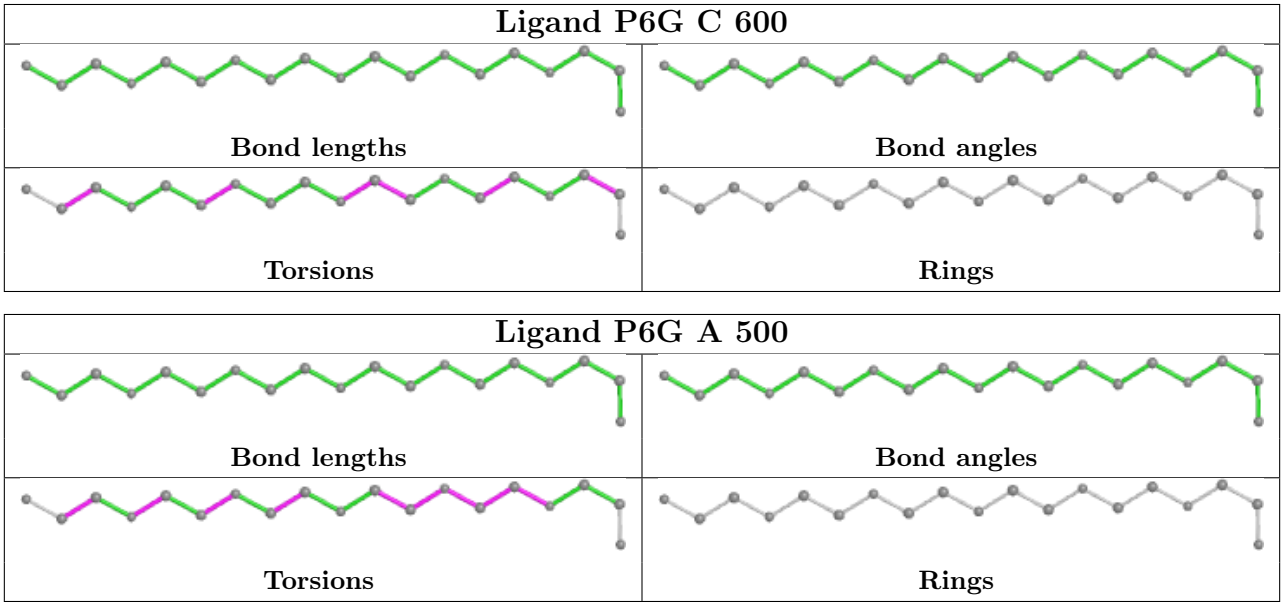
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	P6G	2	0
2	A	500	P6G	2	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.



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	378/379 (99%)	-0.14	1 (0%)	94	94	21, 27, 34, 40	0
1	B	378/379 (99%)	-0.02	7 (1%)	66	71	20, 27, 35, 49	0
1	C	378/379 (99%)	-0.00	4 (1%)	80	84	20, 27, 34, 42	0
1	D	378/379 (99%)	-0.05	7 (1%)	66	71	20, 27, 34, 46	0
All	All	1512/1516 (99%)	-0.05	19 (1%)	77	80	20, 27, 34, 49	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	GLN	6.3
1	B	227	PRO	6.3
1	C	228	GLY	5.5
1	D	227	PRO	5.0
1	D	226	ALA	5.0
1	B	230	PRO	4.9
1	D	228	GLY	4.5
1	D	24	TYR	3.9
1	D	374	PHE	3.8
1	C	54	TYR	3.7
1	B	374	PHE	3.1
1	D	287	GLN	3.0
1	A	241	ARG	2.8
1	D	288	ASP	2.6
1	C	227	PRO	2.4
1	B	65	ASN	2.2
1	B	229	LYS	2.2
1	B	141	ARG	2.2
1	C	141	ARG	2.1

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
1	CSD	D	152	8/9	0.92	0.12	27,29,32,34	0
1	CSD	B	152	8/9	0.93	0.12	26,27,37,37	0
1	CSD	A	152	8/9	0.95	0.11	28,30,33,35	0
1	CSD	C	152	8/9	0.96	0.12	28,29,32,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

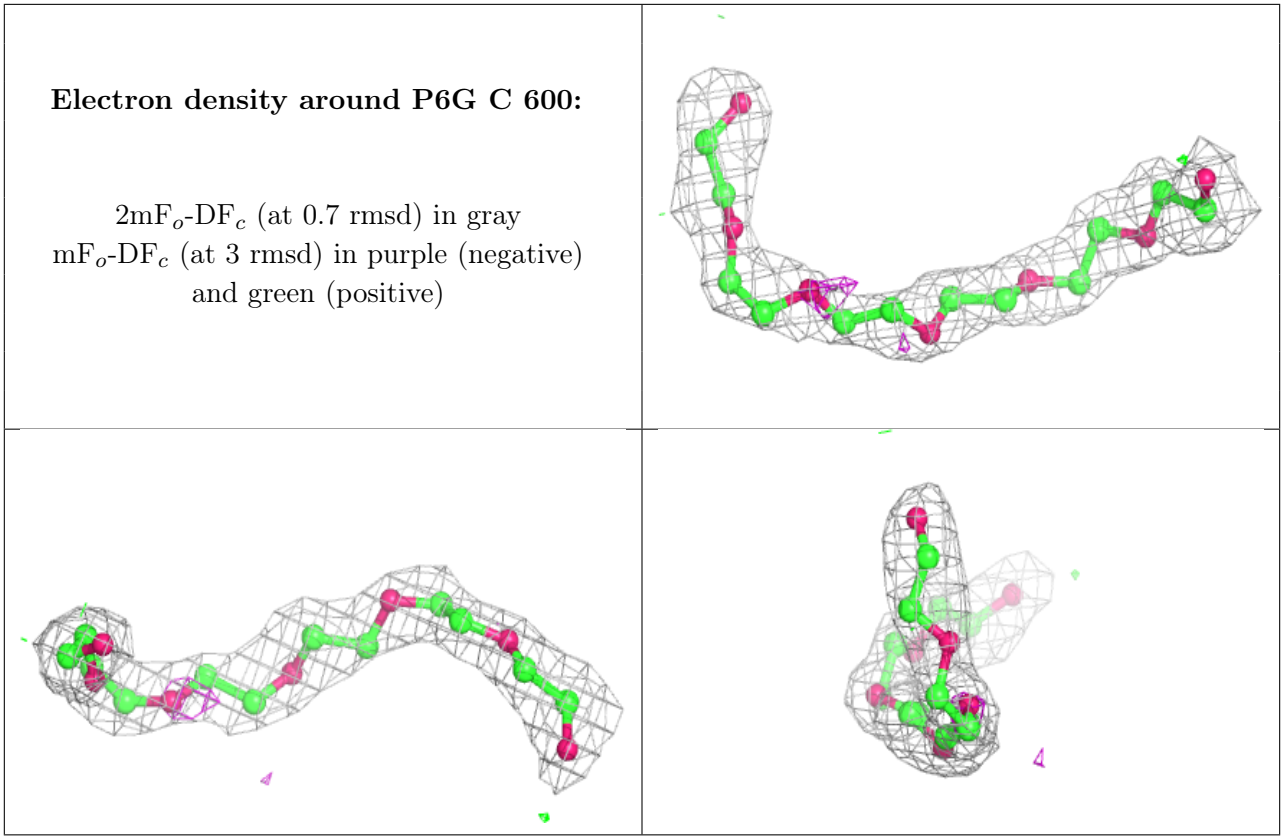
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	P6G	C	600	19/19	0.83	0.23	39,41,45,45	0
2	P6G	A	500	19/19	0.84	0.23	40,42,45,46	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.

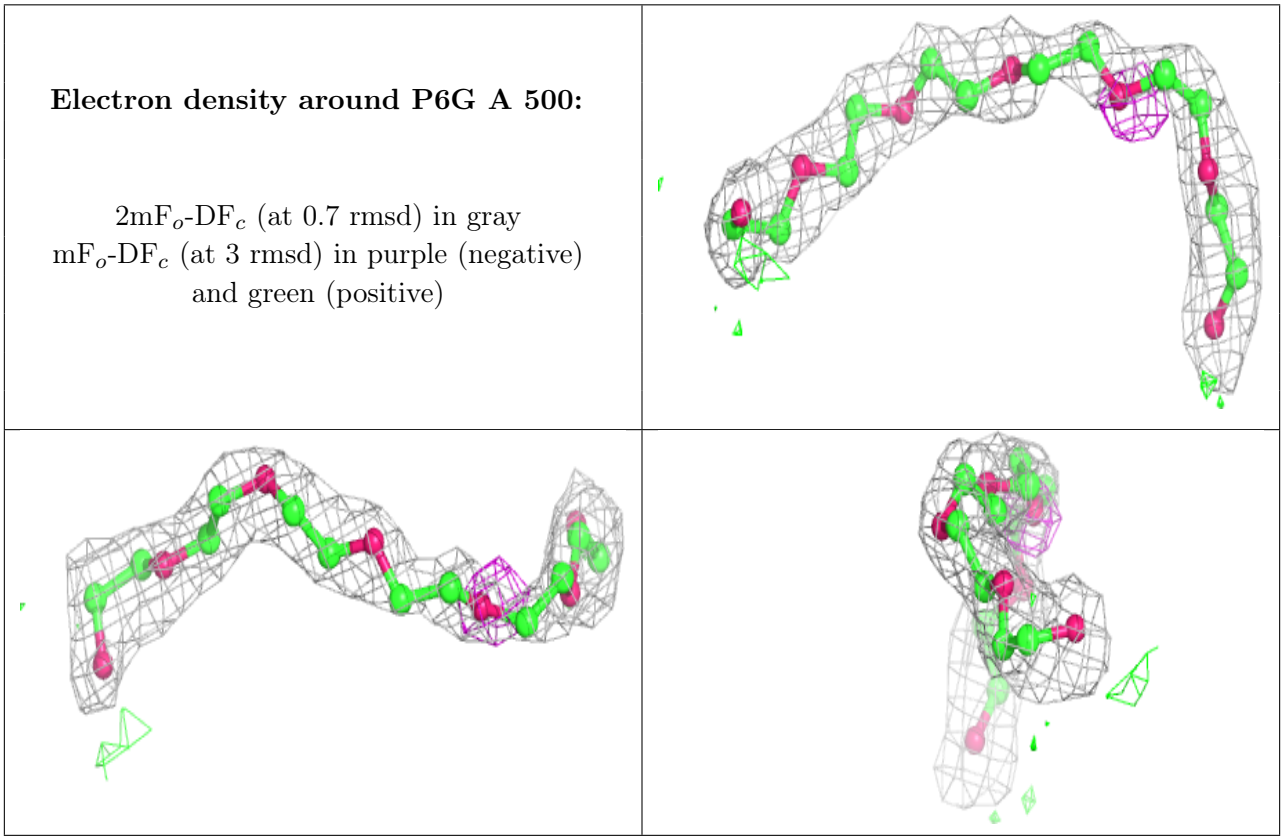
Electron density around P6G C 600:

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



Electron density around P6G A 500:

$2mF_o$-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.