



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 7WLS / pdb_00007wls
Title : Crystal structure of the multidrug efflux transporter BpeB from Burkholderia pseudomallei
Authors : Kato, T.; Hung, L.-W.; Yamashita, E.; Okada, U.; Terwilliger, T.C.; Murakami, S.
Deposited on : 2022-01-13
Resolution : 2.94 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

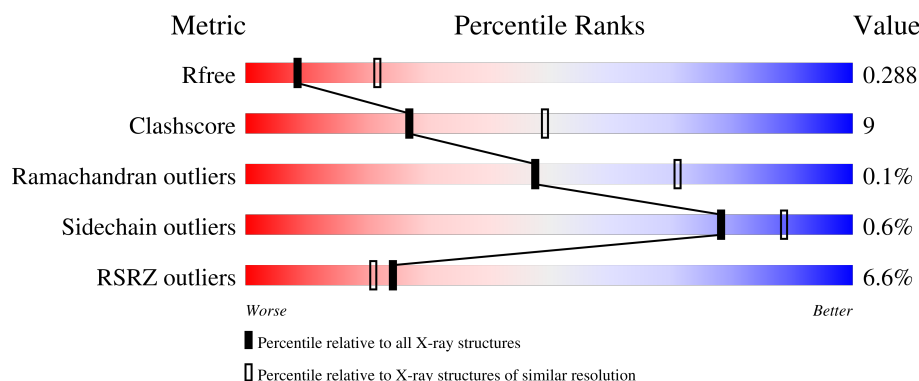
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	1051	6% 76% 21%
1	B	1051	7% 76% 21%
1	C	1051	6% 78% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23250 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			7703	4974	1272	1424	33			
1	B	1024	Total	C	N	O	S	0	0	0
			7744	5002	1278	1431	33			
1	C	1018	Total	C	N	O	S	0	0	0
			7688	4961	1270	1424	33			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q63WS7
A	?	-	HIS	deletion	UNP Q63WS7
A	?	-	GLU	deletion	UNP Q63WS7
A	?	-	HIS	deletion	UNP Q63WS7
A	?	-	MET	deletion	UNP Q63WS7
A	?	-	HIS	deletion	UNP Q63WS7
A	?	-	ARG	deletion	UNP Q63WS7
A	?	-	ASP	deletion	UNP Q63WS7
A	?	-	ASP	deletion	UNP Q63WS7
A	?	-	LYS	deletion	UNP Q63WS7
A	?	-	PRO	deletion	UNP Q63WS7
A	?	-	GLU	deletion	UNP Q63WS7
A	?	-	HIS	deletion	UNP Q63WS7
A	?	-	GLY	deletion	UNP Q63WS7
A	?	-	ASP	deletion	UNP Q63WS7
A	?	-	ASP	deletion	UNP Q63WS7
A	?	-	ALA	deletion	UNP Q63WS7
A	?	-	GLY	deletion	UNP Q63WS7
A	?	-	LYS	deletion	UNP Q63WS7
A	?	-	LYS	deletion	UNP Q63WS7
A	?	-	ASP	deletion	UNP Q63WS7
A	1046	HIS	-	expression tag	UNP Q63WS7
A	1047	HIS	-	expression tag	UNP Q63WS7

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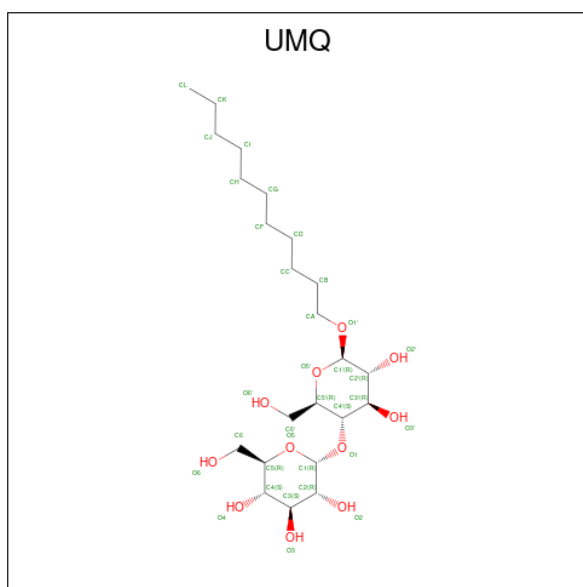
Chain	Residue	Modelled	Actual	Comment	Reference
A	1048	HIS	-	expression tag	UNP Q63WS7
A	1049	HIS	-	expression tag	UNP Q63WS7
A	1050	HIS	-	expression tag	UNP Q63WS7
A	1051	HIS	-	expression tag	UNP Q63WS7
B	?	-	ALA	deletion	UNP Q63WS7
B	?	-	HIS	deletion	UNP Q63WS7
B	?	-	GLU	deletion	UNP Q63WS7
B	?	-	HIS	deletion	UNP Q63WS7
B	?	-	MET	deletion	UNP Q63WS7
B	?	-	HIS	deletion	UNP Q63WS7
B	?	-	ARG	deletion	UNP Q63WS7
B	?	-	ASP	deletion	UNP Q63WS7
B	?	-	ASP	deletion	UNP Q63WS7
B	?	-	LYS	deletion	UNP Q63WS7
B	?	-	PRO	deletion	UNP Q63WS7
B	?	-	GLU	deletion	UNP Q63WS7
B	?	-	HIS	deletion	UNP Q63WS7
B	?	-	GLY	deletion	UNP Q63WS7
B	?	-	ASP	deletion	UNP Q63WS7
B	?	-	ASP	deletion	UNP Q63WS7
B	?	-	ALA	deletion	UNP Q63WS7
B	?	-	GLY	deletion	UNP Q63WS7
B	?	-	LYS	deletion	UNP Q63WS7
B	?	-	LYS	deletion	UNP Q63WS7
B	?	-	ASP	deletion	UNP Q63WS7
B	1046	HIS	-	expression tag	UNP Q63WS7
B	1047	HIS	-	expression tag	UNP Q63WS7
B	1048	HIS	-	expression tag	UNP Q63WS7
B	1049	HIS	-	expression tag	UNP Q63WS7
B	1050	HIS	-	expression tag	UNP Q63WS7
B	1051	HIS	-	expression tag	UNP Q63WS7
C	?	-	ALA	deletion	UNP Q63WS7
C	?	-	HIS	deletion	UNP Q63WS7
C	?	-	GLU	deletion	UNP Q63WS7
C	?	-	HIS	deletion	UNP Q63WS7
C	?	-	MET	deletion	UNP Q63WS7
C	?	-	HIS	deletion	UNP Q63WS7
C	?	-	ARG	deletion	UNP Q63WS7
C	?	-	ASP	deletion	UNP Q63WS7
C	?	-	ASP	deletion	UNP Q63WS7
C	?	-	LYS	deletion	UNP Q63WS7
C	?	-	PRO	deletion	UNP Q63WS7

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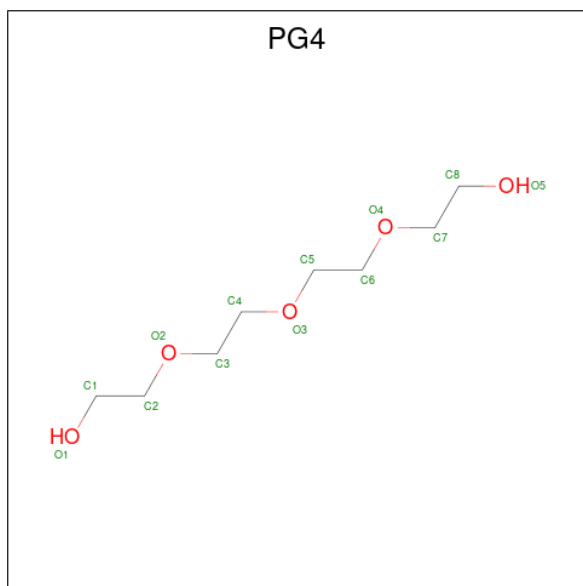
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q63WS7
C	?	-	HIS	deletion	UNP Q63WS7
C	?	-	GLY	deletion	UNP Q63WS7
C	?	-	ASP	deletion	UNP Q63WS7
C	?	-	ASP	deletion	UNP Q63WS7
C	?	-	ALA	deletion	UNP Q63WS7
C	?	-	GLY	deletion	UNP Q63WS7
C	?	-	LYS	deletion	UNP Q63WS7
C	?	-	LYS	deletion	UNP Q63WS7
C	?	-	ASP	deletion	UNP Q63WS7
C	1046	HIS	-	expression tag	UNP Q63WS7
C	1047	HIS	-	expression tag	UNP Q63WS7
C	1048	HIS	-	expression tag	UNP Q63WS7
C	1049	HIS	-	expression tag	UNP Q63WS7
C	1050	HIS	-	expression tag	UNP Q63WS7
C	1051	HIS	-	expression tag	UNP Q63WS7

- Molecule 2 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			34	23	11		
2	B	1	Total	C	O	0	0
			34	23	11		
2	B	1	Total	C	O	0	0
			34	23	11		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

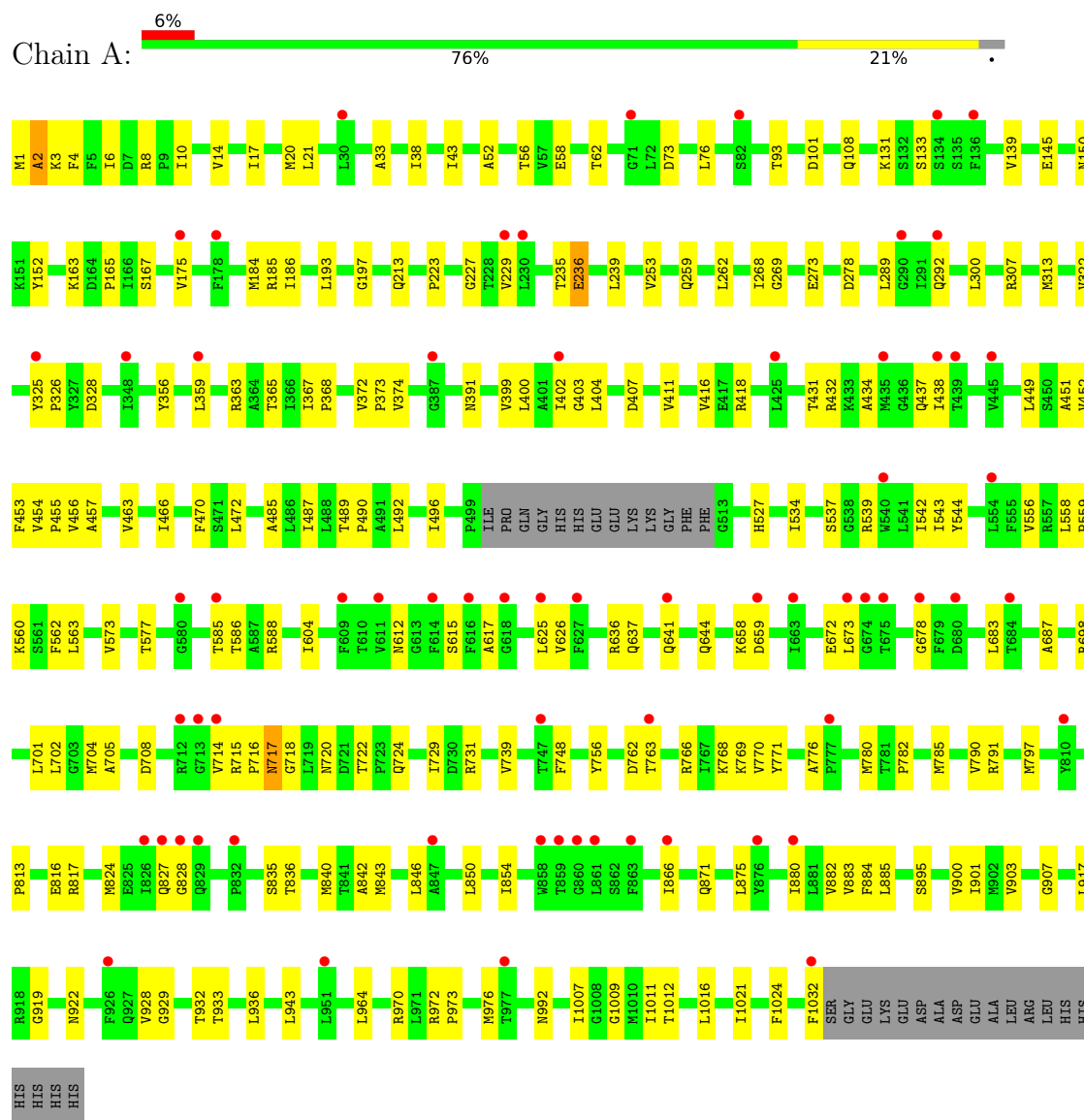


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	8	5		

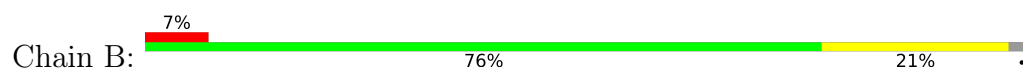
3 Residue-property plots

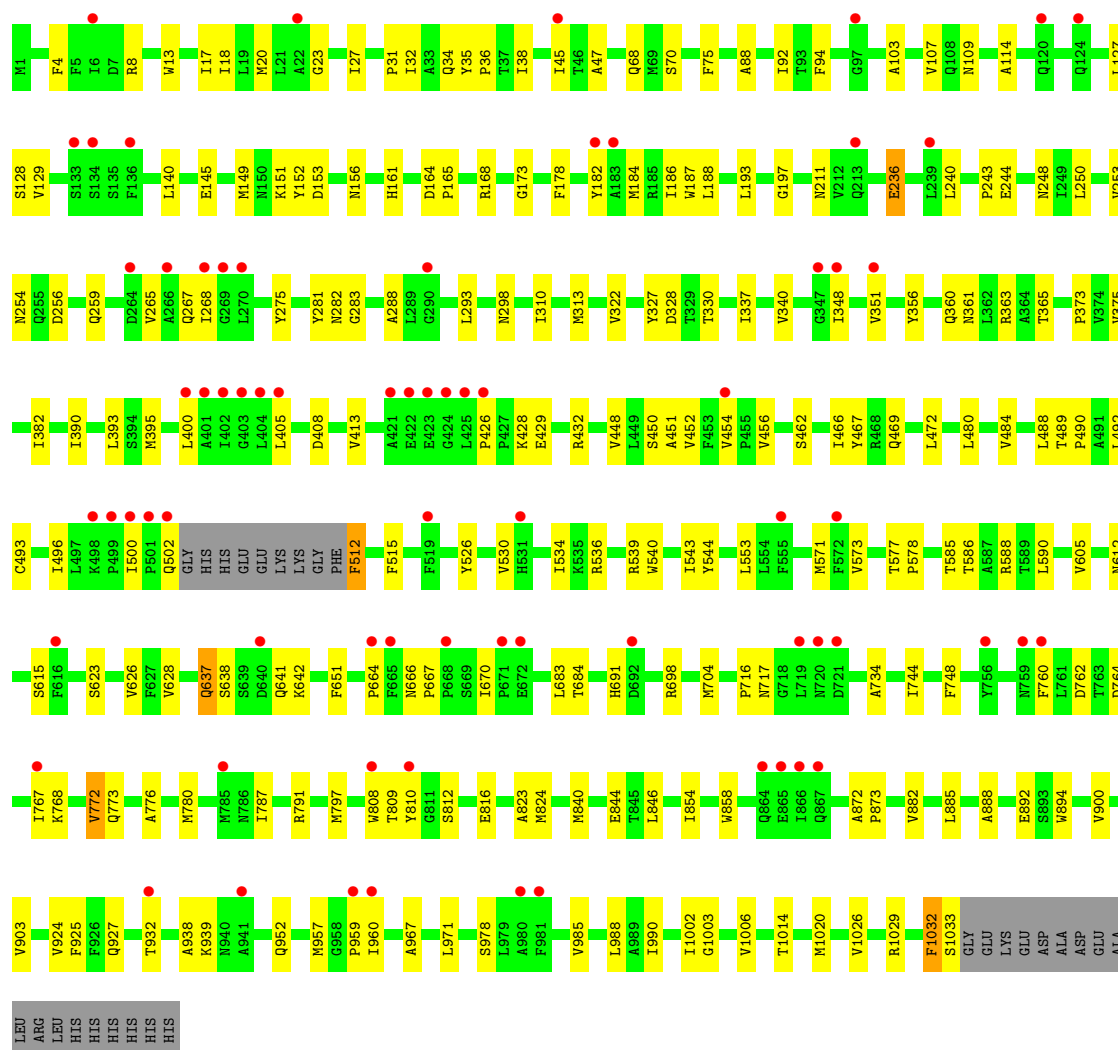
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

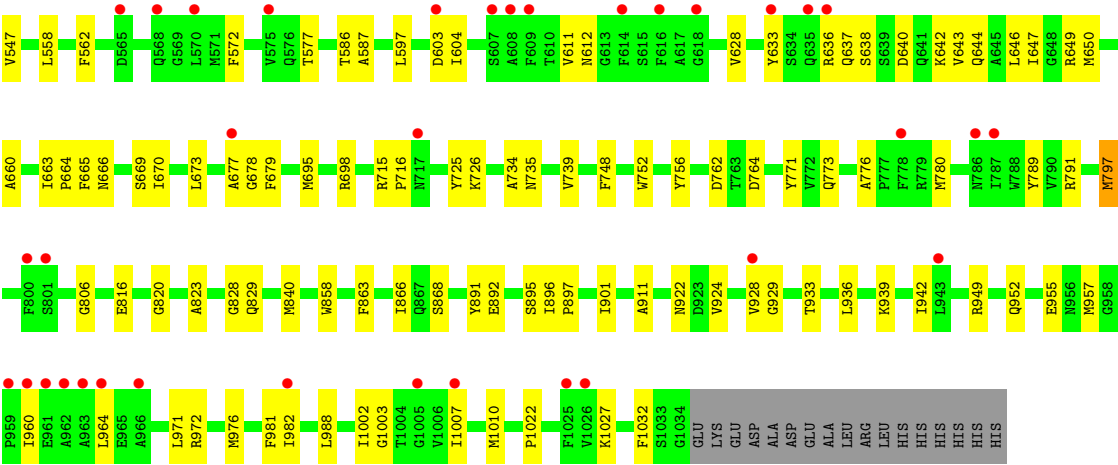
- Molecule 1: Efflux pump membrane transporter



- Molecule 1: Efflux pump membrane transporter







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.88Å 135.98Å 157.82Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	48.80 – 2.94 48.80 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.80-2.94) 99.6 (48.80-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20rc1_4387	Depositor
R, R_{free}	0.230 , 0.284 0.234 , 0.288	Depositor DCC
R_{free} test set	4615 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23250	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, UMQ

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	0/7857	0.74	2/10701 (0.0%)
1	B	0.51	0/7900	0.77	3/10760 (0.0%)
1	C	0.45	0/7839	0.71	1/10674 (0.0%)
All	All	0.48	0/23596	0.74	6/32135 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	GLU	CA-CB-CG	6.85	127.81	114.10
1	B	236	GLU	CB-CA-C	-6.84	96.81	110.42
1	A	235	THR	CA-C-N	-5.80	110.47	121.54
1	A	235	THR	C-N-CA	-5.80	110.47	121.54
1	B	236	GLU	CB-CG-CD	-5.44	103.35	112.60
1	C	797	MET	CB-CG-SD	5.24	128.42	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	GLU	Mainchain

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	7703	0	7890	153	0
1	B	7744	0	7930	163	0
1	C	7688	0	7878	144	0
2	B	102	0	132	5	0
3	B	13	0	18	1	0
All	All	23250	0	23848	435	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 (435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HG22	1:C:213:GLN:HE21	1.13	1.10
1:A:702:LEU:HD11	1:A:716:PRO:HB3	1.37	1.02
1:C:640:ASP:O	1:C:649:ARG:NH1	1.92	1.01
1:C:678:GLY:HA3	1:C:828:GLY:O	1.70	0.90
1:A:717:ASN:ND2	1:A:816:GLU:OE2	2.10	0.85
1:B:32:ILE:HG12	1:B:298:ASN:HB2	1.60	0.81
1:B:254:ASN:ND2	1:B:256:ASP:OD2	2.13	0.81
1:A:56:THR:HG22	1:C:213:GLN:NE2	1.93	0.80
1:A:637:GLN:OE1	1:A:992:ASN:ND2	2.15	0.79
1:B:197:GLY:O	1:B:791:ARG:NH2	2.16	0.79
1:B:164:ASP:OD1	1:B:168:ARG:NH1	2.16	0.79
1:C:403:GLY:HA3	1:C:981:PHE:HA	1.65	0.78
1:C:463:VAL:HG21	1:C:868:SER:HB2	1.66	0.78
1:C:390:ILE:HG23	1:C:395:MET:HE3	1.65	0.77
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.66	0.76
1:C:307:ARG:NH1	1:C:328:ASP:OD2	2.18	0.75
1:C:13:TRP:HH2	1:C:370:ILE:HD11	1.51	0.75
1:B:281:TYR:O	1:B:283:GLY:N	2.21	0.74
1:C:309:LYS:HG3	1:C:313:MET:HE3	1.70	0.73
1:B:978:SER:OG	1:B:1014:THR:HG21	1.89	0.72
1:A:884:PHE:HB2	1:A:901:ILE:HD11	1.70	0.72
1:A:356:TYR:HA	1:A:365:THR:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:TYR:HB2	2:B:1101:UMQ:HI2	1.72	0.71
1:C:663:ILE:HD12	1:C:715:ARG:HD3	1.73	0.70
1:A:133:SER:O	1:A:292:GLN:NE2	2.24	0.70
1:B:408:ASP:OD1	1:B:939:LYS:NZ	2.18	0.69
1:A:704:MET:HB3	1:A:846:LEU:HD22	1.74	0.69
1:B:467:TYR:OH	1:B:927:GLN:OE1	2.13	0.66
1:B:153:ASP:OD1	1:B:182:TYR:OH	2.11	0.66
1:B:236:GLU:O	1:C:726:LYS:NZ	2.23	0.65
1:B:590:LEU:CD1	1:B:612:ASN:HB3	2.27	0.65
1:C:734:ALA:HB1	1:C:739:VAL:HG23	1.79	0.65
1:C:404:LEU:HD11	1:C:936:LEU:HD21	1.77	0.65
1:A:101:ASP:OD1	1:A:131:LYS:NZ	2.30	0.64
1:B:590:LEU:HD12	1:B:612:ASN:HB3	1.80	0.63
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.32	0.63
1:A:20:MET:HE3	1:A:374:VAL:HG22	1.79	0.63
1:A:404:LEU:HD13	1:A:449:LEU:HD11	1.81	0.63
1:A:972:ARG:HB3	1:A:973:PRO:HD3	1.82	0.62
1:B:959:PRO:HG3	2:B:1102:UMQ:HK1	1.81	0.62
1:B:47:ALA:HB3	1:B:88:ALA:HB3	1.82	0.62
1:A:715:ARG:NH2	1:A:827:GLN:OE1	2.32	0.62
1:B:32:ILE:H	1:B:298:ASN:HA	1.64	0.61
1:B:236:GLU:OE2	1:C:748:PHE:HB3	1.99	0.61
1:B:253:VAL:HG22	1:B:259:GLN:HG2	1.82	0.61
1:C:13:TRP:CH2	1:C:370:ILE:HD11	2.35	0.61
1:C:30:LEU:HD21	1:C:384:SER:HB2	1.82	0.61
1:C:466:ILE:HG21	1:C:924:VAL:HG11	1.82	0.61
1:B:340:VAL:HG11	1:B:395:MET:SD	2.40	0.60
1:C:597:LEU:HD13	1:C:628:VAL:HG11	1.83	0.60
1:A:577:THR:HG21	1:A:586:THR:HA	1.83	0.60
1:B:250:LEU:HD13	1:C:735:ASN:HB2	1.83	0.60
1:A:108:GLN:HE21	1:B:109:ASN:HB3	1.67	0.60
1:A:453:PHE:HZ	1:A:932:THR:HG22	1.67	0.59
1:B:990:ILE:O	1:B:990:ILE:HG13	2.03	0.59
1:A:1012:THR:HB	1:A:1016:LEU:HD12	1.85	0.59
1:B:188:LEU:HD13	1:B:193:LEU:HD11	1.85	0.58
1:C:277:PHE:HA	1:C:612:ASN:O	2.03	0.58
1:B:32:ILE:CD1	1:B:390:ILE:HB	2.34	0.58
1:A:636:ARG:HB2	1:A:641:GLN:HB3	1.85	0.58
1:B:426:PRO:HG2	1:B:429:GLU:OE1	2.04	0.58
1:A:456:VAL:HG12	1:A:875:LEU:HD13	1.86	0.57
1:C:642:LYS:O	1:C:646:LEU:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HD13	1:A:131:LYS:HB3	1.86	0.57
1:A:56:THR:CG2	1:C:213:GLN:HE21	2.04	0.57
1:A:558:LEU:HD23	1:A:922:ASN:HB2	1.85	0.57
1:C:188:LEU:HD21	1:C:203:VAL:HG11	1.85	0.57
1:C:379:THR:HG21	1:C:398:LEU:HD21	1.86	0.57
1:A:992:ASN:N	1:A:992:ASN:OD1	2.36	0.57
1:B:168:ARG:NH2	1:C:66:GLU:HB3	2.19	0.57
1:B:348:ILE:HD13	1:B:373:PRO:HG3	1.87	0.57
1:C:279:THR:HG22	1:C:611:VAL:HG12	1.87	0.57
1:B:585:THR:HA	1:B:588:ARG:HH21	1.69	0.57
1:B:1032:PHE:O	1:B:1033:SER:OG	2.20	0.56
1:C:3:LYS:NZ	1:C:436:GLY:HA2	2.20	0.56
1:A:451:ALA:HB1	1:A:882:VAL:HG12	1.88	0.56
1:A:213:GLN:HE21	1:A:239:LEU:H	1.53	0.56
1:C:756:TYR:HB2	1:C:771:TYR:CE1	2.40	0.55
1:C:165:PRO:HG2	1:C:313:MET:HE1	1.89	0.55
1:A:10:ILE:HD12	1:B:894:TRP:NE1	2.21	0.55
1:B:456:VAL:HG12	1:B:467:TYR:HB3	1.89	0.55
1:A:698:ARG:HH22	1:A:720:ASN:HB3	1.70	0.55
1:A:782:PRO:O	1:A:785:MET:HG2	2.06	0.55
1:B:925:PHE:HB3	1:B:1002:ILE:HG22	1.88	0.55
1:A:929:GLY:O	1:A:933:THR:HG23	2.07	0.55
1:B:348:ILE:CD1	1:B:373:PRO:HG3	2.37	0.55
1:B:762:ASP:HB3	1:B:764:ASP:OD1	2.07	0.55
1:B:164:ASP:HB3	1:B:165:PRO:HD3	1.89	0.55
1:A:973:PRO:HA	1:A:976:MET:HB3	1.89	0.55
1:C:399:VAL:HG11	1:C:988:LEU:HD13	1.89	0.55
1:C:929:GLY:O	1:C:933:THR:HG23	2.06	0.55
1:B:32:ILE:CG1	1:B:298:ASN:HB2	2.35	0.54
1:C:725:TYR:OH	1:C:806:GLY:HA3	2.07	0.54
1:A:93:THR:OG1	1:A:673:LEU:HD11	2.07	0.54
1:B:363:ARG:HD3	1:B:496:ILE:O	2.08	0.54
1:A:133:SER:HB2	1:A:672:GLU:HA	1.89	0.54
1:B:267:GLN:C	1:B:268:ILE:HD13	2.32	0.54
1:C:399:VAL:HG11	1:C:988:LEU:CD1	2.37	0.54
1:C:752:TRP:O	1:C:773:GLN:NE2	2.39	0.54
1:A:418:ARG:NH2	1:A:437:GLN:OE1	2.40	0.54
1:B:840:MET:O	1:B:844:GLU:HG3	2.08	0.54
1:C:450:SER:HB2	1:C:475:VAL:HG13	1.89	0.53
1:B:361:ASN:O	1:B:365:THR:HG23	2.08	0.53
1:B:450:SER:O	1:B:454:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HB3	1:B:932:THR:HG21	1.90	0.53
1:C:637:GLN:HB2	1:C:642:LYS:NZ	2.24	0.53
1:C:1003:GLY:O	1:C:1007:ILE:HG12	2.09	0.53
1:B:145:GLU:OE2	1:B:322:VAL:HG11	2.08	0.53
1:A:399:VAL:O	1:A:402:ILE:HG12	2.09	0.53
1:B:691:HIS:CE1	1:B:812:SER:HB2	2.44	0.53
1:B:637:GLN:O	1:B:641:GLN:NE2	2.42	0.53
1:C:188:LEU:HD23	1:C:266:ALA:HB2	1.90	0.53
1:B:356:TYR:O	1:B:360:GLN:N	2.37	0.53
1:C:895:SER:HB3	1:C:1032:PHE:CD2	2.44	0.53
1:B:31:PRO:O	1:B:32:ILE:HD13	2.09	0.52
1:B:526:TYR:CD2	1:B:971:LEU:HD22	2.44	0.52
1:A:884:PHE:CD1	1:A:901:ILE:HD11	2.44	0.52
1:B:173:GLY:O	1:C:70:SER:OG	2.17	0.52
1:A:756:TYR:HB2	1:A:771:TYR:CE2	2.44	0.52
1:B:35:TYR:CD1	1:B:670:ILE:HD11	2.44	0.52
1:B:573:VAL:HB	1:B:626:VAL:HB	1.91	0.52
1:B:577:THR:HG21	1:B:586:THR:HG22	1.91	0.52
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.91	0.52
1:C:519:PHE:HZ	1:C:972:ARG:HG3	1.75	0.52
1:A:724:GLN:HB2	1:C:233:THR:O	2.10	0.52
1:C:558:LEU:HD23	1:C:922:ASN:HB2	1.92	0.52
1:C:695:MET:SD	1:C:698:ARG:NH2	2.83	0.52
1:A:150:ASN:OD1	1:A:152:TYR:N	2.43	0.52
1:A:573:VAL:HB	1:A:626:VAL:HB	1.92	0.52
1:A:756:TYR:CE1	1:A:769:LYS:HD3	2.44	0.52
1:A:716:PRO:O	1:A:718:GLY:N	2.42	0.52
1:B:816:GLU:OE1	1:B:824:MET:HA	2.09	0.52
1:A:236:GLU:HB2	1:B:748:PHE:CE2	2.45	0.51
1:C:955:GLU:O	1:C:957:MET:HG3	2.10	0.51
1:B:571:MET:HE2	1:B:628:VAL:HG11	1.92	0.51
1:C:698:ARG:NH1	1:C:716:PRO:HG3	2.24	0.51
1:C:464:GLY:HA2	1:C:467:TYR:HB2	1.92	0.51
1:A:416:VAL:HG22	1:A:431:THR:HA	1.93	0.51
1:A:907:GLY:O	1:A:1009:GLY:HA2	2.11	0.51
1:C:40:PRO:HD2	1:C:673:LEU:HD13	1.92	0.51
1:B:348:ILE:O	1:B:351:VAL:HG12	2.10	0.51
1:C:463:VAL:HG22	1:C:562:PHE:CE1	2.45	0.51
1:C:463:VAL:HG22	1:C:562:PHE:HE1	1.75	0.51
1:A:560:LYS:HG2	1:A:922:ASN:HB3	1.93	0.51
1:B:526:TYR:O	1:B:530:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:VAL:HG21	1:B:1006:VAL:CG2	2.41	0.51
1:B:38:ILE:HG22	1:B:462:SER:HB3	1.92	0.51
1:A:184:MET:HB3	1:A:770:VAL:HG22	1.92	0.51
1:C:463:VAL:HG21	1:C:868:SER:CB	2.39	0.51
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.45	0.51
1:A:4:PHE:O	1:A:8:ARG:HD2	2.10	0.50
1:C:638:SER:H	1:C:642:LYS:HE2	1.76	0.50
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.94	0.50
1:A:903:VAL:HB	1:A:1021:ILE:HD11	1.93	0.50
1:B:68:GLN:HG3	1:B:114:ALA:CB	2.41	0.50
1:C:891:TYR:OH	1:C:942:ILE:HD11	2.11	0.50
1:A:1:MET:HE3	1:A:487:ILE:HG13	1.93	0.50
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.28	0.50
1:C:218:GLN:CB	1:C:233:THR:HA	2.42	0.50
1:A:705:ALA:HB1	1:A:714:VAL:HG21	1.93	0.50
1:C:26:ALA:HB1	1:C:384:SER:HB2	1.94	0.50
1:C:636:ARG:NH1	1:C:643:VAL:HG23	2.27	0.50
1:A:816:GLU:OE1	1:A:824:MET:HA	2.12	0.50
1:A:253:VAL:HG22	1:A:259:GLN:HG2	1.93	0.49
1:A:17:ILE:O	1:A:21:LEU:HB2	2.12	0.49
1:A:404:LEU:HD21	1:A:936:LEU:CD2	2.42	0.49
1:C:36:PRO:O	1:C:38:ILE:HG23	2.12	0.49
1:A:729:ILE:HD11	1:A:731:ARG:HE	1.76	0.49
1:B:17:ILE:HA	1:B:20:MET:HE3	1.95	0.49
1:B:13:TRP:HD1	1:B:488:LEU:HD11	1.77	0.49
1:B:534:ILE:HG23	1:B:1026:VAL:HG21	1.95	0.49
1:B:168:ARG:CZ	1:C:820:GLY:HA3	2.42	0.49
1:B:704:MET:HB3	1:B:846:LEU:HD22	1.93	0.49
1:C:543:ILE:O	1:C:547:VAL:HG23	2.13	0.49
1:B:32:ILE:HD12	1:B:390:ILE:HB	1.95	0.49
1:C:776:ALA:O	1:C:780:MET:HG2	2.12	0.49
1:A:52:ALA:HB1	1:A:56:THR:OG1	2.12	0.49
1:B:577:THR:HB	1:B:578:PRO:HD2	1.95	0.49
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.95	0.49
1:C:897:PRO:O	1:C:901:ILE:HG12	2.13	0.49
1:C:53:SER:O	1:C:57:VAL:HG23	2.13	0.48
1:C:194:THR:HA	1:C:797:MET:HE2	1.95	0.48
1:A:762:ASP:OD1	1:A:763:THR:N	2.45	0.48
1:C:577:THR:HG22	1:C:660:ALA:HB2	1.95	0.48
1:C:840:MET:HG2	1:C:858:TRP:CZ3	2.48	0.48
1:C:604:ILE:HG22	1:C:636:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLN:CG	1:A:239:LEU:HG	2.43	0.48
1:C:789:TYR:HB3	1:C:797:MET:HE3	1.95	0.48
1:A:108:GLN:NE2	1:B:109:ASN:HB3	2.29	0.48
1:B:184:MET:HE1	1:B:243:PRO:HG3	1.95	0.48
1:C:309:LYS:CG	1:C:313:MET:HE3	2.42	0.48
1:C:457:ALA:O	1:C:468:ARG:NH1	2.39	0.48
1:A:14:VAL:HG13	1:B:885:LEU:HB3	1.95	0.48
1:A:33:ALA:O	1:A:391:ASN:HA	2.14	0.48
1:A:527:HIS:CE1	1:A:964:LEU:HB3	2.49	0.48
1:B:13:TRP:CD1	1:B:488:LEU:HD11	2.49	0.48
1:B:186:ILE:HG23	1:B:268:ILE:HD12	1.95	0.48
1:B:390:ILE:HG23	1:B:395:MET:HE3	1.95	0.48
1:A:400:LEU:HD23	1:A:932:THR:HG21	1.95	0.47
1:B:413:VAL:HG22	1:B:493:CYS:SG	2.54	0.47
1:A:4:PHE:CE1	1:A:8:ARG:CZ	2.97	0.47
1:A:617:ALA:HB1	1:A:718:GLY:HA2	1.96	0.47
1:C:307:ARG:HG2	1:C:325:TYR:CE2	2.50	0.47
1:A:836:THR:O	1:A:840:MET:HG3	2.14	0.47
1:A:932:THR:O	1:A:936:LEU:HG	2.14	0.47
1:B:544:TYR:HB2	1:B:1020:MET:HE1	1.96	0.47
1:C:419:VAL:HG13	1:C:430:ALA:HB1	1.95	0.47
1:B:34:GLN:HG2	1:B:35:TYR:CE2	2.49	0.47
1:C:638:SER:O	1:C:642:LYS:HE2	2.14	0.47
1:A:544:TYR:CD1	1:A:1024:PHE:HZ	2.33	0.47
1:B:451:ALA:HB1	1:B:882:VAL:HG23	1.96	0.47
1:B:900:VAL:O	1:B:903:VAL:HG12	2.15	0.47
1:B:985:VAL:HG21	1:B:1006:VAL:HG23	1.96	0.47
1:B:45:ILE:HG13	1:B:129:VAL:HG22	1.97	0.47
1:C:470:PHE:CD2	1:C:928:VAL:HG11	2.49	0.47
1:A:658:LYS:O	1:A:659:ASP:HB2	2.15	0.47
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.97	0.47
1:B:683:LEU:O	1:B:823:ALA:HA	2.15	0.47
1:C:491:ALA:O	1:C:495:THR:HG22	2.15	0.47
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.96	0.46
1:A:273:GLU:OE2	1:A:769:LYS:HG3	2.15	0.46
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.80	0.46
1:B:13:TRP:HE1	1:B:492:LEU:HD21	1.79	0.46
1:A:739:VAL:HG11	1:A:790:VAL:CG2	2.44	0.46
1:C:76:LEU:HD11	1:C:863:PHE:HE2	1.79	0.46
1:C:251:LEU:HD21	1:C:265:VAL:HG11	1.98	0.46
1:B:791:ARG:HB3	1:B:797:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:HG23	1:B:268:ILE:CD1	2.45	0.46
1:B:637:GLN:O	1:B:641:GLN:HB2	2.15	0.46
1:C:12:ALA:HB1	1:C:488:LEU:HA	1.98	0.46
1:A:559:PRO:HB2	1:A:835:SER:HB3	1.98	0.46
1:A:748:PHE:HZ	1:C:234:ILE:HG21	1.80	0.46
1:C:530:VAL:HG11	1:C:1022:PRO:HG2	1.97	0.46
1:A:485:ALA:HA	1:A:489:THR:HG1	1.80	0.46
1:B:45:ILE:HA	1:B:128:SER:O	2.16	0.46
1:B:68:GLN:HG3	1:B:114:ALA:HB2	1.98	0.46
1:B:536:ARG:NH2	1:B:539:ARG:HG2	2.31	0.46
1:C:37:THR:HG21	1:C:296:ASN:HA	1.98	0.46
1:A:363:ARG:HB3	1:A:496:ILE:HG22	1.98	0.46
1:A:895:SER:HB3	1:A:1032:PHE:CD2	2.51	0.46
1:C:647:ILE:HG23	1:C:664:PRO:HG2	1.97	0.46
1:C:1010:MET:HE3	1:C:1010:MET:HA	1.98	0.46
1:A:840:MET:HE2	1:A:866:ILE:HD11	1.97	0.45
1:C:38:ILE:HD11	1:C:670:ILE:CD1	2.45	0.45
1:A:139:VAL:O	1:A:326:PRO:HD2	2.16	0.45
1:A:186:ILE:HG12	1:A:268:ILE:HD12	1.97	0.45
1:C:218:GLN:HB2	1:C:233:THR:HA	1.97	0.45
1:C:577:THR:CG2	1:C:586:THR:HG22	2.47	0.45
1:A:701:LEU:HB2	1:A:850:LEU:HD11	1.99	0.45
1:C:355:MET:SD	1:C:368:PRO:HB2	2.56	0.45
1:C:603:ASP:OD1	1:C:603:ASP:N	2.49	0.45
1:A:3:LYS:HA	1:A:6:ILE:HD12	1.97	0.45
1:B:382:ILE:HD12	1:B:480:LEU:HD12	1.97	0.45
1:C:298:ASN:OD1	1:C:301:ALA:HB3	2.17	0.45
1:A:885:LEU:HB3	1:C:14:VAL:HG13	1.98	0.45
1:B:615:SER:HB3	1:B:623:SER:OG	2.17	0.45
1:C:46:THR:OG1	1:C:128:SER:OG	2.34	0.45
1:A:678:GLY:HA3	1:A:828:GLY:O	2.16	0.45
1:A:708:ASP:OD2	1:A:842:ALA:HB1	2.17	0.45
1:A:729:ILE:O	1:A:729:ILE:HG13	2.17	0.45
1:B:448:VAL:O	1:B:452:VAL:HG23	2.15	0.45
1:C:530:VAL:CG1	1:C:1022:PRO:HG2	2.46	0.45
1:C:526:TYR:CD2	1:C:971:LEU:HD22	2.52	0.45
1:B:451:ALA:CB	1:B:882:VAL:HG23	2.46	0.45
1:B:456:VAL:CG1	1:B:467:TYR:HB3	2.46	0.45
1:B:888:ALA:O	1:B:892:GLU:N	2.50	0.45
1:B:952:GLN:HG3	1:B:957:MET:O	2.16	0.45
1:A:900:VAL:O	1:A:903:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLY:HA2	1:A:797:MET:SD	2.57	0.44
1:A:717:ASN:CG	1:A:718:GLY:N	2.71	0.44
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.16	0.44
1:C:367:ILE:O	1:C:370:ILE:HG22	2.16	0.44
1:A:943:LEU:O	1:A:970:ARG:HD2	2.17	0.44
1:B:466:ILE:HG21	1:B:924:VAL:HG21	1.99	0.44
1:B:540:TRP:HA	1:B:543:ILE:HB	2.00	0.44
1:B:809:THR:OG1	1:B:810:TYR:N	2.50	0.44
1:B:140:LEU:HD21	1:B:310:ILE:HG13	1.99	0.44
1:C:468:ARG:HA	1:C:471:SER:HB3	1.99	0.44
1:A:307:ARG:HG3	1:A:325:TYR:OH	2.18	0.44
1:A:698:ARG:HD2	1:A:702:LEU:HG	1.99	0.44
1:B:75:PHE:CE1	1:B:92:ILE:HG23	2.53	0.44
1:B:244:GLU:O	1:B:248:ASN:ND2	2.36	0.44
1:B:666:ASN:OD1	1:B:667:PRO:HD2	2.18	0.44
1:B:988:LEU:HD13	1:B:1002:ILE:HD11	2.00	0.44
1:A:453:PHE:CZ	1:A:932:THR:HG22	2.49	0.44
1:B:186:ILE:HG13	1:B:772:VAL:HG12	2.00	0.44
1:C:587:ALA:HB2	1:C:612:ASN:ND2	2.33	0.44
1:A:145:GLU:CD	1:A:322:VAL:HG21	2.43	0.44
1:A:359:LEU:HD22	1:A:976:MET:HE1	2.00	0.44
1:A:457:ALA:HB2	1:A:472:LEU:HD21	2.00	0.44
1:B:211:ASN:OD1	1:B:240:LEU:N	2.46	0.44
1:B:250:LEU:HD13	1:C:735:ASN:CB	2.48	0.44
1:B:1002:ILE:HG13	1:B:1003:GLY:N	2.33	0.43
1:C:666:ASN:HB3	1:C:677:ALA:HB2	2.00	0.43
1:B:8:ARG:HB2	1:C:892:GLU:OE2	2.19	0.43
1:C:393:LEU:HD13	1:C:466:ILE:HG23	2.00	0.43
1:C:541:LEU:HA	1:C:541:LEU:HD23	1.76	0.43
1:C:982:ILE:HG13	1:C:1010:MET:HG2	2.00	0.43
1:A:108:GLN:HG2	1:B:109:ASN:CG	2.43	0.43
1:A:167:SER:O	1:B:70:SER:HB2	2.18	0.43
1:A:489:THR:OG1	1:A:490:PRO:HD3	2.18	0.43
1:A:539:ARG:O	1:A:542:ILE:HB	2.19	0.43
1:A:791:ARG:HB3	1:A:797:MET:SD	2.58	0.43
1:B:45:ILE:HD11	1:B:107:VAL:CG1	2.49	0.43
1:B:156:ASN:OD1	1:B:768:LYS:NZ	2.51	0.43
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.79	0.43
1:B:767:ILE:HG12	1:C:60:THR:HG21	2.00	0.43
1:A:163:LYS:HG3	1:A:175:VAL:HG11	2.01	0.43
1:A:407:ASP:O	1:A:411:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:THR:HG22	1:A:813:PRO:HD3	1.99	0.43
1:A:1007:ILE:O	1:A:1011:ILE:HG12	2.19	0.43
1:B:925:PHE:HB3	1:B:1002:ILE:CG2	2.49	0.43
1:B:328:ASP:OD1	1:B:330:THR:OG1	2.31	0.43
1:B:428:LYS:HB3	1:B:432:ARG:NH2	2.33	0.43
1:C:332:PHE:HB2	1:C:633:TYR:OH	2.19	0.43
1:B:502:GLN:N	1:B:502:GLN:OE1	2.51	0.43
1:C:134:SER:O	1:C:136:PHE:N	2.51	0.43
1:C:939:LYS:O	1:C:942:ILE:HG22	2.19	0.43
1:A:2:ALA:O	1:A:6:ILE:HG13	2.18	0.43
1:A:615:SER:HA	1:A:625:LEU:HG	2.01	0.43
1:B:651:PHE:CE1	1:B:664:PRO:HD2	2.54	0.43
1:C:196:TYR:HB2	1:C:198:LEU:HD23	2.01	0.43
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.83	0.43
1:B:23:GLY:O	1:B:27:ILE:HG12	2.19	0.43
1:B:638:SER:O	1:B:642:LYS:HE2	2.18	0.43
1:B:4:PHE:CE2	1:B:8:ARG:HD2	2.54	0.43
1:B:161:HIS:O	1:B:313:MET:HE1	2.19	0.43
1:C:136:PHE:HD1	1:C:136:PHE:HA	1.67	0.43
1:C:791:ARG:HB3	1:C:797:MET:SD	2.59	0.43
1:A:470:PHE:CE2	1:A:928:VAL:HB	2.54	0.42
1:A:485:ALA:HA	1:A:489:THR:OG1	2.19	0.42
1:A:776:ALA:O	1:A:780:MET:HG2	2.19	0.42
1:A:973:PRO:O	1:A:976:MET:HB3	2.19	0.42
1:B:734:ALA:HB1	1:B:744:ILE:HD11	2.01	0.42
1:A:58:GLU:HA	1:A:62:THR:HB	2.01	0.42
1:A:227:GLY:O	1:A:229:VAL:HG13	2.18	0.42
1:B:467:TYR:CE1	1:B:924:VAL:HG23	2.54	0.42
1:B:577:THR:OG1	1:B:586:THR:HG22	2.19	0.42
1:B:698:ARG:HD2	1:B:716:PRO:HB3	2.01	0.42
1:C:399:VAL:HG11	1:C:988:LEU:CD2	2.49	0.42
1:A:683:LEU:HG	1:A:854:ILE:CG2	2.49	0.42
1:A:1012:THR:O	1:A:1016:LEU:HB2	2.19	0.42
1:C:141:ALA:HB1	1:C:286:THR:HG21	2.01	0.42
1:C:419:VAL:CG1	1:C:430:ALA:HB1	2.50	0.42
1:A:3:LYS:HE2	1:A:432:ARG:HD3	2.00	0.42
1:A:300:LEU:N	1:A:300:LEU:HD12	2.35	0.42
1:A:687:ALA:HB2	1:C:316:TYR:CD1	2.54	0.42
1:B:762:ASP:HB2	1:B:768:LYS:HE3	2.01	0.42
1:B:960:ILE:HD12	2:B:1102:UMQ:HD1	2.02	0.42
1:C:840:MET:HE1	1:C:866:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB3	1:B:153:ASP:HB2	2.02	0.42
1:B:571:MET:HB3	1:B:628:VAL:HG13	2.01	0.42
1:C:816:GLU:HB2	1:C:823:ALA:O	2.19	0.42
1:A:165:PRO:HG2	1:A:313:MET:HE1	2.02	0.42
1:A:644:GLN:OE1	1:A:644:GLN:N	2.52	0.42
1:B:903:VAL:HG11	1:B:938:ALA:HA	2.01	0.42
1:C:388:PHE:HE2	1:C:469:GLN:HA	1.84	0.42
1:C:891:TYR:CD2	1:C:896:ILE:HG21	2.54	0.42
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.91	0.42
1:A:766:ARG:HB3	1:A:768:LYS:HE3	2.01	0.42
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.77	0.42
1:B:526:TYR:OH	1:B:967:ALA:HB1	2.20	0.42
1:B:872:ALA:N	1:B:873:PRO:HD2	2.34	0.42
1:C:34:GLN:HB2	1:C:333:VAL:HG13	2.01	0.42
1:A:278:ASP:HB3	1:A:612:ASN:HB3	2.02	0.42
1:B:684:THR:HG22	1:B:823:ALA:HB2	2.02	0.42
1:C:949:ARG:NH2	1:C:952:GLN:OE1	2.52	0.42
1:C:960:ILE:O	1:C:964:LEU:HG	2.19	0.42
1:A:185:ARG:HB2	1:A:269:GLY:O	2.19	0.42
1:A:454:VAL:N	1:A:455:PRO:CD	2.83	0.42
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.71	0.42
1:B:187:TRP:HA	1:B:773:GLN:O	2.20	0.41
1:B:787:ILE:HD13	1:B:787:ILE:HG21	1.87	0.41
2:B:1102:UMQ:H2'1	2:B:1102:UMQ:HB2	2.02	0.41
1:C:193:LEU:HD23	1:C:265:VAL:HG21	2.02	0.41
1:C:358:PHE:CD2	1:C:976:MET:HG2	2.55	0.41
1:A:372:VAL:HB	1:A:373:PRO:HD3	2.01	0.41
1:A:701:LEU:HD21	1:A:843:MET:HE1	2.02	0.41
1:B:854:ILE:HG23	1:B:854:ILE:HD12	1.79	0.41
1:B:1029:ARG:O	1:B:1033:SER:HB2	2.20	0.41
1:B:186:ILE:CG1	1:B:772:VAL:HG12	2.50	0.41
1:C:137:LEU:HD11	1:C:299:ALA:HB1	2.02	0.41
1:C:679:PHE:CE2	1:C:828:GLY:HA3	2.56	0.41
1:C:911:ALA:HB2	1:C:933:THR:HG21	2.03	0.41
1:A:463:VAL:HG21	1:A:871:GLN:HG3	2.02	0.41
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.55	0.41
1:B:760:PHE:CE1	1:B:768:LYS:HB2	2.56	0.41
1:C:637:GLN:HA	1:C:642:LYS:HD3	2.03	0.41
1:B:178:PHE:HB2	1:B:288:ALA:HB3	2.03	0.41
1:B:512:PHE:O	1:B:515:PHE:N	2.53	0.41
1:C:470:PHE:CE1	1:C:1002:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:PHE:HB2	1:C:665:PHE:CE2	2.56	0.41
1:A:213:GLN:HG3	1:A:239:LEU:HG	2.02	0.41
1:A:452:VAL:HG22	1:A:883:VAL:HG11	2.01	0.41
1:B:808:TRP:HB3	3:B:1104:PG4:H31	2.02	0.41
1:A:38:ILE:HD13	1:A:466:ILE:HD11	2.02	0.41
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.41
1:B:337:ILE:O	1:B:340:VAL:HG12	2.21	0.41
1:A:402:ILE:HG13	1:A:403:GLY:N	2.36	0.41
1:B:151:LYS:HE2	1:B:152:TYR:CZ	2.56	0.41
1:C:414:GLU:HG2	1:C:972:ARG:HH21	1.85	0.41
1:B:553:LEU:HD23	1:B:553:LEU:HA	1.79	0.41
1:B:605:VAL:HG13	1:B:628:VAL:HG23	2.02	0.41
1:B:1033:SER:O	2:B:1102:UMQ:HL2	2.21	0.41
1:C:202:ASP:OD2	1:C:791:ARG:NH1	2.54	0.41
1:C:286:THR:HG22	1:C:287:ALA:N	2.36	0.41
1:C:597:LEU:HD21	1:C:650:MET:SD	2.61	0.41
1:C:638:SER:N	1:C:642:LYS:HE2	2.35	0.41
1:A:10:ILE:HD12	1:B:894:TRP:CE2	2.56	0.41
1:A:604:ILE:HD11	1:A:641:GLN:O	2.20	0.41
1:A:917:LEU:C	1:A:919:GLY:H	2.29	0.41
1:C:399:VAL:O	1:C:402:ILE:HG12	2.20	0.41
1:A:562:PHE:CE2	1:A:563:LEU:HD23	2.56	0.40
1:B:38:ILE:CG2	1:B:462:SER:HB3	2.52	0.40
1:A:434:ALA:O	1:A:438:ILE:HG12	2.21	0.40
1:A:739:VAL:HG11	1:A:790:VAL:HG23	2.02	0.40
1:B:186:ILE:HB	1:B:772:VAL:HG12	2.03	0.40
1:B:840:MET:HG2	1:B:858:TRP:CH2	2.56	0.40
1:C:3:LYS:HE2	1:C:439:THR:HG21	2.04	0.40
1:A:3:LYS:CE	1:A:432:ARG:HD3	2.52	0.40
1:A:58:GLU:OE2	1:A:817:ARG:HD3	2.20	0.40
1:A:534:ILE:O	1:A:537:SER:HB2	2.21	0.40
1:A:585:THR:HG22	1:A:588:ARG:NH1	2.36	0.40
1:A:880:ILE:HA	1:A:883:VAL:HG22	2.04	0.40
1:C:135:SER:O	1:C:137:LEU:N	2.55	0.40
1:A:1:MET:HE3	1:A:487:ILE:CG1	2.51	0.40
1:A:4:PHE:HE1	1:A:8:ARG:CZ	2.35	0.40
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.74	0.40
1:B:776:ALA:O	1:B:780:MET:HG2	2.21	0.40
1:C:58:GLU:HA	1:C:62:THR:HB	2.03	0.40
1:C:762:ASP:HB3	1:C:764:ASP:OD1	2.22	0.40
1:C:1027:LYS:HD3	1:C:1027:LYS:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:LEU:HD23	1:B:472:LEU:HA	1.85	0.40
1:C:3:LYS:HZ3	1:C:436:GLY:HA2	1.87	0.40
1:C:663:ILE:HD12	1:C:715:ARG:HB3	2.02	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	1015/1051 (97%)	973 (96%)	40 (4%)	2 (0%)	43	65
1	B	1020/1051 (97%)	1000 (98%)	19 (2%)	1 (0%)	48	71
1	C	1014/1051 (96%)	989 (98%)	25 (2%)	0	100	100
All	All	3049/3153 (97%)	2962 (97%)	84 (3%)	3 (0%)	48	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	ASN
1	A	717	ASN
1	A	2	ALA

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	828/855 (97%)	826 (100%)	2 (0%)	87	95
1	B	833/855 (97%)	825 (99%)	8 (1%)	68	81
1	C	827/855 (97%)	821 (99%)	6 (1%)	76	86
All	All	2488/2565 (97%)	2472 (99%)	16 (1%)	78	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	543	ILE
1	A	556	VAL
1	B	18	ILE
1	B	405	LEU
1	B	500	ILE
1	B	512	PHE
1	B	637	GLN
1	B	717	ASN
1	B	772	VAL
1	B	1032	PHE
1	C	136	PHE
1	C	277	PHE
1	C	463	VAL
1	C	644	GLN
1	C	669	SER
1	C	829	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	360	GLN
1	A	516	ASN
1	A	527	HIS
1	A	531	HIS
1	A	956	ASN
1	B	48	ASN
1	B	87	ASN
1	B	213	GLN
1	B	576	GLN
1	B	583	GLN
1	B	637	GLN
1	B	641	GLN

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Mol	Chain	Res	Type
1	B	952	GLN
1	C	68	GLN
1	C	74	ASN
1	C	437	GLN
1	C	635	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 [i](#)

4 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	UMQ	B	1102	-	35,35,35	2.44	15 (42%)	46,46,46	2.04	14 (30%)
3	PG4	B	1104	-	12,12,12	0.58	0	11,11,11	0.55	0
2	UMQ	B	1101	-	35,35,35	1.61	7 (20%)	46,46,46	1.75	15 (32%)
2	UMQ	B	1103	-	35,35,35	1.68	5 (14%)	46,46,46	1.62	9 (19%)

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	UMQ	B	1102	-	-	12/20/60/60	0/2/2/2
3	PG4	B	1104	-	-	4/10/10/10	-
2	UMQ	B	1101	-	-	8/20/60/60	0/2/2/2
2	UMQ	B	1103	-	-	10/20/60/60	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1102	UMQ	C3'-C2'	5.51	1.66	1.52
2	B	1102	UMQ	O1'-C1'	5.16	1.48	1.40
2	B	1102	UMQ	C1'-C2'	4.94	1.67	1.52
2	B	1101	UMQ	C3-C4	4.45	1.63	1.52
2	B	1102	UMQ	C3-C4	4.44	1.63	1.52
2	B	1101	UMQ	C4-C5	4.38	1.62	1.53
2	B	1103	UMQ	C3'-C2'	4.15	1.63	1.52
2	B	1102	UMQ	C4'-C5'	4.05	1.63	1.52
2	B	1102	UMQ	O5-C1	3.20	1.50	1.41
2	B	1103	UMQ	O1'-C1'	3.18	1.45	1.40
2	B	1102	UMQ	CB-CA	2.99	1.63	1.51
2	B	1102	UMQ	C3'-C4'	2.96	1.60	1.52
2	B	1102	UMQ	C1-C2	2.68	1.60	1.52
2	B	1102	UMQ	O1'-CA	2.67	1.50	1.43
2	B	1103	UMQ	CB-CA	2.51	1.61	1.51
2	B	1101	UMQ	C1-C2	2.50	1.59	1.52
2	B	1102	UMQ	CF-CD	2.46	1.64	1.51
2	B	1101	UMQ	O1'-C1'	2.38	1.44	1.40
2	B	1101	UMQ	CH-CG	2.38	1.63	1.51
2	B	1103	UMQ	O5-C1	2.25	1.47	1.41
2	B	1101	UMQ	O1-C4'	-2.24	1.38	1.43
2	B	1102	UMQ	CD-CC	2.21	1.62	1.51
2	B	1102	UMQ	CG-CF	2.12	1.62	1.51
2	B	1102	UMQ	O5'-C1'	2.10	1.47	1.41
2	B	1103	UMQ	CH-CG	2.10	1.62	1.51
2	B	1102	UMQ	CH-CG	2.09	1.62	1.51
2	B	1101	UMQ	O2'-C2'	-2.04	1.37	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1102	UMQ	O5'-C5'-C4'	5.14	120.35	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	UMQ	O3-C3-C2	-4.62	99.49	110.38
2	B	1102	UMQ	O1'-C1'-C2'	4.53	115.16	108.27
2	B	1102	UMQ	CA-O1'-C1'	4.49	121.35	113.68
2	B	1103	UMQ	C3'-C4'-C5'	-4.37	101.25	110.93
2	B	1101	UMQ	O5'-C5'-C4'	3.81	117.60	109.72
2	B	1102	UMQ	O3-C3-C2	-3.66	101.74	110.38
2	B	1102	UMQ	O5-C1-C2	3.61	117.80	110.37
2	B	1102	UMQ	O6-C6-C5	-3.07	100.87	111.33
2	B	1103	UMQ	O5'-C5'-C4'	3.07	116.06	109.72
2	B	1103	UMQ	O5'-C1'-C2'	-2.98	104.25	110.37
2	B	1101	UMQ	O2'-C2'-C1'	-2.94	103.07	110.08
2	B	1101	UMQ	O3'-C3'-C4'	-2.85	102.62	109.94
2	B	1103	UMQ	O1-C4'-C3'	2.84	114.45	107.23
2	B	1101	UMQ	C6'-C5'-C4'	-2.81	105.47	113.38
2	B	1103	UMQ	C1-O5-C5	2.77	119.13	113.72
2	B	1102	UMQ	C1-O5-C5	2.77	119.13	113.72
2	B	1102	UMQ	O6'-C6'-C5'	-2.73	102.04	111.33
2	B	1103	UMQ	CA-O1'-C1'	2.71	118.31	113.68
2	B	1102	UMQ	O5-C5-C4	2.70	114.56	109.70
2	B	1101	UMQ	C3-C4-C5	2.65	115.04	110.23
2	B	1101	UMQ	O2-C2-C3	-2.63	104.17	110.38
2	B	1101	UMQ	O5-C5-C4	2.59	114.36	109.70
2	B	1101	UMQ	C4-C3-C2	2.49	115.20	110.83
2	B	1102	UMQ	O3'-C3'-C2'	2.48	116.22	110.38
2	B	1103	UMQ	O5-C5-C4	2.35	113.93	109.70
2	B	1101	UMQ	O5'-C1'-O1'	-2.31	104.59	110.04
2	B	1102	UMQ	C1'-C2'-C3'	2.30	114.85	110.01
2	B	1103	UMQ	O1'-C1'-C2'	2.30	111.76	108.27
2	B	1101	UMQ	C3'-C4'-C5'	-2.27	105.89	110.93
2	B	1103	UMQ	O1-C4'-C5'	2.23	115.32	109.48
2	B	1101	UMQ	O6-C6-C5	-2.23	103.75	111.33
2	B	1101	UMQ	C2'-C3'-C4'	2.18	114.63	109.68
2	B	1102	UMQ	O1-C4'-C3'	2.16	112.73	107.23
2	B	1102	UMQ	C6'-C5'-C4'	-2.15	107.32	113.38
2	B	1102	UMQ	O3-C3-C4	2.11	115.34	110.38
2	B	1101	UMQ	C1'-O5'-C5'	2.06	117.75	113.72
2	B	1101	UMQ	O2'-C2'-C3'	-2.04	105.56	110.38

There are no chirality outliers.

All (34) torsion outliers are listed below:

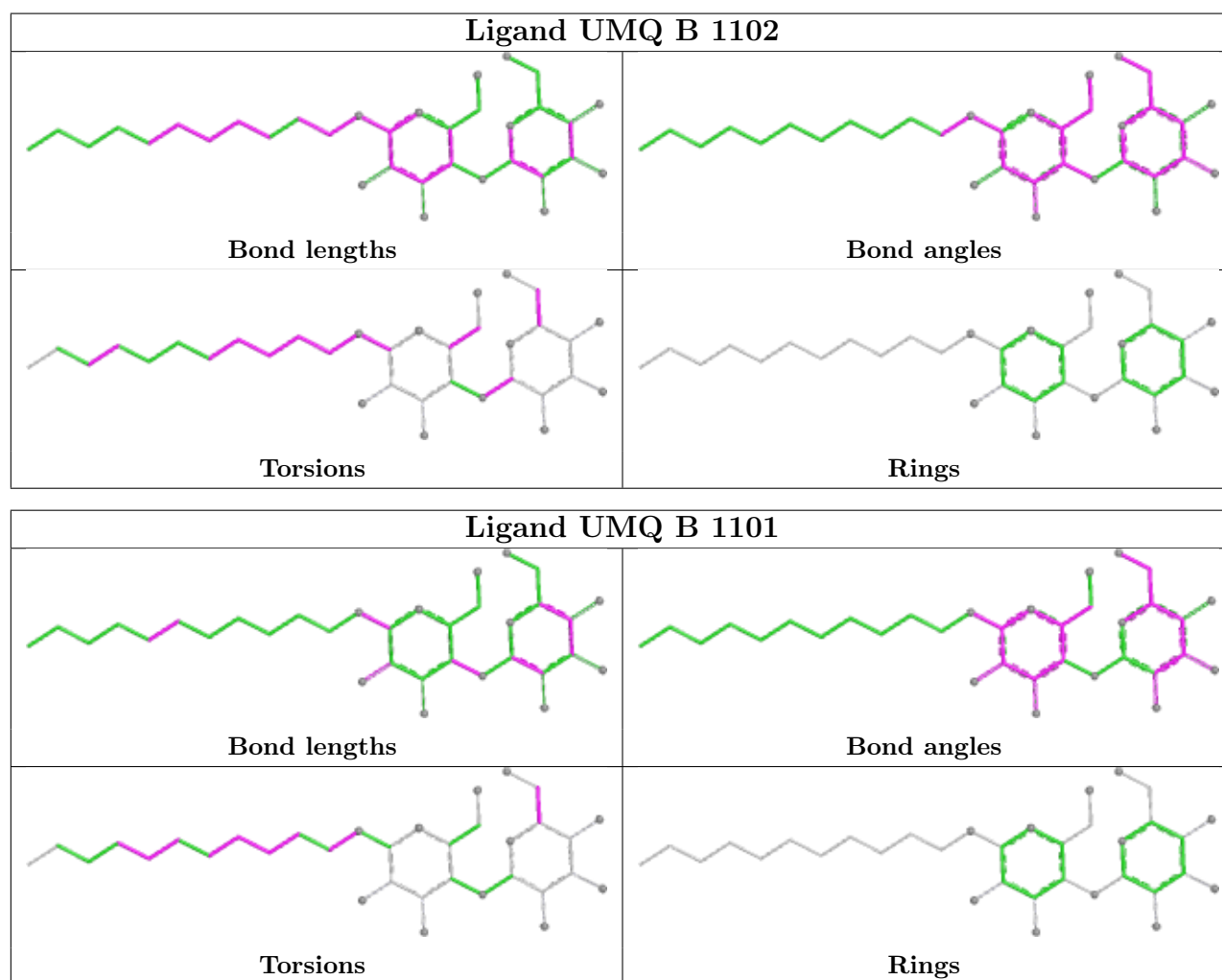
Mol	Chain	Res	Type	Atoms
2	B	1102	UMQ	O5-C1-O1-C4'
2	B	1102	UMQ	C2'-C1'-O1'-CA
2	B	1102	UMQ	O5'-C1'-O1'-CA
2	B	1101	UMQ	O5-C5-C6-O6
2	B	1102	UMQ	O5-C5-C6-O6
2	B	1101	UMQ	C4-C5-C6-O6
2	B	1102	UMQ	C4-C5-C6-O6
2	B	1103	UMQ	O5-C5-C6-O6
2	B	1102	UMQ	O5'-C5'-C6'-O6'
2	B	1103	UMQ	CC-CD-CF-CG
2	B	1103	UMQ	C4-C5-C6-O6
2	B	1101	UMQ	CF-CG-CH-CI
2	B	1101	UMQ	CA-CB-CC-CD
2	B	1101	UMQ	CB-CC-CD-CF
2	B	1102	UMQ	O1'-CA-CB-CC
2	B	1103	UMQ	CB-CC-CD-CF
2	B	1102	UMQ	CH-CI-CJ-CK
3	B	1104	PG4	O4-C7-C8-O5
2	B	1103	UMQ	CF-CG-CH-CI
2	B	1102	UMQ	CC-CD-CF-CG
2	B	1101	UMQ	CG-CH-CI-CJ
2	B	1101	UMQ	CB-CA-O1'-C1'
2	B	1102	UMQ	CB-CA-O1'-C1'
2	B	1103	UMQ	CH-CI-CJ-CK
2	B	1102	UMQ	CB-CC-CD-CF
2	B	1103	UMQ	O1'-CA-CB-CC
2	B	1103	UMQ	CD-CF-CG-CH
3	B	1104	PG4	C5-C6-O4-C7
2	B	1102	UMQ	CA-CB-CC-CD
2	B	1103	UMQ	CB-CA-O1'-C1'
2	B	1103	UMQ	CA-CB-CC-CD
3	B	1104	PG4	O1-C1-C2-O2
2	B	1101	UMQ	CC-CD-CF-CG
3	B	1104	PG4	O3-C5-C6-O4

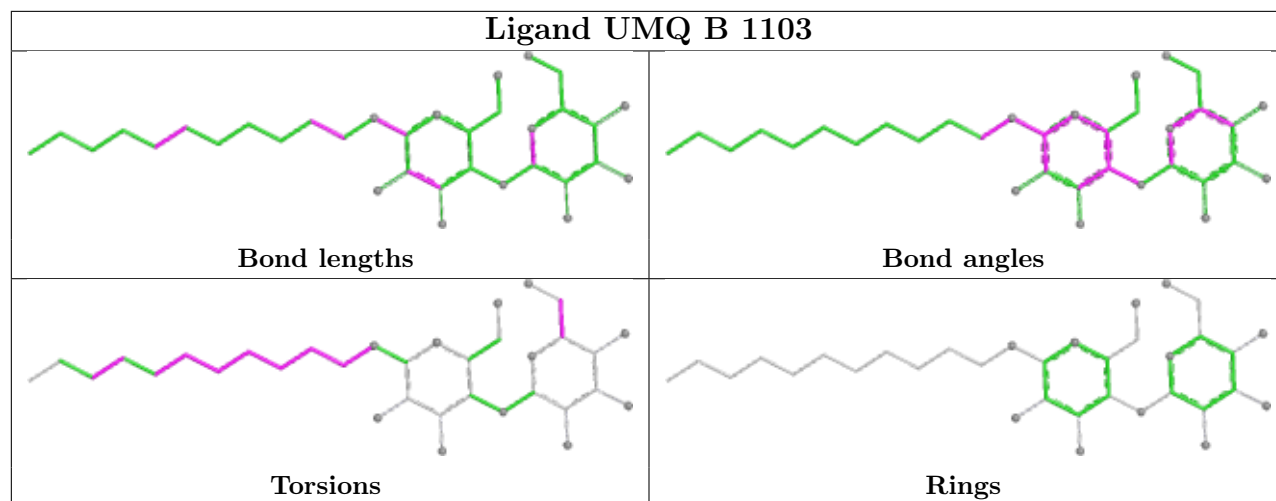
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1102	UMQ	4	0
3	B	1104	PG4	1	0
2	B	1101	UMQ	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	1019/1051 (96%)	0.38	66 (6%) 25 21	68, 120, 184, 336	0
1	B	1024/1051 (97%)	0.34	72 (7%) 22 19	72, 110, 147, 206	0
1	C	1018/1051 (96%)	0.39	65 (6%) 25 21	72, 125, 190, 294	0
All	All	3061/3153 (97%)	0.37	203 (6%) 24 21	68, 116, 176, 336	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	PRO	10.7
1	C	1026	VAL	7.6
1	B	500	ILE	7.2
1	C	226	PRO	6.9
1	A	675	THR	6.7
1	B	424	GLY	6.7
1	B	97	GLY	5.9
1	B	401	ALA	5.8
1	B	499	PRO	5.6
1	C	49	TYR	5.5
1	A	713	GLY	5.3
1	C	568	GLN	5.2
1	B	134	SER	5.2
1	B	866	ILE	5.2
1	B	423	GLU	5.1
1	B	348	ILE	5.0
1	C	786	ASN	4.6
1	B	239	LEU	4.5
1	C	635	GLN	4.5
1	C	565	ASP	4.5
1	A	680	ASP	4.5
1	B	759	ASN	4.4
1	B	502	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	633	TYR	4.2
1	C	119	PRO	4.2
1	C	229	VAL	4.2
1	A	230	LEU	4.1
1	A	674	GLY	4.1
1	B	421	ALA	4.0
1	B	767	ILE	4.0
1	C	960	ILE	4.0
1	C	964	LEU	4.0
1	A	445	VAL	4.0
1	B	347	GLY	4.0
1	B	268	ILE	3.9
1	B	402	ILE	3.9
1	B	960	ILE	3.9
1	C	570	LEU	3.8
1	C	609	PHE	3.8
1	B	403	GLY	3.8
1	C	373	PRO	3.8
1	B	405	LEU	3.8
1	A	348	ILE	3.7
1	B	404	LEU	3.7
1	C	966	ALA	3.7
1	B	264	ASP	3.7
1	A	175	VAL	3.7
1	A	540	TRP	3.6
1	B	213	GLN	3.6
1	B	182	TYR	3.6
1	A	616	PHE	3.6
1	C	17	ILE	3.6
1	B	351	VAL	3.6
1	A	673	LEU	3.5
1	A	810	TYR	3.5
1	C	227	GLY	3.5
1	C	1025	PHE	3.5
1	A	136	PHE	3.4
1	A	614	PHE	3.4
1	A	609	PHE	3.4
1	A	1032	PHE	3.4
1	C	24	VAL	3.4
1	C	961	GLU	3.4
1	B	864	GLN	3.4
1	C	800	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	134	SER	3.4
1	B	183	ALA	3.4
1	C	801	SER	3.4
1	A	684	THR	3.4
1	B	959	PRO	3.3
1	C	1	MET	3.3
1	C	21	LEU	3.3
1	A	827	GLN	3.3
1	A	860	GLY	3.3
1	C	370	ILE	3.2
1	A	951	LEU	3.2
1	A	829	GLN	3.2
1	A	425	LEU	3.2
1	B	756	TYR	3.2
1	C	963	ALA	3.2
1	B	290	GLY	3.2
1	C	50	PRO	3.2
1	C	281	TYR	3.2
1	A	178	PHE	3.2
1	A	290	GLY	3.2
1	B	865	GLU	3.2
1	C	122	VAL	3.1
1	B	270	LEU	3.1
1	A	659	ASP	3.1
1	A	714	VAL	3.1
1	A	439	THR	3.1
1	B	45	ILE	3.1
1	C	228	THR	3.1
1	B	671	PRO	3.0
1	B	425	LEU	3.0
1	C	943	LEU	3.0
1	B	454	VAL	3.0
1	B	981	PHE	3.0
1	B	498	LYS	2.9
1	C	158	VAL	2.9
1	B	808	TRP	2.8
1	C	543	ILE	2.8
1	C	1005	GLY	2.8
1	B	668	PRO	2.8
1	C	778	PHE	2.8
1	C	230	LEU	2.8
1	A	82	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	664	PRO	2.7
1	A	826	ILE	2.7
1	C	377	LEU	2.7
1	C	787	ILE	2.7
1	B	640	ASP	2.7
1	C	288	ALA	2.7
1	A	859	THR	2.7
1	A	292	GLN	2.7
1	B	720	ASN	2.7
1	A	402	ILE	2.6
1	C	982	ILE	2.6
1	B	672	GLU	2.6
1	A	663	ILE	2.6
1	A	866	ILE	2.6
1	B	616	PHE	2.6
1	C	616	PHE	2.6
1	C	618	GLY	2.6
1	A	611	VAL	2.6
1	A	627	PHE	2.6
1	C	51	GLY	2.6
1	A	625	LEU	2.6
1	A	747	THR	2.6
1	B	136	PHE	2.6
1	B	400	LEU	2.5
1	A	880	ILE	2.5
1	A	763	THR	2.5
1	B	867	GLN	2.5
1	B	980	ALA	2.5
1	B	133	SER	2.5
1	A	777	PRO	2.5
1	A	847	ALA	2.5
1	B	721	ASP	2.5
1	C	113	LEU	2.5
1	C	603	ASP	2.4
1	A	229	VAL	2.4
1	B	555	PHE	2.4
1	C	120	GLN	2.4
1	C	167	SER	2.4
1	C	186	ILE	2.4
1	C	337	ILE	2.4
1	B	572	PHE	2.3
1	C	614	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1007	ILE	2.3
1	A	30	LEU	2.3
1	A	876	TYR	2.3
1	B	932	THR	2.3
1	B	692	ASP	2.3
1	A	71	GLY	2.3
1	A	618	GLY	2.3
1	C	147	GLY	2.3
1	C	607	SER	2.3
1	B	810	TYR	2.3
1	A	678	GLY	2.3
1	B	22	ALA	2.2
1	C	717	ASN	2.2
1	A	832	PRO	2.2
1	A	641	GLN	2.2
1	B	6	ILE	2.2
1	A	585	THR	2.2
1	A	858	TRP	2.2
1	B	426	PRO	2.2
1	A	861	LEU	2.2
1	C	677	ALA	2.2
1	C	117	ILE	2.2
1	B	519	PHE	2.2
1	B	719	LEU	2.2
1	B	266	ALA	2.2
1	C	636	ARG	2.2
1	B	124	GLN	2.2
1	A	977	THR	2.2
1	B	269	GLY	2.2
1	B	941	ALA	2.2
1	A	438	ILE	2.1
1	A	359	LEU	2.1
1	A	863	PHE	2.1
1	C	169	ILE	2.1
1	B	531	HIS	2.1
1	C	928	VAL	2.1
1	C	959	PRO	2.1
1	A	926	PHE	2.1
1	A	712	ARG	2.1
1	B	120	GLN	2.1
1	A	554	LEU	2.1
1	C	515	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	325	TYR	2.1
1	A	387	GLY	2.0
1	B	665	PHE	2.0
1	C	608	ALA	2.0
1	C	575	VAL	2.0
1	A	580	GLY	2.0
1	A	828	GLY	2.0
1	B	760	PHE	2.0
1	C	962	ALA	2.0
1	B	422	GLU	2.0
1	A	435	MET	2.0
1	B	785	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

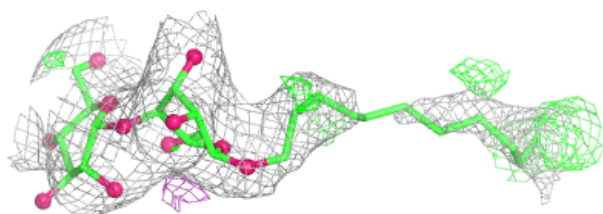
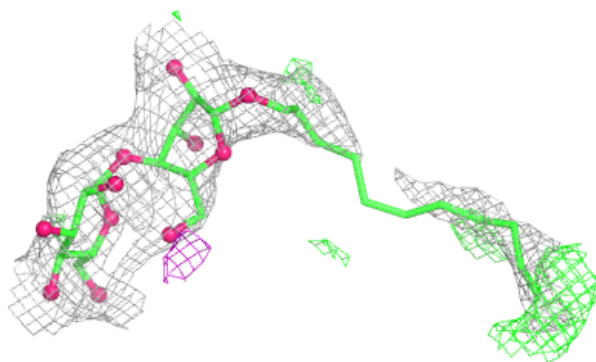
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	UMQ	B	1102	34/34	0.75	0.18	111,120,129,131	0
3	PG4	B	1104	13/13	0.83	0.17	99,103,117,119	0
2	UMQ	B	1103	34/34	0.86	0.13	104,121,125,128	0
2	UMQ	B	1101	34/34	0.89	0.11	97,113,121,124	0

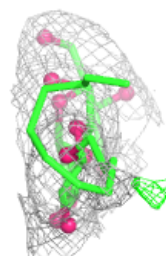
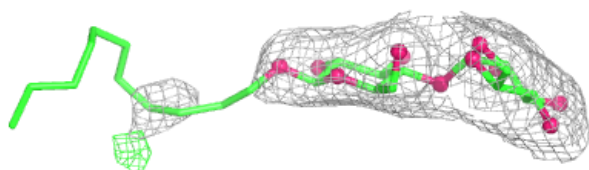
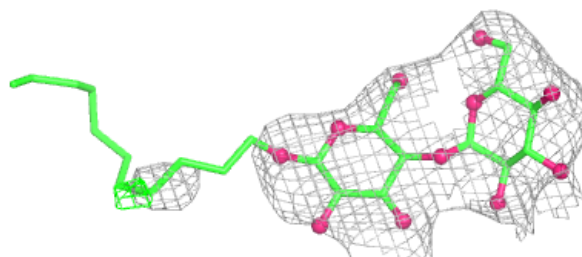
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMQ B 1102:

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

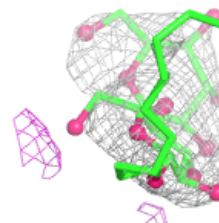
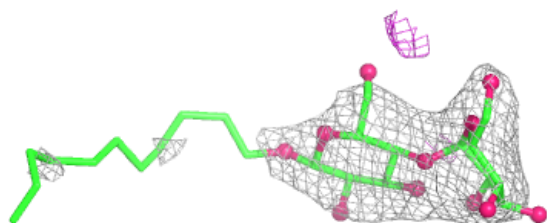
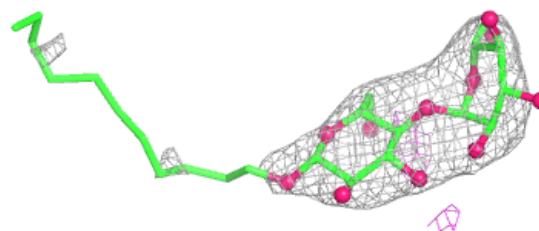
**Electron density around UMQ B 1103:**

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



Electron density around UMQ B 1101:

$2mF_o - DF_c$ (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.