



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 11:54 AM BST

PDB ID : 5CTG
Title : The 3.1 Å resolution structure of a eukaryotic SWEET transporter
Authors : Tao, Y.; Perry, K.; Feng, L.
Deposited on : 2015-07-24
Resolution : 3.10 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 : 2.13.1
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) : 2.13.1

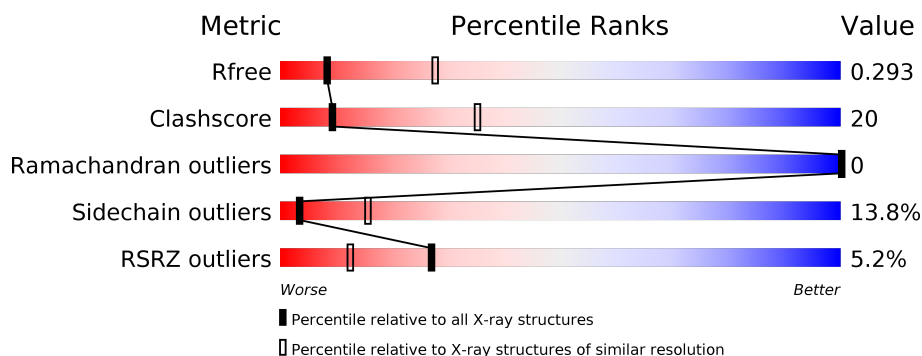
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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 $\leq 5\%$. 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	224	
1	B	224	
1	C	224	

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
4	TRS	C	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5019 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 Bidirectional sugar transporter SWEET2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1630	1096	250	272	12			
1	B	220	Total	C	N	O	S	0	0	0
			1671	1122	256	281	12			
1	C	215	Total	C	N	O	S	0	0	0
			1625	1094	248	271	12			

There are 27 discrepancies between the modelled and reference sequences:

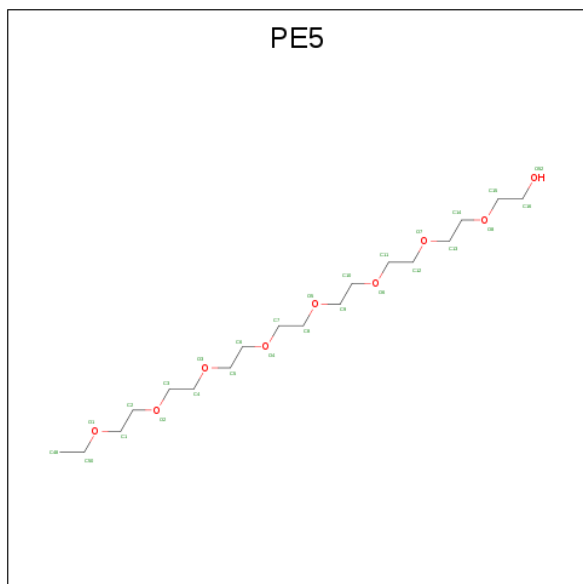
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	SER	-	expression tag	UNP Q5N8J1
A	217	ASN	-	expression tag	UNP Q5N8J1
A	218	SER	-	expression tag	UNP Q5N8J1
A	219	LEU	-	expression tag	UNP Q5N8J1
A	220	GLU	-	expression tag	UNP Q5N8J1
A	221	VAL	-	expression tag	UNP Q5N8J1
A	222	LEU	-	expression tag	UNP Q5N8J1
A	223	PHE	-	expression tag	UNP Q5N8J1
A	224	GLN	-	expression tag	UNP Q5N8J1
B	216	SER	-	expression tag	UNP Q5N8J1
B	217	ASN	-	expression tag	UNP Q5N8J1
B	218	SER	-	expression tag	UNP Q5N8J1
B	219	LEU	-	expression tag	UNP Q5N8J1
B	220	GLU	-	expression tag	UNP Q5N8J1
B	221	VAL	-	expression tag	UNP Q5N8J1
B	222	LEU	-	expression tag	UNP Q5N8J1
B	223	PHE	-	expression tag	UNP Q5N8J1
B	224	GLN	-	expression tag	UNP Q5N8J1
C	216	SER	-	expression tag	UNP Q5N8J1
C	217	ASN	-	expression tag	UNP Q5N8J1
C	218	SER	-	expression tag	UNP Q5N8J1
C	219	LEU	-	expression tag	UNP Q5N8J1
C	220	GLU	-	expression tag	UNP Q5N8J1

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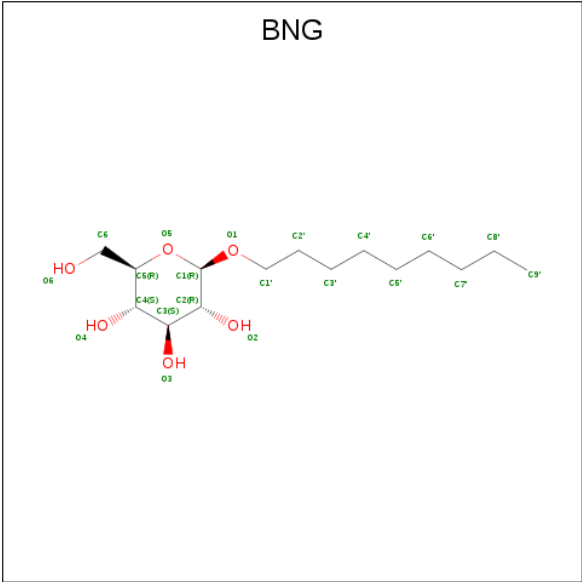
Chain	Residue	Modelled	Actual	Comment	Reference
C	221	VAL	-	expression tag	UNP Q5N8J1
C	222	LEU	-	expression tag	UNP Q5N8J1
C	223	PHE	-	expression tag	UNP Q5N8J1
C	224	GLN	-	expression tag	UNP Q5N8J1

- Molecule 2 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



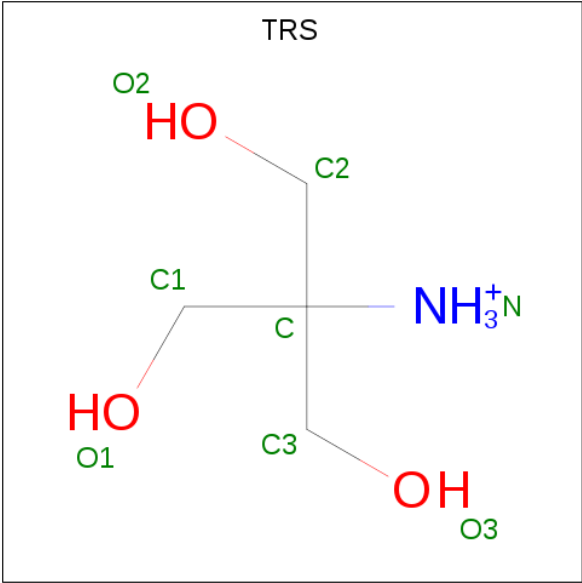
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	16	8		
2	B	1	Total	C	O	0	0
			24	16	8		

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

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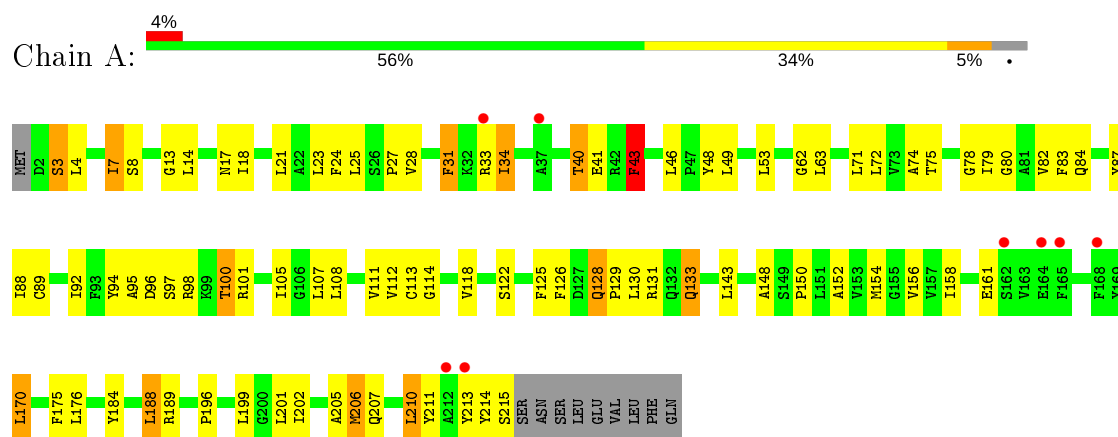
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

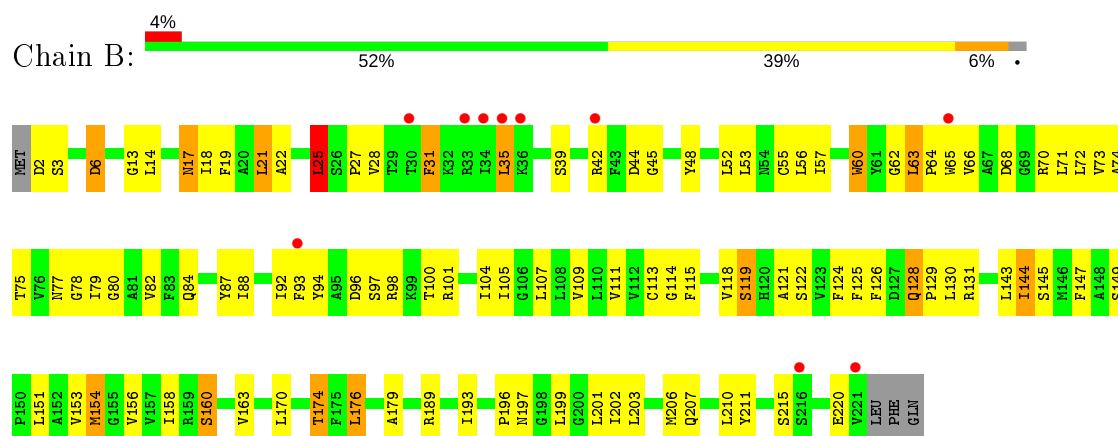
3 Residue-property plots [i](#)

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.

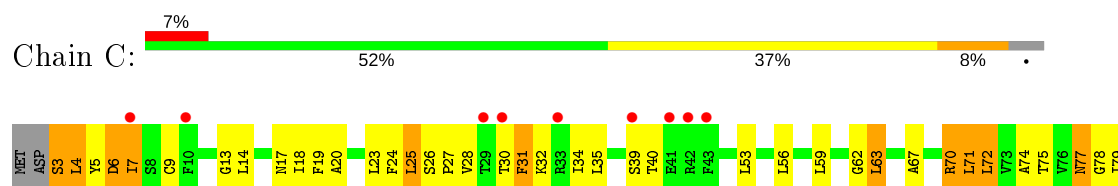
- Molecule 1: Bidirectional sugar transporter SWEET2b

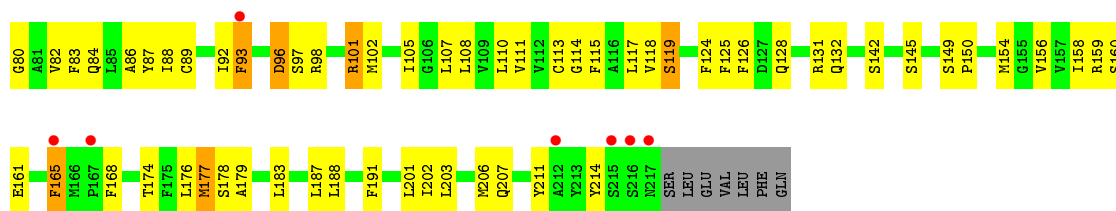


- Molecule 1: Bidirectional sugar transporter SWEET2b



- Molecule 1: Bidirectional sugar transporter SWEET2b





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.83Å 142.24Å 81.57Å 90.00° 93.36° 90.00°	Depositor
Resolution (Å)	29.90 – 3.10 48.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.90-3.10) 91.0 (48.62-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.253 , 0.291 0.259 , 0.293	Depositor DCC
R_{free} test set	973 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 102.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PE5, TRS, BNG

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	0.48	1/1672 (0.1%)	0.68	0/2275
1	B	0.46	0/1714	0.71	3/2334 (0.1%)
1	C	0.35	0/1667	0.61	0/2270
All	All	0.43	1/5053 (0.0%)	0.67	3/6879 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	PHE	CE2-CZ	-5.13	1.27	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	LEU	CB-CG-CD2	5.80	120.86	111.00
1	B	25	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	144	ILE	CG1-CB-CG2	-5.22	99.92	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1630	0	1647	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1671	0	1682	71	1
1	C	1625	0	1634	74	0
2	A	24	0	28	0	0
2	B	24	0	28	4	0
3	A	21	0	30	1	0
4	A	8	0	12	0	0
4	B	8	0	12	0	0
4	C	8	0	12	3	0
All	All	5019	0	5085	200	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 20.

All (200) 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:B:128:GLN:HG3	1:B:129:PRO:HA	1.55	0.86
1:B:113:CYS:HB3	1:C:202:ILE:HD13	1.61	0.82
1:A:34:ILE:CD1	1:A:40:THR:HA	2.10	0.82
1:A:40:THR:OG1	1:A:94:TYR:O	1.98	0.81
1:A:199:LEU:HD23	1:C:117:LEU:HD23	1.66	0.78
1:A:202:ILE:HD13	1:C:113:CYS:HB3	1.70	0.73
1:C:77:ASN:HD22	1:C:78:GLY:H	1.38	0.71
1:C:23:LEU:HD21	1:C:174:THR:HG23	1.72	0.71
1:A:34:ILE:HD12	1:A:40:THR:HA	1.72	0.70
1:C:203:LEU:HD23	1:C:206:MET:HE3	1.74	0.69
1:A:23:LEU:HA	1:A:170:LEU:HD11	1.75	0.69
1:B:60:TRP:HA	1:B:63:LEU:HD22	1.74	0.68
1:B:73:VAL:O	1:B:77:ASN:ND2	2.26	0.67
1:B:17:ASN:ND2	1:B:75:THR:OG1	2.22	0.67
1:B:68:ASP:O	1:B:70:ARG:NH1	2.29	0.66
1:A:34:ILE:HG12	1:A:43:PHE:HE2	1.59	0.66
1:A:13:GLY:O	1:A:17:ASN:ND2	2.28	0.65
1:C:156:VAL:HG11	1:C:165:PHE:HD2	1.62	0.64
1:C:27:PRO:HG2	1:C:87:TYR:CE2	2.33	0.63
1:A:96:ASP:O	1:A:97:SER:OG	2.15	0.63
1:C:3:SER:OG	1:C:4:LEU:N	2.31	0.62
1:C:77:ASN:HD22	1:C:78:GLY:N	1.97	0.62
1:B:174:THR:HG21	2:B:301:PE5:H142	1.80	0.61
1:C:101:ARG:O	1:C:105:ILE:HG13	2.00	0.61
1:C:17:ASN:OD1	1:C:75:THR:OG1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:O	1:A:206:MET:HG3	2.01	0.61
1:C:23:LEU:HD11	1:C:174:THR:HA	1.82	0.61
1:C:14:LEU:O	1:C:18:ILE:HG12	2.01	0.61
1:A:113:CYS:HB3	1:B:202:ILE:HD13	1.83	0.60
1:B:75:THR:O	1:B:79:ILE:HG13	2.01	0.60
1:C:13:GLY:HA3	1:C:72:LEU:HD23	1.81	0.60
1:C:71:LEU:H	1:C:71:LEU:HD12	1.66	0.60
1:C:74:ALA:O	1:C:77:ASN:ND2	2.34	0.60
1:A:53:LEU:HB2	1:A:111:VAL:HG13	1.84	0.60
1:C:114:GLY:O	1:C:118:VAL:HG12	2.02	0.59
4:C:301:TRS:O1	4:C:301:TRS:O3	2.15	0.59
1:C:96:ASP:O	1:C:97:SER:OG	2.20	0.59
1:C:27:PRO:O	1:C:30:THR:HG22	2.02	0.59
1:A:143:LEU:HD23	1:A:196:PRO:HB2	1.85	0.59
1:A:31:PHE:HE2	1:A:48:TYR:HE2	1.51	0.58
1:B:88:ILE:O	1:B:92:ILE:HG13	2.04	0.58
1:C:71:LEU:O	1:C:75:THR:HG23	2.03	0.58
1:C:24:PHE:HB3	1:C:83:PHE:CD1	2.38	0.58
1:A:184:TYR:CE1	1:A:188:LEU:HD21	2.39	0.58
1:C:168:PHE:HB2	1:C:211:TYR:CZ	2.37	0.57
1:B:80:GLY:O	1:B:84:GLN:HG2	2.04	0.57
1:A:161:GLU:HA	1:A:214:TYR:HE2	1.69	0.57
1:B:45:GLY:HA2	1:B:48:TYR:HE2	1.70	0.57
1:C:4:LEU:O	1:C:7:ILE:HG12	2.05	0.57
1:A:189:ARG:NH1	1:C:125:PHE:O	2.38	0.56
1:B:73:VAL:HG21	1:B:193:ILE:HD13	1.88	0.56
1:B:96:ASP:O	1:B:97:SER:OG	2.23	0.56
1:A:154:MET:O	1:A:158:ILE:HG13	2.06	0.56
1:B:122:SER:HA	1:B:126:PHE:HD2	1.71	0.55
1:C:67:ALA:CB	1:C:70:ARG:HG3	2.37	0.55
1:C:9:CYS:SG	1:C:187:LEU:HD11	2.48	0.54
1:A:96:ASP:O	1:A:100:THR:OG1	2.24	0.54
1:C:19:PHE:CE1	1:C:176:LEU:HB3	2.43	0.54
1:C:62:GLY:HA3	1:C:74:ALA:HB2	1.90	0.53
1:B:17:ASN:HD22	1:B:72:LEU:HD12	1.74	0.53
1:B:19:PHE:CE2	1:B:176:LEU:HB3	2.43	0.53
1:C:75:THR:O	1:C:79:ILE:HG13	2.08	0.53
1:A:78:GLY:O	1:A:82:VAL:HG23	2.09	0.53
1:A:148:ALA:HB2	3:A:302:BNG:H5	1.91	0.53
1:A:107:LEU:O	1:A:111:VAL:HG23	2.09	0.53
1:B:197:ASN:HD21	2:B:301:PE5:H22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLN:NE2	4:C:301:TRS:O2	2.42	0.53
1:B:126:PHE:HB2	1:B:131:ARG:HG3	1.90	0.53
1:C:13:GLY:O	1:C:17:ASN:ND2	2.35	0.53
1:B:122:SER:HA	1:B:126:PHE:CD2	2.43	0.52
1:C:154:MET:O	1:C:158:ILE:HG13	2.10	0.52
1:B:14:LEU:O	1:B:18:ILE:HG13	2.10	0.52
1:B:207:GLN:OE1	2:B:301:PE5:H132	2.10	0.52
1:B:25:LEU:O	1:B:28:VAL:HG12	2.10	0.52
1:A:31:PHE:HE2	1:A:48:TYR:CE2	2.27	0.52
1:C:34:ILE:HD12	1:C:40:THR:HG22	1.91	0.51
1:A:4:LEU:O	1:A:7:ILE:HG12	2.10	0.51
1:B:55:CYS:O	1:B:77:ASN:HB3	2.11	0.51
1:A:184:TYR:O	1:A:188:LEU:HD22	2.11	0.51
1:A:125:PHE:O	1:B:189:ARG:NH2	2.43	0.51
1:A:18:ILE:O	1:A:21:LEU:HB2	2.10	0.51
1:C:82:VAL:O	1:C:86:ALA:N	2.39	0.51
1:C:20:ALA:HB1	1:C:24:PHE:CE2	2.46	0.50
1:C:89:CYS:O	1:C:92:ILE:HG12	2.11	0.50
1:A:34:ILE:HD11	1:A:40:THR:HA	1.93	0.50
1:B:65:TRP:HB2	1:B:131:ARG:NH2	2.26	0.50
1:C:67:ALA:HB3	1:C:70:ARG:HG3	1.92	0.50
1:B:149:SER:O	1:B:153:VAL:HG13	2.12	0.50
1:C:156:VAL:HG11	1:C:165:PHE:CD2	2.46	0.50
1:C:115:PHE:O	1:C:119:SER:HB2	2.12	0.49
1:B:154:MET:HG2	1:B:210:LEU:HD12	1.92	0.49
1:C:31:PHE:O	1:C:34:ILE:HB	2.13	0.49
1:A:40:THR:OG1	1:A:95:ALA:HA	2.13	0.49
1:C:154:MET:CE	1:C:207:GLN:HG3	2.42	0.49
1:C:32:LYS:O	1:C:35:LEU:HB3	2.11	0.49
1:A:80:GLY:O	1:A:84:GLN:HG2	2.12	0.49
1:B:27:PRO:O	1:B:31:PHE:N	2.43	0.49
1:B:60:TRP:CE3	1:B:66:VAL:HG21	2.48	0.49
1:C:98:ARG:HG2	1:C:102:MET:HE2	1.95	0.49
1:B:151:LEU:HA	1:B:154:MET:HE3	1.95	0.48
1:A:75:THR:O	1:A:79:ILE:HG13	2.12	0.48
1:B:143:LEU:HD23	1:B:196:PRO:HB2	1.95	0.48
1:A:126:PHE:O	1:A:131:ARG:NH2	2.47	0.48
1:B:179:ALA:HA	1:B:201:LEU:HD12	1.96	0.48
1:A:211:TYR:O	1:A:215:SER:N	2.37	0.48
1:A:14:LEU:O	1:A:18:ILE:HG12	2.12	0.48
1:C:56:LEU:O	1:C:59:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLN:O	1:C:88:ILE:HG13	2.13	0.48
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.66	0.47
1:B:211:TYR:O	1:B:215:SER:HB3	2.14	0.47
1:B:53:LEU:HD13	1:B:111:VAL:HG13	1.95	0.47
1:B:19:PHE:CD2	1:B:176:LEU:HB3	2.49	0.47
1:A:27:PRO:HB2	1:A:87:TYR:CE1	2.49	0.47
1:B:115:PHE:O	1:B:119:SER:OG	2.25	0.47
1:B:62:GLY:HA3	1:B:74:ALA:HB2	1.96	0.47
1:B:78:GLY:O	1:B:82:VAL:HG23	2.14	0.47
1:C:83:PHE:O	1:C:87:TYR:HD1	1.97	0.47
1:B:21:LEU:HD12	1:B:22:ALA:N	2.30	0.47
1:A:25:LEU:O	1:A:28:VAL:HG12	2.15	0.47
1:B:114:GLY:O	1:B:118:VAL:HG12	2.14	0.47
1:B:156:VAL:O	1:B:160:SER:HB2	2.15	0.47
1:B:170:LEU:O	1:B:174:THR:OG1	2.33	0.47
1:A:133:GLN:HG2	1:A:133:GLN:H	1.43	0.47
1:B:27:PRO:HG2	1:B:87:TYR:CZ	2.50	0.47
1:C:177:MET:HG3	1:C:178:SER:N	2.30	0.47
1:B:17:ASN:HD21	1:B:75:THR:HG1	1.56	0.46
1:A:126:PHE:CD1	1:A:130:LEU:HD23	2.50	0.46
1:B:100:THR:O	1:B:104:ILE:HG12	2.14	0.46
1:A:46:LEU:O	1:A:49:LEU:HB2	2.16	0.46
1:B:84:GLN:O	1:B:88:ILE:HG13	2.15	0.46
1:C:158:ILE:HA	1:C:214:TYR:OH	2.15	0.46
1:A:128:GLN:HB2	1:A:128:GLN:HE21	1.60	0.46
1:B:107:LEU:O	1:B:111:VAL:HG23	2.14	0.46
1:C:19:PHE:HE1	1:C:176:LEU:HB3	1.81	0.46
1:C:59:LEU:O	1:C:63:LEU:HD22	2.16	0.46
1:A:114:GLY:O	1:A:118:VAL:HG12	2.15	0.46
1:C:126:PHE:HB2	1:C:131:ARG:HG2	1.97	0.46
1:A:122:SER:O	1:A:126:PHE:HB2	2.15	0.46
1:C:154:MET:HE1	1:C:206:MET:HB3	1.98	0.46
1:A:3:SER:O	1:A:7:ILE:HG23	2.16	0.45
1:B:154:MET:O	1:B:158:ILE:HG13	2.16	0.45
1:C:168:PHE:HB2	1:C:211:TYR:CE1	2.52	0.45
1:B:144:ILE:O	1:B:147:PHE:HB2	2.17	0.45
1:A:189:ARG:HG2	1:C:124:PHE:HE2	1.82	0.45
1:B:3:SER:H	1:B:6:ASP:HB2	1.80	0.45
1:B:94:TYR:N	1:B:94:TYR:CD1	2.85	0.45
1:C:142:SER:O	1:C:145:SER:OG	2.26	0.45
1:C:149:SER:HB3	1:C:150:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:MET:HE3	1:C:207:GLN:HG3	1.98	0.45
1:C:150:PRO:O	1:C:154:MET:HG3	2.17	0.45
1:C:25:LEU:O	1:C:28:VAL:HG12	2.17	0.44
1:C:80:GLY:O	1:C:84:GLN:HG2	2.17	0.44
1:A:24:PHE:O	1:A:27:PRO:HD2	2.18	0.44
1:C:3:SER:N	1:C:6:ASP:OD2	2.50	0.44
1:A:158:ILE:HD11	1:A:210:LEU:HD21	1.99	0.44
1:B:121:ALA:O	1:B:125:PHE:HD2	2.00	0.44
1:B:143:LEU:HA	1:B:143:LEU:HD12	1.73	0.44
1:B:63:LEU:HA	1:B:64:PRO:HD3	1.87	0.44
1:A:101:ARG:O	1:A:105:ILE:HG13	2.18	0.44
1:B:53:LEU:O	1:B:57:ILE:HG13	2.17	0.44
1:B:105:ILE:O	1:B:109:VAL:HG23	2.19	0.43
1:C:174:THR:O	1:C:177:MET:HG2	2.19	0.43
1:B:154:MET:HE1	1:B:203:LEU:HD22	2.01	0.43
1:B:101:ARG:O	1:B:105:ILE:HG12	2.17	0.43
1:C:179:ALA:O	1:C:183:LEU:HD13	2.18	0.43
1:C:26:SER:N	1:C:27:PRO:HD2	2.34	0.43
1:A:213:TYR:CD1	1:A:213:TYR:N	2.85	0.43
1:B:44:ASP:HA	1:B:45:GLY:HA3	1.75	0.43
1:B:28:VAL:HA	1:B:31:PHE:HB2	2.00	0.42
1:A:150:PRO:O	1:A:154:MET:HG3	2.20	0.42
1:C:126:PHE:CB	1:C:131:ARG:HG2	2.49	0.42
1:B:144:ILE:HA	1:B:147:PHE:CD2	2.55	0.42
1:B:176:LEU:HA	1:B:176:LEU:HD13	1.79	0.42
1:A:152:ALA:O	1:A:156:VAL:HG23	2.20	0.42
1:A:62:GLY:HA3	1:A:74:ALA:HB2	2.02	0.42
1:C:161:GLU:HA	1:C:214:TYR:HE1	1.85	0.42
1:C:92:ILE:HG13	1:C:93:PHE:N	2.34	0.41
1:A:24:PHE:HB3	1:A:83:PHE:CD2	2.55	0.41
1:A:128:GLN:HG3	1:A:129:PRO:HA	2.02	0.41
1:B:18:ILE:O	1:B:21:LEU:HG	2.21	0.41
1:C:53:LEU:HA	1:C:56:LEU:HD12	2.02	0.41
1:A:108:LEU:O	1:A:112:VAL:HG23	2.21	0.41
1:A:175:PHE:HE1	1:A:205:ALA:HB2	1.86	0.41
1:B:56:LEU:HD23	1:B:115:PHE:CD2	2.56	0.41
2:B:301:PE5:H71	2:B:301:PE5:H51	1.84	0.41
1:B:13:GLY:O	1:B:17:ASN:HB2	2.21	0.41
1:C:187:LEU:HD12	1:C:188:LEU:N	2.36	0.41
1:A:17:ASN:OD1	1:A:75:THR:OG1	2.39	0.41
1:B:130:LEU:O	1:B:130:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:CE2	1:B:199:LEU:HB3	2.56	0.41
1:C:107:LEU:O	1:C:111:VAL:HG23	2.20	0.41
1:C:19:PHE:CD2	1:C:19:PHE:N	2.87	0.41
1:C:88:ILE:O	1:C:92:ILE:HG23	2.21	0.41
1:A:206:MET:O	1:A:210:LEU:HB2	2.20	0.40
1:A:48:TYR:N	1:A:48:TYR:CD1	2.86	0.40
1:A:88:ILE:O	1:A:92:ILE:HG13	2.22	0.40
1:B:52:LEU:O	1:B:56:LEU:HD13	2.21	0.40
1:B:65:TRP:HB2	1:B:131:ARG:HH21	1.85	0.40
1:B:124:PHE:HD2	1:B:125:PHE:CD2	2.39	0.40
1:C:191:PHE:H	4:C:301:TRS:C1	2.34	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:B:2:ASP:N	1:B:220:GLU:OE2[1_455]	2.18	0.02

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	212/224 (95%)	211 (100%)	1 (0%)	0	100	100
1	B	218/224 (97%)	214 (98%)	4 (2%)	0	100	100
1	C	213/224 (95%)	209 (98%)	4 (2%)	0	100	100
All	All	643/672 (96%)	634 (99%)	9 (1%)	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 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	168/187 (90%)	145 (86%)	23 (14%)	3	16
1	B	173/187 (92%)	151 (87%)	22 (13%)	4	18
1	C	166/187 (89%)	141 (85%)	25 (15%)	3	12
All	All	507/561 (90%)	437 (86%)	70 (14%)	3	16

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	7	ILE
1	A	8	SER
1	A	31	PHE
1	A	33	ARG
1	A	34	ILE
1	A	40	THR
1	A	41	GLU
1	A	43	PHE
1	A	63	LEU
1	A	71	LEU
1	A	89	CYS
1	A	98	ARG
1	A	100	THR
1	A	128	GLN
1	A	133	GLN
1	A	170	LEU
1	A	176	LEU
1	A	188	LEU
1	A	201	LEU
1	A	206	MET
1	A	207	GLN
1	A	210	LEU
1	B	6	ASP
1	B	17	ASN
1	B	21	LEU

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Mol	Chain	Res	Type
1	B	25	LEU
1	B	31	PHE
1	B	35	LEU
1	B	39	SER
1	B	42	ARG
1	B	60	TRP
1	B	63	LEU
1	B	71	LEU
1	B	93	PHE
1	B	98	ARG
1	B	119	SER
1	B	128	GLN
1	B	145	SER
1	B	154	MET
1	B	160	SER
1	B	163	VAL
1	B	174	THR
1	B	176	LEU
1	B	206	MET
1	C	3	SER
1	C	4	LEU
1	C	5	TYR
1	C	6	ASP
1	C	7	ILE
1	C	25	LEU
1	C	31	PHE
1	C	39	SER
1	C	63	LEU
1	C	70	ARG
1	C	71	LEU
1	C	72	LEU
1	C	77	ASN
1	C	93	PHE
1	C	96	ASP
1	C	101	ARG
1	C	108	LEU
1	C	110	LEU
1	C	119	SER
1	C	128	GLN
1	C	159	ARG
1	C	160	SER
1	C	165	PHE

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Mol	Chain	Res	Type
1	C	177	MET
1	C	201	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	54	ASN
1	B	197	ASN
1	C	77	ASN
1	C	132	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	TRS	A	303	-	7,7,7	0.35	0	9,9,9	0.58	0
2	PE5	B	301	-	23,23,26	0.73	0	22,22,25	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PE5	A	301	-	23,23,26	0.82	1 (4%)	22,22,25	0.26	0
4	TRS	B	302	-	7,7,7	0.34	0	9,9,9	0.31	0
4	TRS	C	301	-	7,7,7	0.37	0	9,9,9	0.40	0
3	BNG	A	302	-	21,21,21	1.04	1 (4%)	26,26,26	1.39	3 (11%)

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
4	TRS	A	303	-	-	3/9/9/9	-
2	PE5	B	301	-	-	13/21/21/24	-
2	PE5	A	301	-	-	12/21/21/24	-
4	TRS	B	302	-	-	8/9/9/9	-
4	TRS	C	301	-	-	6/9/9/9	-
3	BNG	A	302	-	-	10/12/32/32	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	BNG	O5-C1	2.86	1.49	1.41
2	A	301	PE5	C8-C7	2.06	1.59	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	BNG	C3-C4-C5	4.00	117.37	110.24
3	A	302	BNG	C4-C3-C2	2.93	115.94	110.82
3	A	302	BNG	O5-C5-C4	2.87	114.90	109.69

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	TRS	N-C-C2-O2
4	B	302	TRS	N-C-C1-O1
4	B	302	TRS	C1-C-C2-O2
4	B	302	TRS	C3-C-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	301	TRS	N-C-C1-O1
4	C	301	TRS	C1-C-C2-O2
4	C	301	TRS	C3-C-C2-O2
3	A	302	BNG	C2-C1-O1-C1'
3	A	302	BNG	O5-C1-O1-C1'
3	A	302	BNG	C2'-C1'-O1-C1
3	A	302	BNG	O5-C5-C6-O6
2	B	301	PE5	O1-C1-C2-O2
2	B	301	PE5	O3-C5-C6-O4
2	B	301	PE5	O7-C13-C14-O8
2	B	301	PE5	O6-C10-C9-O5
2	A	301	PE5	O7-C13-C14-O8
2	B	301	PE5	O4-C7-C8-O5
2	B	301	PE5	O2-C3-C4-O3
2	B	301	PE5	O6-C11-C12-O7
3	A	302	BNG	C4-C5-C6-O6
3	A	302	BNG	C4'-C5'-C6'-C7'
3	A	302	BNG	C1'-C2'-C3'-C4'
2	A	301	PE5	C7-C8-O5-C9
4	A	303	TRS	C3-C-C2-O2
4	B	302	TRS	C3-C-C1-O1
3	A	302	BNG	C3'-C4'-C5'-C6'
3	A	302	BNG	O1-C1'-C2'-C3'
2	A	301	PE5	O6-C10-C9-O5
2	B	301	PE5	C5-C6-O4-C7
2	A	301	PE5	O1-C1-C2-O2
2	A	301	PE5	O2-C3-C4-O3
2	A	301	PE5	O4-C7-C8-O5
2	A	301	PE5	C2-C1-O1-C50
2	B	301	PE5	C11-C12-O7-C13
2	A	301	PE5	C4-C3-O2-C2
2	B	301	PE5	C7-C8-O5-C9
4	B	302	TRS	N-C-C2-O2
4	B	302	TRS	C2-C-C3-O3
4	C	301	TRS	C3-C-C1-O1
4	C	301	TRS	N-C-C2-O2
2	A	301	PE5	C10-C9-O5-C8
2	B	301	PE5	C8-C7-O4-C6
2	A	301	PE5	C13-C14-O8-C15
4	B	302	TRS	C1-C-C3-O3
2	B	301	PE5	C6-C5-O3-C4
2	A	301	PE5	O6-C11-C12-O7

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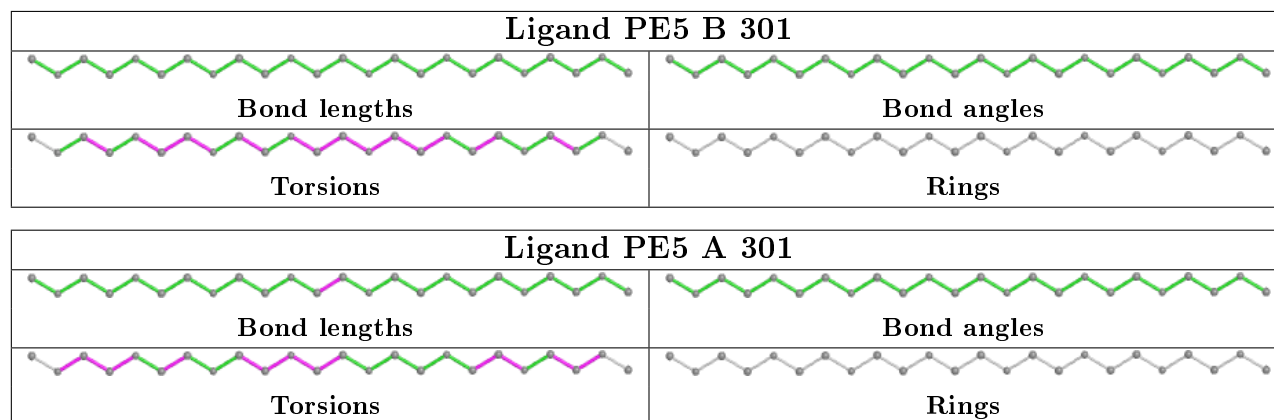
Mol	Chain	Res	Type	Atoms
3	A	302	BNG	C5'-C6'-C7'-C8'
2	B	301	PE5	C12-C11-O6-C10
4	A	303	TRS	C1-C-C2-O2
4	B	302	TRS	N-C-C3-O3
4	C	301	TRS	C2-C-C1-O1
2	A	301	PE5	C14-C13-O7-C12

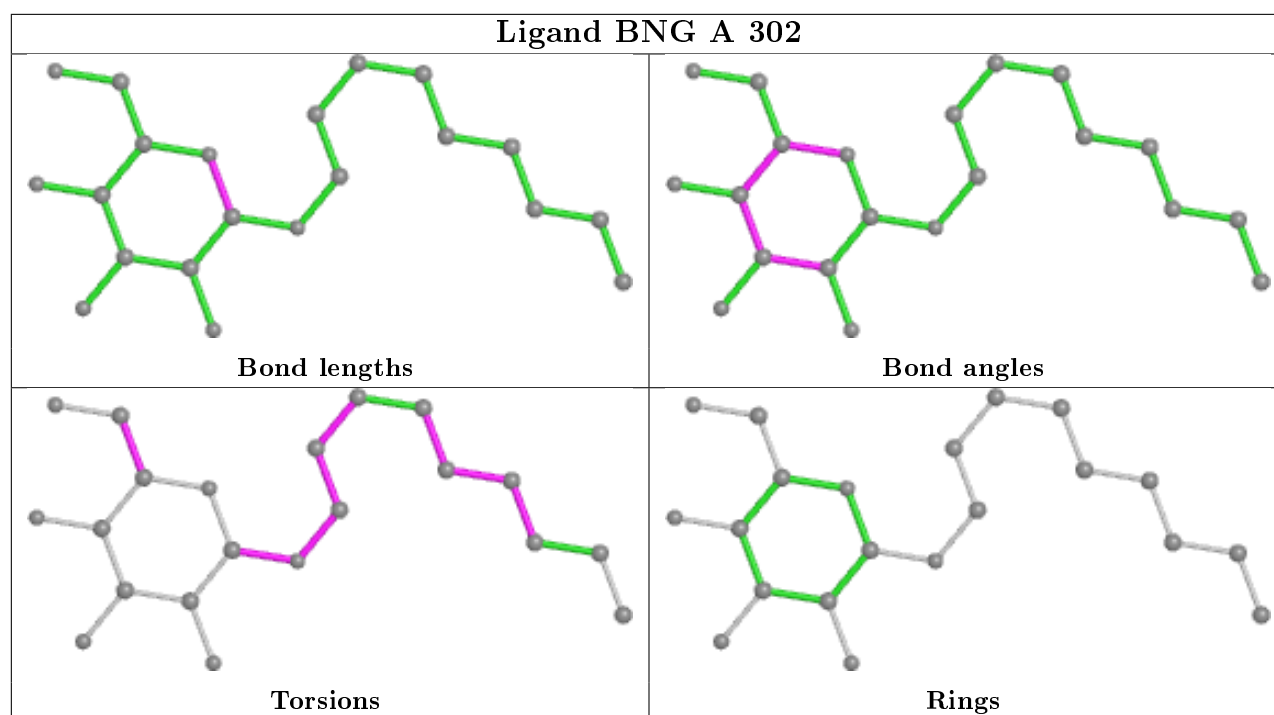
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PE5	4	0
4	C	301	TRS	3	0
3	A	302	BNG	1	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 than 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, 95th 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	214/224 (95%)	-0.13	8 (3%) 41 21	27, 74, 131, 153	0
1	B	220/224 (98%)	-0.08	10 (4%) 33 16	30, 72, 140, 161	0
1	C	215/224 (95%)	0.35	16 (7%) 14 5	76, 133, 200, 230	0
All	All	649/672 (96%)	0.05	34 (5%) 27 12	27, 89, 174, 230	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	PHE	7.2
1	C	217	ASN	7.2
1	C	216	SER	6.4
1	C	39	SER	5.3
1	C	212	ALA	5.1
1	B	33	ARG	4.8
1	B	35	LEU	3.7
1	B	30	THR	3.7
1	A	165	PHE	3.5
1	C	30	THR	3.5
1	C	42	ARG	3.5
1	C	93	PHE	3.3
1	C	41	GLU	3.3
1	C	33	ARG	3.2
1	B	65	TRP	3.1
1	A	37	ALA	3.1
1	A	33	ARG	3.0
1	B	93	PHE	2.9
1	A	164	GLU	2.9
1	C	7	ILE	2.9
1	B	36	LYS	2.7
1	A	212	ALA	2.6
1	C	215	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	216	SER	2.5
1	B	221	VAL	2.5
1	A	168	PHE	2.5
1	C	10	PHE	2.4
1	B	34	ILE	2.4
1	A	213	TYR	2.4
1	B	42	ARG	2.3
1	C	43	PHE	2.2
1	A	162	SER	2.2
1	C	167	PRO	2.0
1	C	29	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

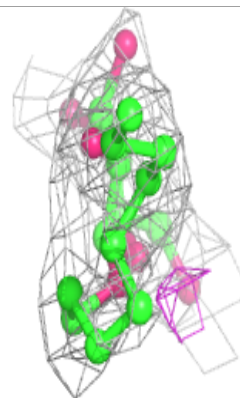
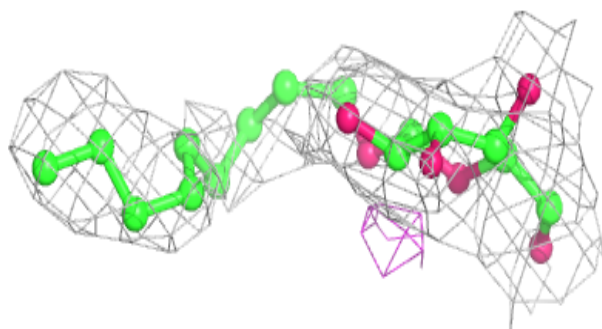
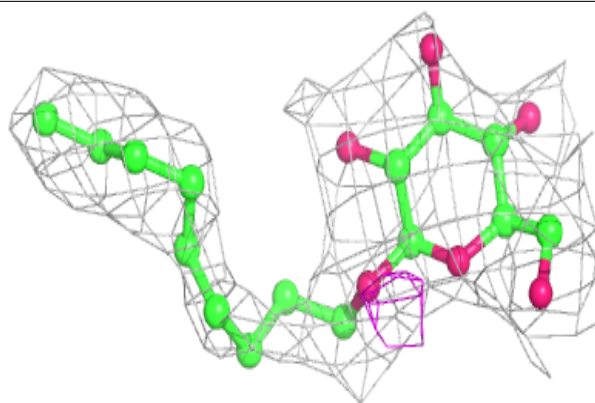
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRS	B	302	8/8	0.70	0.38	100,123,130,141	0
4	TRS	C	301	8/8	0.72	0.46	104,141,143,145	0
3	BNG	A	302	21/21	0.75	0.30	63,106,117,121	0
2	PE5	A	301	24/27	0.77	0.38	86,93,110,115	0
4	TRS	A	303	8/8	0.77	0.26	86,107,117,117	0
2	PE5	B	301	24/27	0.93	0.21	56,76,89,94	0

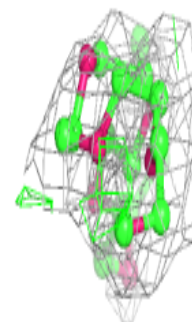
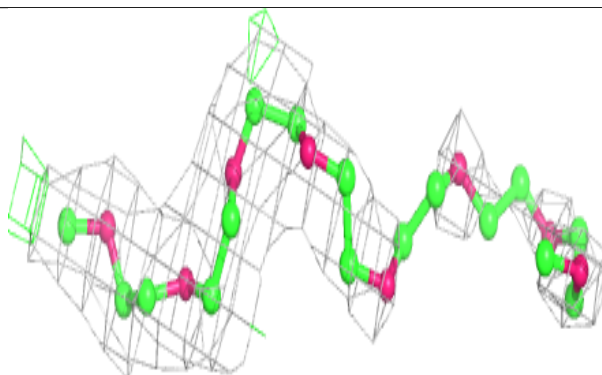
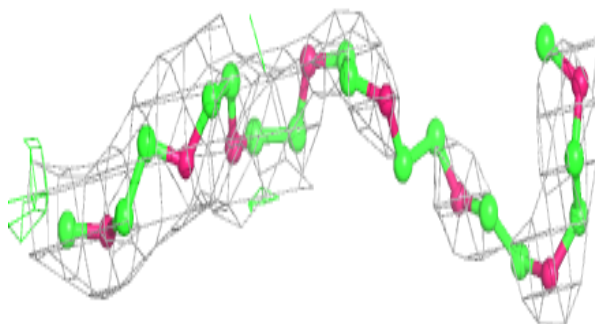
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG A 302:

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

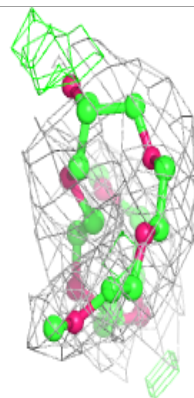
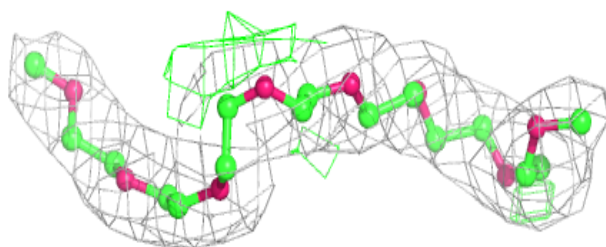
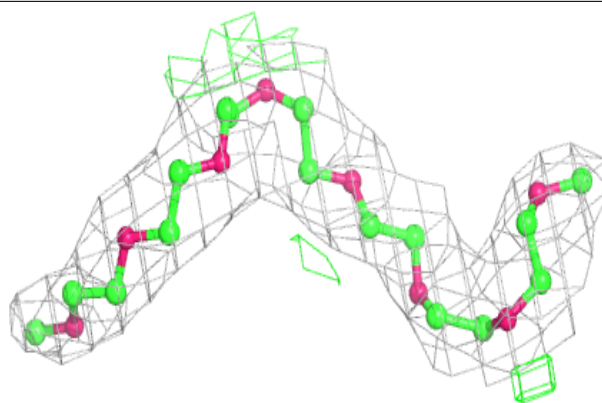
**Electron density around PE5 A 301:**

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



Electron density around PE5 B 301:

$2mF_o-DF_c$ (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.