



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:45 PM UTC

PDB ID : 5CTG / pdb_00005ctg
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

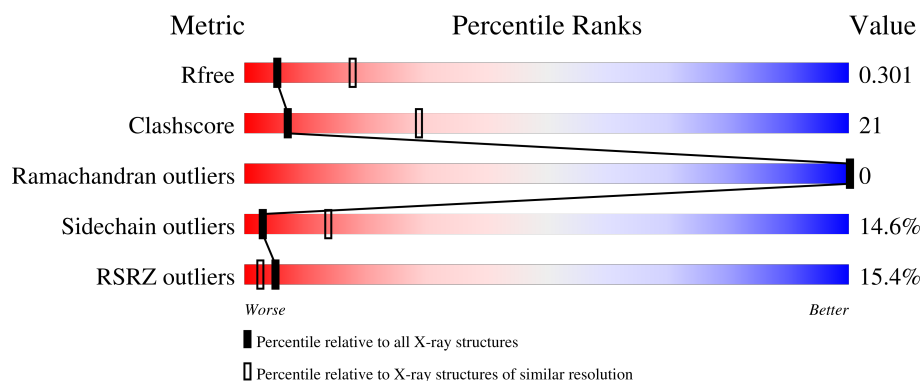
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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 $\leq 5\%$. 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	14% 54% 35% 6% .
1	B	224	16% 50% 43% 6% .
1	C	224	15% 48% 41% 7% .

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:

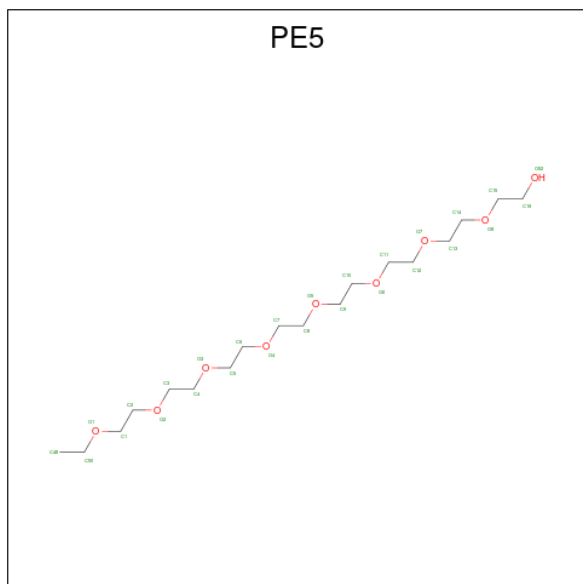
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	SER	-	expression tag	UNP Q5N8J1
A	217	ASN	-	expression tag	UNP Q5N8J1
A	218	SER	-	expression tag	UNP Q5N8J1
A	219	LEU	-	expression tag	UNP Q5N8J1
A	220	GLU	-	expression tag	UNP Q5N8J1
A	221	VAL	-	expression tag	UNP Q5N8J1
A	222	LEU	-	expression tag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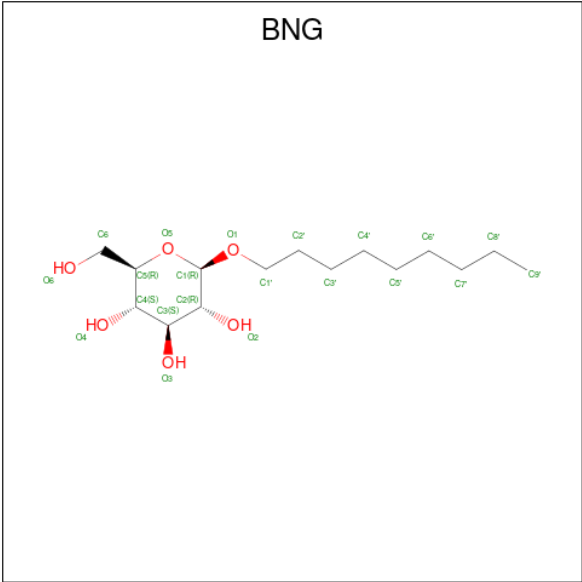
Chain	Residue	Modelled	Actual	Comment	Reference
C	221	VAL	-	expression tag	UNP Q5N8J1
C	222	LEU	-	expression tag	UNP Q5N8J1
C	223	PHE	-	expression tag	UNP Q5N8J1
C	224	GLN	-	expression tag	UNP Q5N8J1

- Molecule 2 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: $C_{18}H_{38}O_9$).



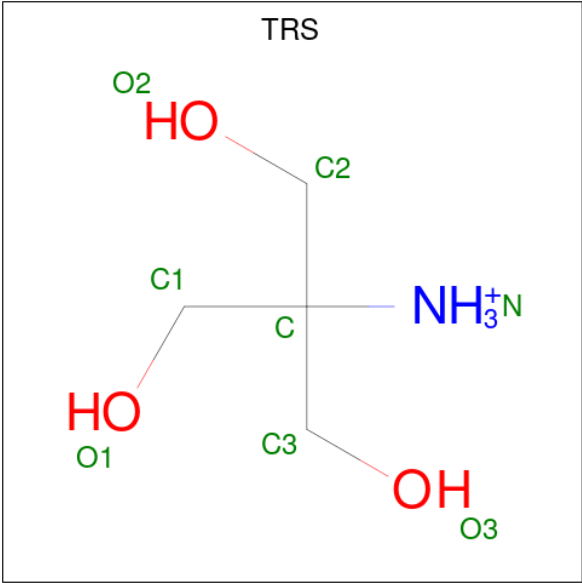
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	16	8		
2	B	1	Total	C	O	0	0
			24	16	8		

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: $C_{15}H_{30}O_6$).



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 (CCD ID: 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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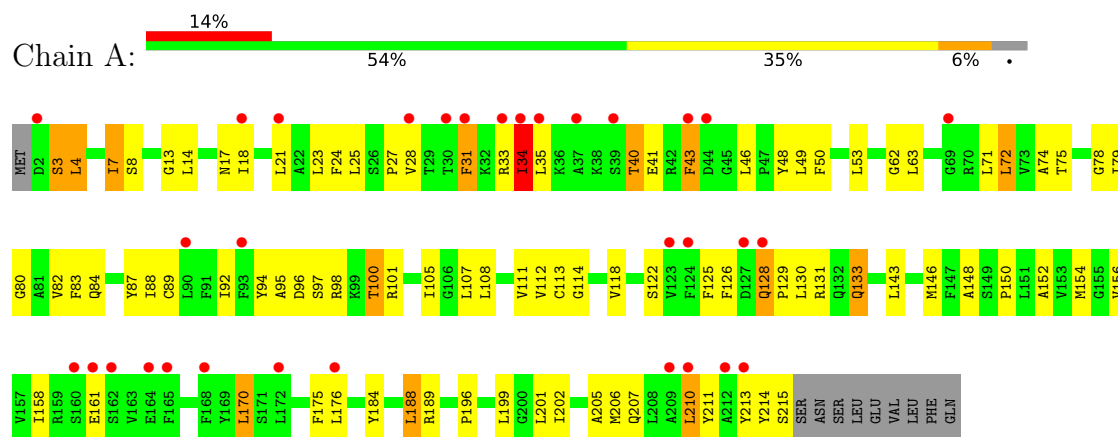
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

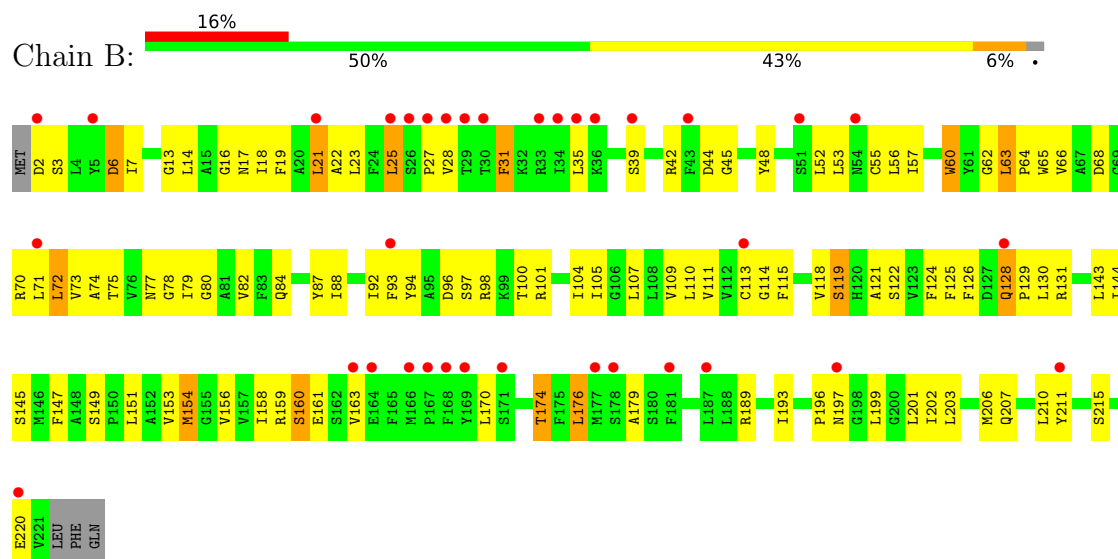
3 Residue-property plots [i](#)

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

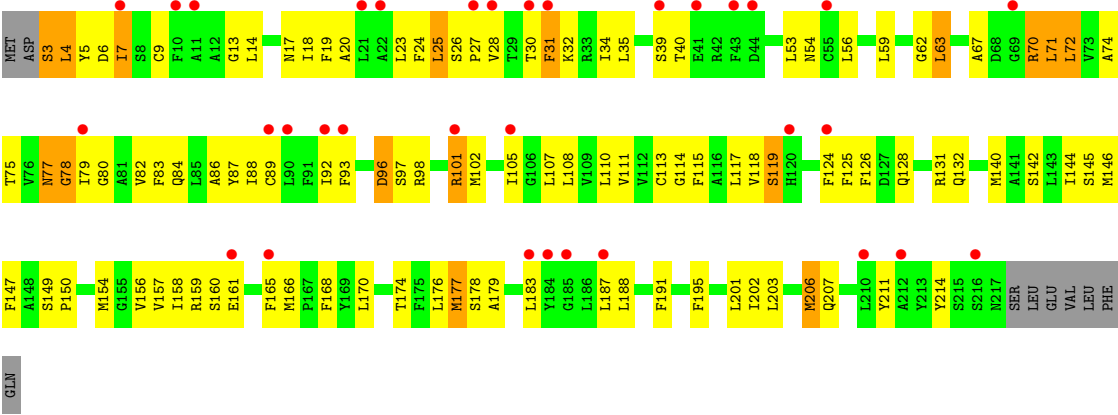


• Molecule 1: Bidirectional sugar transporter SWEET2b



• 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 29.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.90-3.10) 90.9 (29.90-3.10)	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 0.273 , 0.301	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)	0.21 , 69.5	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	0.88	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: TRS, PE5, 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	0.58	0/1672	1.02	2/2275 (0.1%)
1	B	0.58	0/1714	1.04	2/2334 (0.1%)
1	C	0.49	0/1667	0.98	1/2270 (0.0%)
All	All	0.55	0/5053	1.01	5/6879 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	N-CA-C	-6.82	103.84	111.28
1	B	16	GLY	N-CA-C	-5.56	105.65	112.77
1	B	161	GLU	N-CA-C	-5.52	106.49	113.23
1	C	78	GLY	N-CA-C	-5.17	106.52	112.73
1	A	34	ILE	CB-CA-C	-5.12	105.23	112.14

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	62	0
1	B	1671	0	1682	72	1
1	C	1625	0	1634	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	210	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 21.

All (210) 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: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:77:ASN:HD22	1:C:78:GLY:N	1.97	0.62
1:C:3:SER:OG	1:C:4:LEU:N	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:C:71:LEU:H	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:O3	4:C:301:TRS:O1	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:C:54:ASN:HB2	1:C:146:MET:HE3	1.86	0.56
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: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:B:115:PHE:O	1:B:119:SER:OG	2.25	0.54
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:C:142:SER:O	1:C:145:SER:OG	2.26	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:B:151:LEU:HA	1:B:154:MET:HE3	1.90	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:C:154:MET:HE1	1:C:206:MET:HB3	1.90	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:18:ILE:O	1:A:21:LEU:HB2	2.10	0.51
1:A:125:PHE:O	1:B:189:ARG:NH2	2.43	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:96:ASP:O	1:B:97:SER:OG	2.23	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:32:LYS:O	1:C:35:LEU:HB3	2.11	0.49
1:C:154:MET:CE	1:C:207:GLN:HG3	2.42	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: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:HD23	1:A:72:LEU:HA	1.66	0.47
1:B:211:TYR:O	1:B:215:SER:HB3	2.14	0.47
1:B:19:PHE:CD2	1:B:176:LEU:HB3	2.49	0.47
1:B:53:LEU:HD13	1:B:111:VAL:HG13	1.95	0.47
1:B:17:ASN:HD21	1:B:75:THR:HG1	1.55	0.47
1:A:27:PRO:HB2	1:A:87:TYR:CE1	2.49	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:H	1:A:133:GLN:HG2	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: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:HE21	1:A:128:GLN:HB2	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: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:154:MET:HE2	1:C:207:GLN:HG3	1.98	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:B:154:MET:HE1	1:B:203:LEU:HD22	1.98	0.45
1:C:98:ARG:HG2	1:C:102:MET:HE2	1.98	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: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:A:50:PHE:HB3	1:A:146:MET:HE1	1.99	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:A:211:TYR:C	1:A:211:TYR:CD2	2.95	0.44
1:C:3:SER:N	1:C:6:ASP:OD2	2.50	0.44
1:C:203:LEU:HA	1:C:206:MET:HE3	2.00	0.44
1:A:158:ILE:HD11	1:A:210:LEU:HD21	1.99	0.44
1:B:63:LEU:HA	1:B:64:PRO:HD3	1.87	0.44
1:B:121:ALA:O	1:B:125:PHE:HD2	2.00	0.44
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.73	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:C:140:MET:HE1	1:C:191:PHE:CE2	2.53	0.43
1:B:105:ILE:O	1:B:109:VAL:HG23	2.19	0.43
1:B:110:LEU:HD13	1:C:206:MET:HE1	2.00	0.43
1:C:174:THR:O	1:C:177:MET:HG2	2.19	0.43
1:B:101:ARG:O	1:B:105:ILE:HG12	2.17	0.43
1:C:147:PHE:C	1:C:150:PRO:HD2	2.43	0.43
1:C:157:VAL:HG21	1:C:166:MET:HE2	2.00	0.43
1:C:26:SER:N	1:C:27:PRO:HD2	2.34	0.43
1:C:179:ALA:O	1:C:183:LEU:HD13	2.18	0.43
1:A:213:TYR:N	1:A:213:TYR:CD1	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:HD13	1:B:176:LEU:HA	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:C:187:LEU:C	1:C:187:LEU:HD12	2.45	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:140:MET:HE3	1:C:195:PHE:HD2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H51	2:B:301:PE5:H71	1.84	0.41
1:A:17:ASN:OD1	1:A:75:THR:OG1	2.39	0.41
1:B:13:GLY:O	1:B:17:ASN:HB2	2.21	0.41
1:B:130:LEU:O	1:B:130:LEU:HD23	2.20	0.41
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:187:LEU:HD12	1:C:188:LEU:N	2.36	0.41
1:C:19:PHE:N	1:C:19:PHE:CD2	2.87	0.41
1:C:88:ILE:O	1:C:92:ILE:HG23	2.21	0.41
1:A:48:TYR:CD1	1:A:48:TYR:N	2.86	0.40
1:A:88:ILE:O	1:A:92:ILE:HG13	2.22	0.40
1:A:206:MET:O	1:A:210:LEU:HB2	2.20	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:C:54:ASN:CB	1:C:146:MET:HE3	2.52	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	144 (86%)	24 (14%)	3	14
1	B	173/187 (92%)	148 (86%)	25 (14%)	3	14
1	C	166/187 (89%)	141 (85%)	25 (15%)	3	13
All	All	507/561 (90%)	433 (85%)	74 (15%)	3	14

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	LEU
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	72	LEU
1	A	89	CYS
1	A	98	ARG
1	A	100	THR

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Mol	Chain	Res	Type
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	207	GLN
1	A	210	LEU
1	B	6	ASP
1	B	7	ILE
1	B	21	LEU
1	B	23	LEU
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	72	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	159	ARG
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	7	ILE
1	C	25	LEU
1	C	31	PHE
1	C	39	SER
1	C	63	LEU
1	C	70	ARG

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Mol	Chain	Res	Type
1	C	71	LEU
1	C	72	LEU
1	C	77	ASN
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	144	ILE
1	C	159	ARG
1	C	160	SER
1	C	170	LEU
1	C	177	MET
1	C	201	LEU
1	C	206	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	54	ASN
1	B	128	GLN
1	B	197	ASN
1	C	77	ASN
1	C	120	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry

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	0.36	0	9,9,9	0.64	0
3	BNG	A	302	-	21,21,21	1.04	1 (4%)	26,26,26	1.39	3 (11%)
2	PE5	A	301	-	23,23,26	0.83	1 (4%)	22,22,25	0.26	0
4	TRS	B	302	-	7,7,7	0.36	0	9,9,9	0.31	0
4	TRS	C	301	-	7,7,7	0.38	0	9,9,9	0.41	0
2	PE5	B	301	-	23,23,26	0.74	0	22,22,25	0.30	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
4	TRS	A	303	-	-	3/9/9/9	-
3	BNG	A	302	-	-	10/12/32/32	0/1/1/1
2	PE5	A	301	-	-	12/21/21/24	-
4	TRS	B	302	-	-	9/9/9/9	-
4	TRS	C	301	-	-	8/9/9/9	-
2	PE5	B	301	-	-	13/21/21/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	BNG	O5-C1	2.83	1.49	1.41
2	A	301	PE5	C8-C7	2.10	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	3.94	117.37	110.23
3	A	302	BNG	C4-C3-C2	2.91	115.94	110.83
3	A	302	BNG	O5-C5-C4	2.89	114.90	109.70

There are no chirality outliers.

All (55) torsion outliers are listed below:

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

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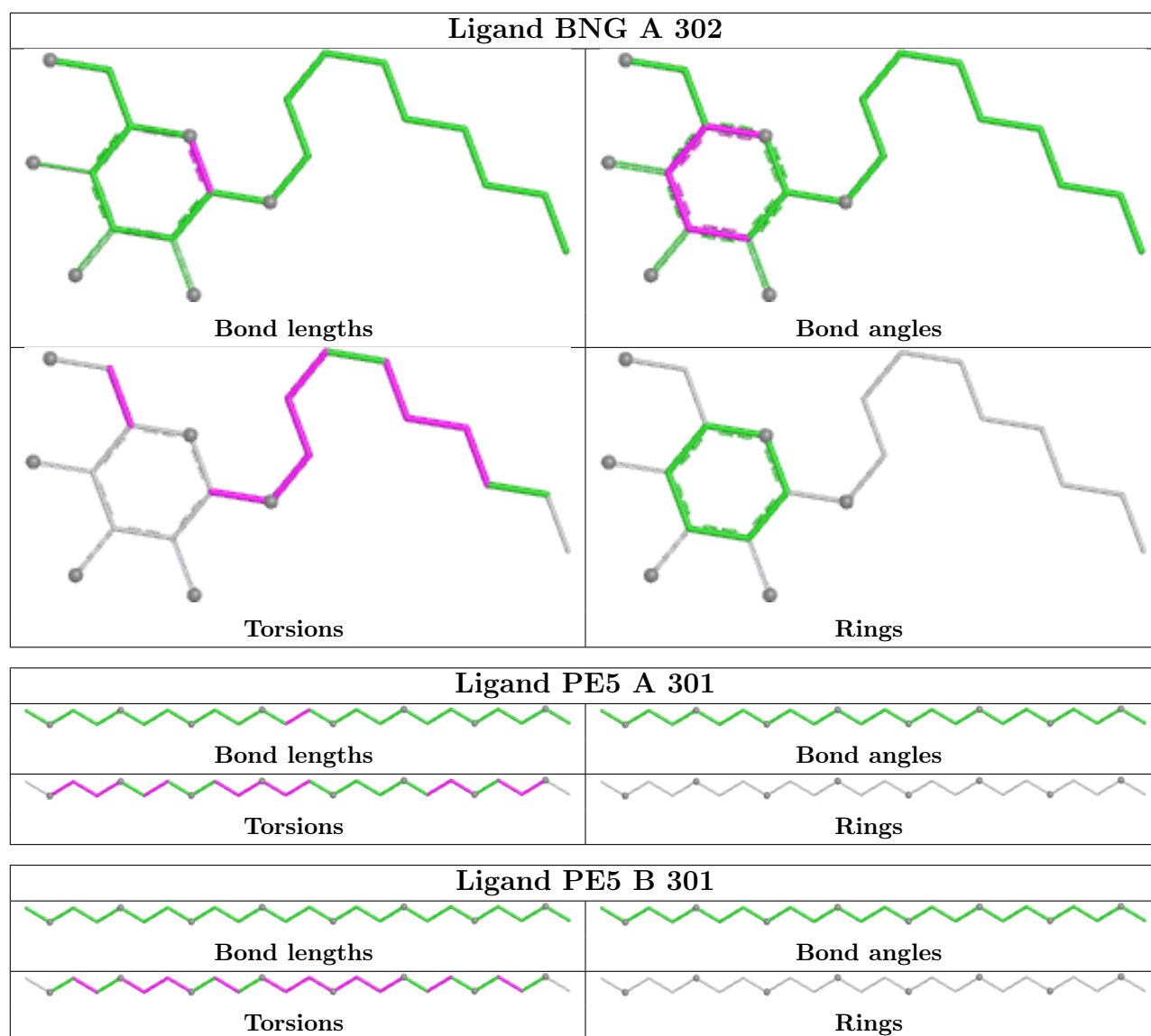
Mol	Chain	Res	Type	Atoms
2	A	301	PE5	O4-C7-C8-O5
2	A	301	PE5	C2-C1-O1-C50
2	B	301	PE5	C11-C12-O7-C13
2	A	301	PE5	C4-C3-O2-C2
2	B	301	PE5	C7-C8-O5-C9
2	A	301	PE5	C10-C9-O5-C8
4	B	302	TRS	C1-C-C3-O3
2	B	301	PE5	C8-C7-O4-C6
4	A	303	TRS	C1-C-C2-O2
4	B	302	TRS	N-C-C3-O3
4	C	301	TRS	C2-C-C1-O1
2	A	301	PE5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

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	BNG	1	0
4	C	301	TRS	3	0
2	B	301	PE5	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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%)	0.71	32 (14%) 5 3	27, 74, 131, 153	0
1	B	220/224 (98%)	0.96	35 (15%) 5 2	30, 72, 140, 161	0
1	C	215/224 (95%)	1.08	33 (15%) 5 3	76, 133, 200, 230	0
All	All	649/672 (96%)	0.92	100 (15%) 5 2	27, 89, 174, 230	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	SER	8.4
1	C	10	PHE	7.5
1	B	168	PHE	7.1
1	A	37	ALA	6.9
1	B	30	THR	6.7
1	C	90	LEU	6.4
1	B	25	LEU	6.3
1	B	113	CYS	6.2
1	B	167	PRO	5.8
1	B	21	LEU	5.1
1	C	93	PHE	4.9
1	C	89	CYS	4.7
1	B	5	TYR	4.7
1	A	164	GLU	4.6
1	C	165	PHE	4.6
1	A	161	GLU	4.5
1	A	213	TYR	4.5
1	C	41	GLU	4.3
1	C	212	ALA	4.3
1	B	197	ASN	4.3
1	C	124	PHE	4.2
1	A	2	ASP	4.1
1	C	187	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	4.0
1	A	35	LEU	3.9
1	A	90	LEU	3.9
1	C	92	ILE	3.8
1	A	93	PHE	3.8
1	C	120	HIS	3.8
1	B	164	GLU	3.7
1	A	172	LEU	3.7
1	A	212	ALA	3.6
1	C	7	ILE	3.6
1	C	184	TYR	3.5
1	B	178	SER	3.4
1	C	185	GLY	3.4
1	A	43	PHE	3.3
1	A	124	PHE	3.3
1	B	166	MET	3.3
1	C	44	ASP	3.2
1	C	55	CYS	3.2
1	A	162	SER	3.1
1	C	161	GLU	3.1
1	A	123	VAL	3.1
1	C	39	SER	3.0
1	C	30	THR	3.0
1	C	79	ILE	3.0
1	B	26	SER	2.9
1	B	128	GLN	2.9
1	B	177	MET	2.9
1	B	2	ASP	2.8
1	B	28	VAL	2.8
1	A	176	LEU	2.8
1	B	169	TYR	2.8
1	B	71	LEU	2.8
1	A	18	ILE	2.8
1	C	216	SER	2.7
1	C	43	PHE	2.7
1	B	54	ASN	2.7
1	B	220	GLU	2.6
1	A	39	SER	2.6
1	B	211	TYR	2.6
1	A	127	ASP	2.6
1	A	33	ARG	2.6
1	A	44	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	105	ILE	2.5
1	B	171	SER	2.5
1	C	69	GLY	2.5
1	B	163	VAL	2.5
1	A	34	ILE	2.5
1	A	28	VAL	2.5
1	A	168	PHE	2.5
1	A	30	THR	2.5
1	A	21	LEU	2.5
1	C	31	PHE	2.4
1	B	34	ILE	2.4
1	B	51	SER	2.4
1	B	187	LEU	2.4
1	B	29	THR	2.4
1	B	93	PHE	2.4
1	A	128	GLN	2.4
1	A	69	GLY	2.3
1	B	35	LEU	2.3
1	C	21	LEU	2.3
1	B	43	PHE	2.3
1	B	36	LYS	2.3
1	A	209	ALA	2.2
1	C	28	VAL	2.2
1	A	165	PHE	2.2
1	B	33	ARG	2.2
1	C	101	ARG	2.2
1	B	181	PHE	2.2
1	C	11	ALA	2.1
1	C	27	PRO	2.1
1	C	210	LEU	2.1
1	C	22	ALA	2.1
1	A	31	PHE	2.1
1	B	27	PRO	2.1
1	B	39	SER	2.0
1	A	210	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

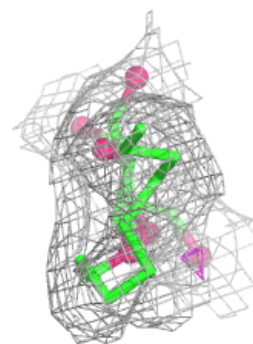
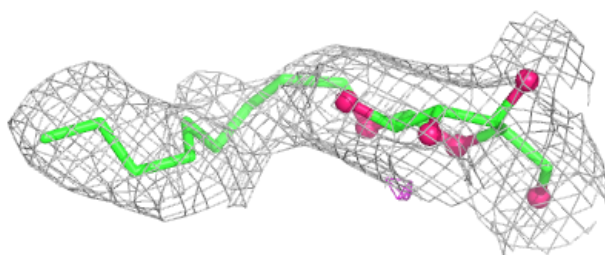
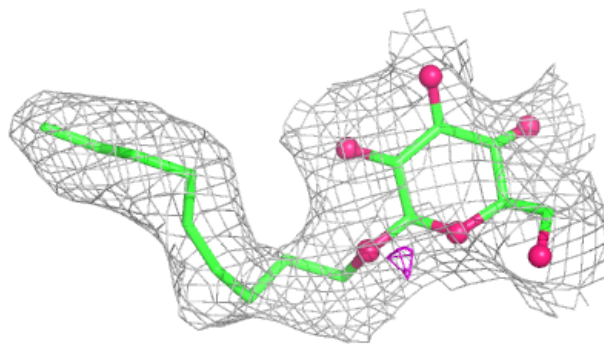
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BNG	A	302	21/21	0.56	0.16	63,106,117,121	0
4	TRS	A	303	8/8	0.74	0.22	86,107,117,117	0
4	TRS	C	301	8/8	0.76	0.18	104,141,143,145	0
4	TRS	B	302	8/8	0.82	0.31	100,123,130,141	0
2	PE5	A	301	24/27	0.82	0.24	86,93,110,115	0
2	PE5	B	301	24/27	0.89	0.20	56,76,89,94	0

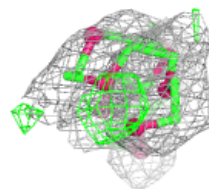
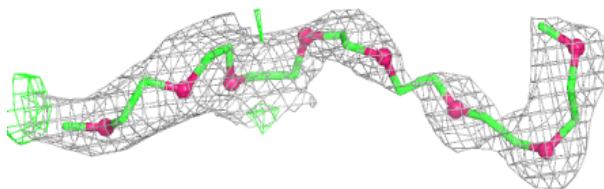
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

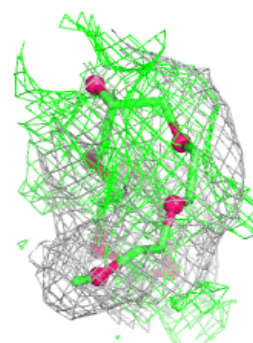
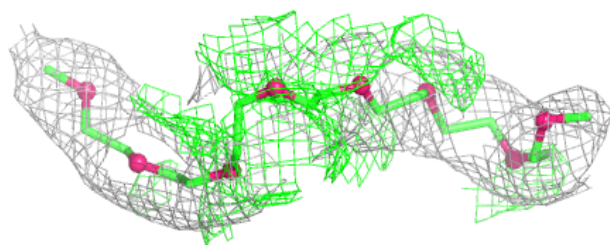
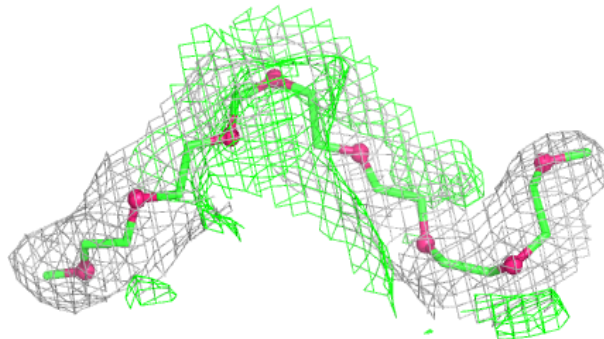
**Electron density around PE5 A 301:**

$2mF_o-DF_c$ (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.