



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 6TEJ / pdb_00006tej
Title : Structure of apo IrtAB devoid SID in complex with sybody Syb_NL5
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mann, L.M.
Deposited on : 2019-11-12
Resolution : 2.70 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

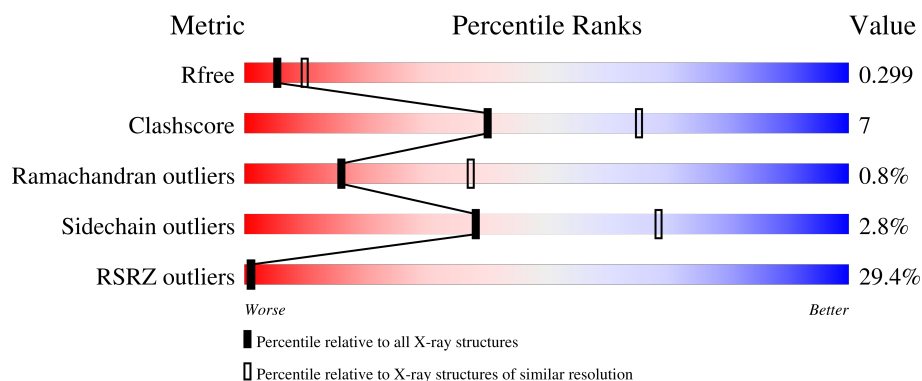
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	908	16% 52% 9% 38%
2	B	586	35% 81% 19%
3	C	124	19% 89% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9422 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 Drug ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4179	2747	671	753	8			

- Molecule 2 is a protein called Drug ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	585	Total	C	N	O	S	0	0	0
			4227	2743	683	796	5			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	580	ALA	-	expression tag	UNP A0A100XE85
B	581	LEU	-	expression tag	UNP A0A100XE85
B	582	GLU	-	expression tag	UNP A0A100XE85
B	583	VAL	-	expression tag	UNP A0A100XE85
B	584	LEU	-	expression tag	UNP A0A100XE85
B	585	PHE	-	expression tag	UNP A0A100XE85
B	586	GLN	-	expression tag	UNP A0A100XE85

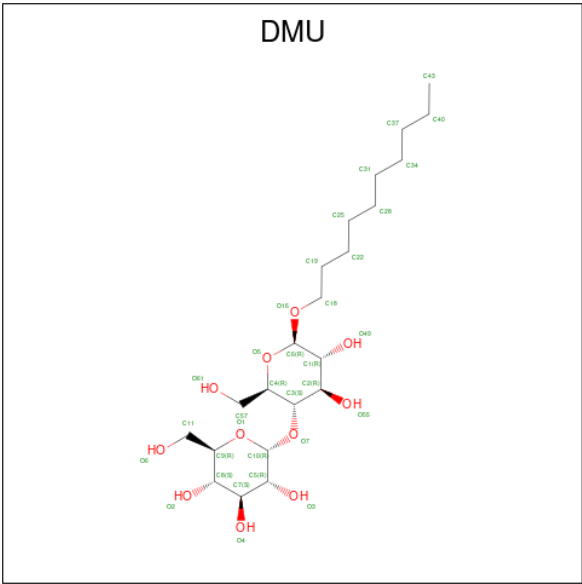
- Molecule 3 is a protein called Syb_NL5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	124	Total	C	N	O	S	0	0	0
			928	592	151	180	5			

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		

- Molecule 5 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).

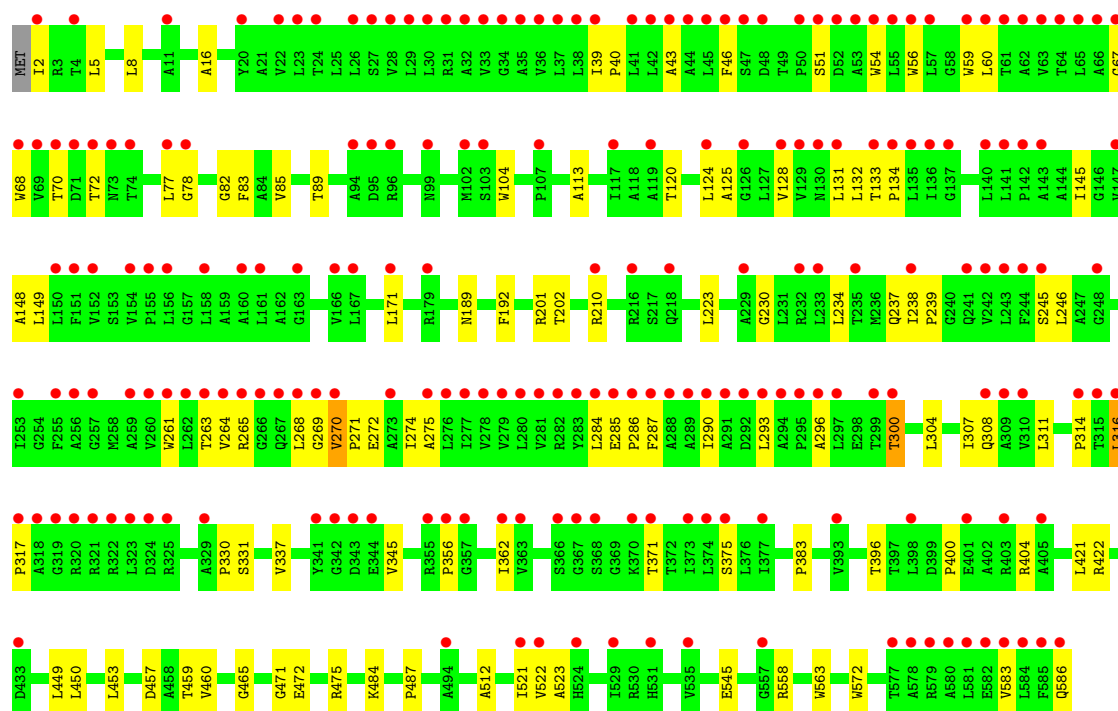


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			33	22	11		

- Molecule 6 is water.

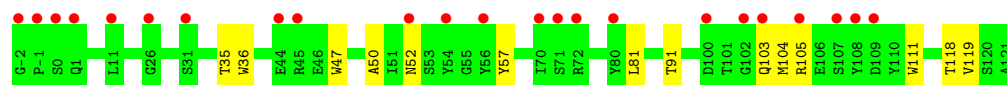
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	22	Total	O	0	0
			22	22		
6	C	5	Total	O	0	0
			5	5		

Chain B: 



• Molecule 3: Syb_NL5

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 78.58Å 133.57Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	47.43 – 2.70 47.43 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.43-2.70) 99.9 (47.43-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.264 , 0.296 0.268 , 0.299	Depositor DCC
R_{free} test set	2919 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9422	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: NI, DMU

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	0.16	0/4248	0.36	0/5760
2	B	0.16	0/4292	0.37	0/5850
3	C	0.18	0/946	0.38	0/1275
All	All	0.16	0/9486	0.37	0/12885

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4179	0	4233	54	0
2	B	4227	0	4242	69	0
3	C	928	0	865	9	0
4	A	1	0	0	0	0
5	B	33	0	42	2	0
6	A	27	0	0	0	0
6	B	22	0	0	0	0
6	C	5	0	0	0	0
All	All	9422	0	9382	124	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 7.

All (124) 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)
2:B:375:SER:HB3	5:B:601:DMU:H19	1.71	0.72
1:A:545:TRP:CZ3	1:A:545:TRP:CZ2	2.77	0.71
2:B:56:TRP:CZ2	2:B:56:TRP:CZ3	2.77	0.71
2:B:104:TRP:CZ3	2:B:104:TRP:CZ2	2.77	0.71
1:A:567:TRP:CZ2	1:A:567:TRP:CZ3	2.77	0.71
2:B:59:TRP:CZ3	2:B:59:TRP:CZ2	2.77	0.71
3:C:47:TRP:CZ3	3:C:47:TRP:CZ2	2.76	0.71
2:B:261:TRP:CZ3	2:B:261:TRP:CZ2	2.77	0.71
1:A:391:TRP:CZ3	1:A:391:TRP:CZ2	2.77	0.71
1:A:502:TRP:CZ3	1:A:502:TRP:CZ2	2.76	0.71
1:A:468:TRP:CZ3	1:A:468:TRP:CZ2	2.77	0.70
2:B:54:TRP:CZ3	2:B:54:TRP:CZ2	2.77	0.70
1:A:368:TRP:CZ3	1:A:368:TRP:CZ2	2.77	0.70
3:C:36:TRP:CZ3	3:C:36:TRP:CZ2	2.77	0.70
2:B:572:TRP:CZ3	2:B:572:TRP:CZ2	2.76	0.70
3:C:111:TRP:CZ3	3:C:111:TRP:CZ2	2.77	0.69
1:A:418:TRP:CZ3	1:A:418:TRP:CZ2	2.77	0.69
2:B:563:TRP:CZ3	2:B:563:TRP:CZ2	2.76	0.69
2:B:68:TRP:CZ3	2:B:68:TRP:CZ2	2.76	0.69
1:A:885:TRP:CZ3	1:A:885:TRP:CZ2	2.77	0.68
1:A:592:LEU:HD21	2:B:274:ILE:HG12	1.75	0.67
2:B:512:ALA:O	3:C:52:ASN:ND2	2.27	0.67
1:A:350:LEU:HD11	1:A:374:ALA:HB2	1.75	0.66
1:A:561:ARG:H	1:A:562:PRO:HD2	1.60	0.66
1:A:547:ARG:H	1:A:548:PRO:HD2	1.62	0.64
1:A:568:ILE:HA	1:A:571:VAL:HG22	1.79	0.63
2:B:404:ARG:O	2:B:484:LYS:NZ	2.31	0.62
2:B:89:THR:HG21	2:B:304:LEU:HD11	1.81	0.62
1:A:337:GLN:HE21	1:A:388:MET:HE1	1.65	0.62
1:A:660:SER:HB2	1:A:708:GLN:HB2	1.82	0.60
2:B:271:PRO:O	2:B:275:ALA:N	2.29	0.60
1:A:542:LEU:HA	1:A:545:TRP:CD1	2.37	0.59
1:A:454:VAL:HA	1:A:457:VAL:HG12	1.86	0.58
2:B:314:PRO:HB2	2:B:316:LEU:HD23	1.85	0.58
1:A:485:MET:HE3	1:A:557:ASP:OD2	2.06	0.56
1:A:716:ARG:HG2	1:A:721:LEU:HD21	1.88	0.56
1:A:485:MET:HE1	1:A:554:THR:HG22	1.89	0.55
1:A:426:SER:HB2	1:A:428:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ALA:HA	2:B:307:ILE:HD11	1.88	0.54
1:A:749:ALA:HA	1:A:805:LEU:HD23	1.90	0.54
2:B:270:VAL:HG22	2:B:271:PRO:HD3	1.90	0.54
3:C:103:GLN:O	3:C:105:ARG:N	2.41	0.54
1:A:585:VAL:HG12	1:A:588:LEU:HD13	1.90	0.53
2:B:371:THR:HG22	5:B:601:DMU:H18	1.90	0.53
1:A:459:VAL:HG21	1:A:593:LEU:HB3	1.89	0.53
1:A:450:VAL:HA	1:A:453:VAL:HG22	1.89	0.53
1:A:445:ALA:HB1	1:A:611:ILE:HG12	1.90	0.53
3:C:52:ASN:HB2	3:C:57:TYR:HB3	1.91	0.53
2:B:286:PRO:O	2:B:290:ILE:N	2.40	0.52
2:B:284:LEU:HA	2:B:287:PHE:HB2	1.91	0.52
2:B:263:THR:C	2:B:265:ARG:H	2.18	0.51
2:B:449:LEU:HD22	2:B:472:GLU:HB3	1.93	0.51
2:B:16:ALA:HB1	2:B:77:LEU:HD11	1.93	0.51
2:B:422:ARG:HD2	2:B:457:ASP:OD2	2.11	0.50
1:A:393:HIS:HB3	2:B:234:LEU:HD13	1.93	0.50
2:B:128:VAL:HG23	2:B:132:LEU:HD23	1.93	0.50
1:A:469:ARG:O	1:A:473:VAL:N	2.44	0.50
1:A:389:THR:HG23	2:B:238:ILE:HD12	1.94	0.50
1:A:547:ARG:HB2	2:B:83:PHE:HE2	1.77	0.49
1:A:541:PHE:O	1:A:544:SER:OG	2.27	0.49
2:B:83:PHE:CE1	2:B:125:ALA:HB1	2.47	0.49
2:B:237:GLN:H	2:B:239:PRO:HD2	1.78	0.49
1:A:591:LEU:HD12	2:B:274:ILE:HG21	1.95	0.48
2:B:337:VAL:HG13	2:B:383:PRO:HB3	1.95	0.48
2:B:131:LEU:C	2:B:134:PRO:HD2	2.39	0.48
2:B:133:THR:OG1	2:B:134:PRO:HD3	2.14	0.48
1:A:502:TRP:O	1:A:506:MET:HB2	2.14	0.47
1:A:686:VAL:HG12	1:A:845:ALA:HB3	1.95	0.47
2:B:192:PHE:HD1	2:B:223:LEU:HD22	1.80	0.47
2:B:8:LEU:HB3	2:B:85:VAL:HG23	1.95	0.47
1:A:547:ARG:N	1:A:548:PRO:HD2	2.28	0.46
3:C:35:THR:HG23	3:C:50:ALA:HB2	1.97	0.46
2:B:293:LEU:HA	2:B:296:ALA:HB3	1.97	0.46
2:B:317:PRO:HD2	2:B:396:THR:O	2.15	0.46
2:B:330:PRO:HD3	2:B:487:PRO:HB2	1.98	0.46
1:A:585:VAL:HA	1:A:588:LEU:HB2	1.98	0.46
2:B:521:ILE:HG12	2:B:523:ALA:HB2	1.98	0.46
1:A:729:ARG:HA	1:A:809:PRO:HD2	1.99	0.45
1:A:349:VAL:HG23	1:A:462:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:GLY:HA2	2:B:70:THR:HG22	1.99	0.45
1:A:470:VAL:O	1:A:473:VAL:HG12	2.17	0.44
2:B:453:LEU:HD22	2:B:459:THR:HG21	1.99	0.44
2:B:545:GLU:OE2	2:B:558:ARG:N	2.49	0.44
2:B:545:GLU:OE2	2:B:558:ARG:HB2	2.17	0.44
3:C:36:TRP:CG	3:C:81:LEU:HD22	2.52	0.44
2:B:471:GLY:O	2:B:475:ARG:HD3	2.17	0.44
2:B:128:VAL:HA	2:B:132:LEU:HB3	2.00	0.44
1:A:584:PRO:HG2	2:B:46:PHE:CG	2.53	0.44
2:B:78:GLY:O	2:B:82:GLY:N	2.40	0.43
2:B:89:THR:HG23	2:B:304:LEU:HD21	1.98	0.43
1:A:675:LEU:HD21	1:A:858:VAL:HG21	2.00	0.43
1:A:574:VAL:O	1:A:576:LEU:N	2.51	0.43
1:A:346:ALA:N	1:A:347:PRO:HD2	2.33	0.43
2:B:230:GLY:O	2:B:234:LEU:HG	2.18	0.43
1:A:495:LYS:HD2	1:A:541:PHE:CE1	2.53	0.43
2:B:39:ILE:HB	2:B:40:PRO:HD3	2.01	0.43
2:B:56:TRP:O	2:B:60:LEU:N	2.46	0.43
2:B:300:THR:O	2:B:304:LEU:HB2	2.19	0.43
1:A:694:SER:HA	1:A:844:ILE:HD13	1.99	0.43
2:B:268:LEU:O	2:B:271:PRO:HD2	2.18	0.43
2:B:201:ARG:HG3	2:B:202:THR:HG23	1.99	0.43
2:B:421:LEU:HD22	2:B:450:LEU:HD21	2.01	0.42
1:A:488:MET:HB2	1:A:488:MET:HE3	1.75	0.42
2:B:269:GLY:O	2:B:272:GLU:HB2	2.19	0.42
2:B:145:ILE:O	2:B:149:LEU:N	2.53	0.42
2:B:189:ASN:HA	2:B:192:PHE:HB2	2.02	0.42
2:B:316:LEU:HD13	2:B:400:PRO:HG3	2.00	0.42
1:A:323:LEU:HD11	1:A:441:LEU:HD21	2.02	0.42
2:B:145:ILE:HA	2:B:148:ALA:HB3	2.02	0.41
2:B:460:VAL:HG23	2:B:465:GLY:HA3	2.02	0.41
1:A:816:ALA:HA	1:A:819:PHE:CE1	2.55	0.41
2:B:120:THR:HB	2:B:124:LEU:HD13	2.02	0.41
2:B:331:SER:HB3	2:B:356:PRO:HD3	2.02	0.41
2:B:362:ILE:HB	2:B:522:VAL:HG22	2.02	0.41
1:A:403:LEU:HD21	1:A:621:ILE:HG21	2.03	0.41
2:B:287:PHE:HA	2:B:290:ILE:HG12	2.03	0.41
3:C:91:THR:HG23	3:C:118:THR:HA	2.03	0.41
1:A:484:LEU:HD22	1:A:553:LYS:HE3	2.03	0.41
1:A:539:ILE:HG13	1:A:540:ASP:N	2.36	0.41
1:A:588:LEU:O	1:A:591:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLN:O	2:B:311:LEU:HG	2.21	0.41
1:A:555:LEU:HD11	2:B:72:THR:O	2.20	0.40
1:A:833:ASN:O	1:A:837:ARG:HG3	2.21	0.40
2:B:43:ALA:HB1	2:B:268:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	557/908 (61%)	524 (94%)	26 (5%)	7 (1%)	9	25
2	B	583/586 (100%)	548 (94%)	33 (6%)	2 (0%)	36	60
3	C	122/124 (98%)	117 (96%)	4 (3%)	1 (1%)	16	37
All	All	1262/1618 (78%)	1189 (94%)	63 (5%)	10 (1%)	16	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	ALA
1	A	576	LEU
1	A	362	ALA
1	A	562	PRO
3	C	104	MET
2	B	51	SER
2	B	264	VAL
1	A	548	PRO
1	A	561	ARG
1	A	493	GLY

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	447/711 (63%)	433 (97%)	14 (3%)	35	65
2	B	438/439 (100%)	425 (97%)	13 (3%)	36	66
3	C	101/101 (100%)	100 (99%)	1 (1%)	68	86
All	All	986/1251 (79%)	958 (97%)	28 (3%)	38	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	LEU
1	A	363	GLU
1	A	428	LYS
1	A	457	VAL
1	A	460	LEU
1	A	473	VAL
1	A	475	PHE
1	A	480	VAL
1	A	506	MET
1	A	542	LEU
1	A	554	THR
1	A	586	ASN
1	A	588	LEU
1	A	790	LEU
2	B	2	ILE
2	B	5	LEU
2	B	171	LEU
2	B	210	ARG
2	B	245	SER
2	B	246	LEU
2	B	270	VAL
2	B	285	GLU
2	B	300	THR
2	B	316	LEU
2	B	345	VAL
2	B	583	VAL

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Mol	Chain	Res	Type
2	B	586	GLN
3	C	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	439	HIS
2	B	237	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMU	B	601	-	34,34,34	1.51	8 (23%)	45,45,45	1.50	8 (17%)

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
5	DMU	B	601	-	-	7/19/59/59	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	DMU	O1-C9	4.18	1.54	1.44
5	B	601	DMU	C7-C5	-2.85	1.44	1.52
5	B	601	DMU	C11-C9	-2.82	1.42	1.51
5	B	601	DMU	O1-C10	2.37	1.47	1.41
5	B	601	DMU	O3-C5	2.26	1.48	1.43
5	B	601	DMU	O4-C7	2.26	1.48	1.43
5	B	601	DMU	C8-C9	2.13	1.57	1.53
5	B	601	DMU	O5-C6	2.05	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	DMU	C1-C2-C3	3.67	118.00	109.68
5	B	601	DMU	C7-C8-C9	3.55	116.67	110.23
5	B	601	DMU	C10-O7-C3	-3.34	110.05	117.98
5	B	601	DMU	C10-O1-C9	2.81	119.20	113.72
5	B	601	DMU	O1-C9-C8	2.72	114.59	109.70
5	B	601	DMU	C2-C3-C4	2.70	116.92	110.93
5	B	601	DMU	O16-C6-C1	2.47	112.03	108.27
5	B	601	DMU	C6-O5-C4	-2.36	109.11	113.72

There are no chirality outliers.

All (7) torsion outliers are listed below:

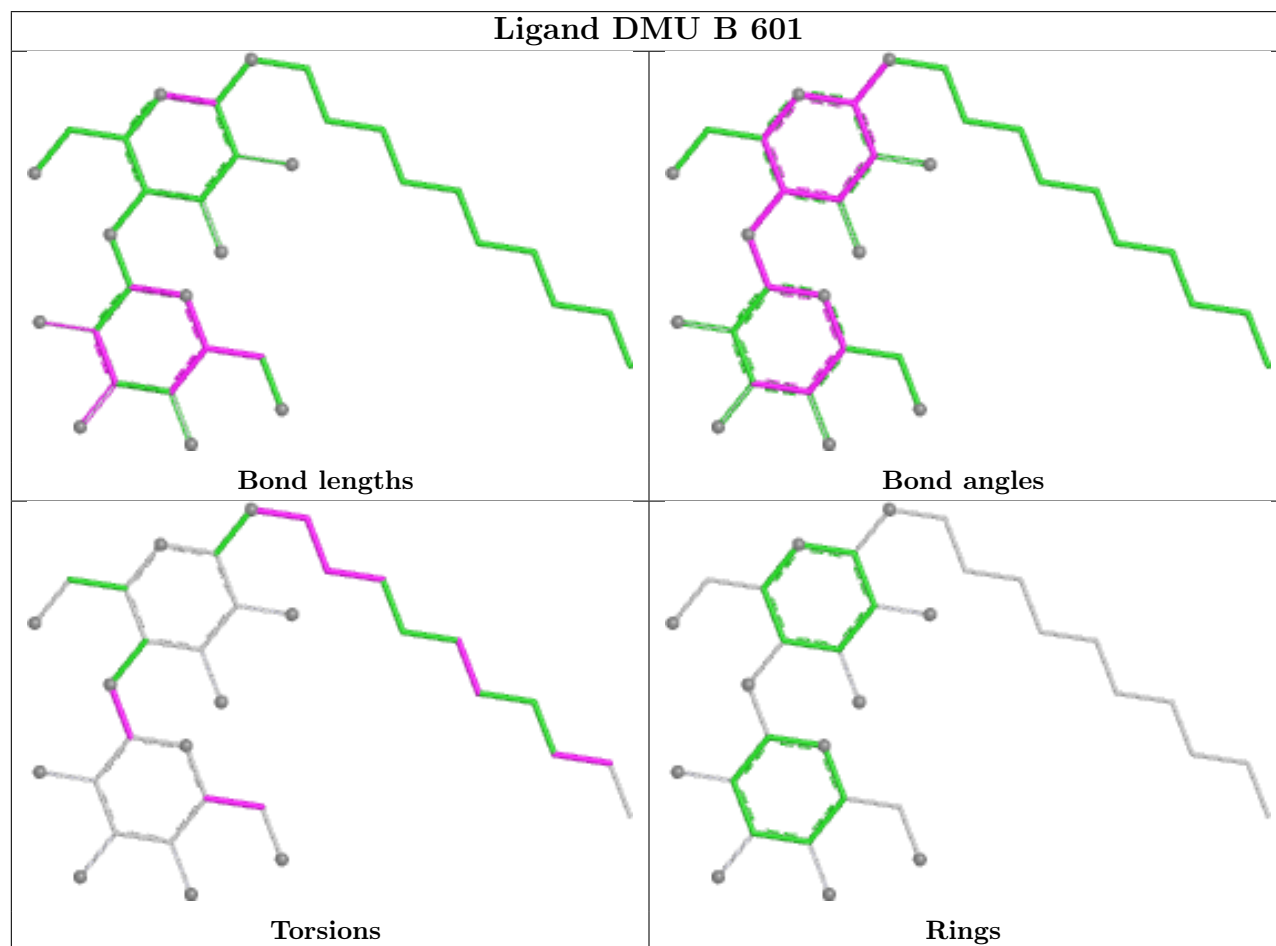
Mol	Chain	Res	Type	Atoms
5	B	601	DMU	C18-C19-C22-C25
5	B	601	DMU	C19-C18-O16-C6
5	B	601	DMU	O6-C11-C9-C8
5	B	601	DMU	O16-C18-C19-C22
5	B	601	DMU	C34-C37-C40-C43
5	B	601	DMU	C25-C28-C31-C34
5	B	601	DMU	O1-C10-O7-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	DMU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	561/908 (61%)	1.39	143 (25%)  	39, 80, 150, 171	0
2	B	585/586 (99%)	1.77	208 (35%)  	37, 97, 156, 183	0
3	C	124/124 (100%)	1.22	23 (18%)  	44, 70, 111, 132	0
All	All	1270/1618 (78%)	1.55	374 (29%)  	37, 84, 153, 183	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	282	ARG	12.9
2	B	279	VAL	11.4
2	B	284	LEU	10.8
2	B	578	ALA	10.2
2	B	285	GLU	10.1
1	A	564	THR	9.9
2	B	280	LEU	9.7
2	B	278	VAL	9.5
1	A	595	THR	8.6
2	B	318	ALA	8.5
1	A	556	MET	8.5
1	A	563	ALA	8.5
2	B	281	VAL	8.4
1	A	608	LEU	7.6
2	B	71	ASP	7.3
2	B	343	ASP	7.1
1	A	596	THR	6.5
1	A	566	LEU	6.5
2	B	54	TRP	6.4
1	A	565	PHE	6.3
1	A	561	ARG	6.3
2	B	53	ALA	6.3
1	A	558	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	599	ALA	6.1
2	B	64	THR	6.0
1	A	348	PHE	5.9
2	B	137	GLY	5.8
2	B	577	THR	5.7
2	B	147	VAL	5.7
1	A	515	GLU	5.7
2	B	33	VAL	5.6
1	A	787	GLY	5.4
2	B	35	ALA	5.3
2	B	324	ASP	5.3
1	A	593	LEU	5.2
1	A	560	THR	5.1
2	B	67	GLY	5.1
1	A	559	VAL	5.0
2	B	264	VAL	5.0
2	B	276	LEU	5.0
2	B	398	LEU	4.9
1	A	606	TYR	4.9
1	A	607	GLY	4.8
1	A	368	TRP	4.8
2	B	69	VAL	4.8
2	B	68	TRP	4.7
2	B	582	GLU	4.7
1	A	890	TYR	4.7
2	B	287	PHE	4.7
2	B	277	ILE	4.7
2	B	31	ARG	4.7
2	B	30	LEU	4.6
2	B	260	VAL	4.6
2	B	283	TYR	4.6
2	B	266	GLY	4.6
2	B	72	THR	4.6
2	B	232	ARG	4.5
2	B	2	ILE	4.5
2	B	317	PRO	4.5
1	A	634	ASP	4.4
2	B	63	VAL	4.3
1	A	592	LEU	4.3
2	B	316	LEU	4.3
2	B	47	SER	4.3
3	C	52	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	505	ARG	4.3
2	B	580	ALA	4.3
3	C	-1	PRO	4.3
2	B	288	ALA	4.2
1	A	367	LEU	4.2
1	A	470	VAL	4.2
3	C	72	ARG	4.2
2	B	315	THR	4.2
2	B	243	LEU	4.2
2	B	261	TRP	4.1
1	A	562	PRO	4.1
2	B	273	ALA	4.1
2	B	24	THR	4.1
2	B	95	ASP	4.1
2	B	102	MET	4.1
2	B	585	PHE	4.1
1	A	578	VAL	4.1
1	A	316	ALA	4.1
2	B	309	ALA	4.1
2	B	367	GLY	4.1
1	A	568	ILE	4.1
2	B	42	LEU	4.1
1	A	354	LEU	4.1
2	B	322	ARG	4.0
2	B	154	VAL	4.0
2	B	70	THR	4.0
3	C	102	GLY	4.0
1	A	574	VAL	4.0
2	B	325	ARG	3.9
2	B	256	ALA	3.9
2	B	259	ALA	3.9
2	B	275	ALA	3.9
1	A	741	HIS	3.9
2	B	140	LEU	3.9
1	A	600	ARG	3.9
2	B	321	ARG	3.9
3	C	0	SER	3.9
2	B	368	SER	3.9
2	B	557	GLY	3.9
2	B	166	VAL	3.8
2	B	55	LEU	3.8
2	B	156	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	659	VAL	3.8
1	A	370	LEU	3.8
1	A	569	ILE	3.8
2	B	45	LEU	3.7
2	B	28	VAL	3.7
2	B	268	LEU	3.7
1	A	468	TRP	3.7
1	A	594	GLY	3.7
2	B	66	ALA	3.7
2	B	310	VAL	3.7
2	B	265	ARG	3.6
2	B	233	LEU	3.6
1	A	469	ARG	3.6
1	A	508	GLY	3.6
1	A	572	ALA	3.6
2	B	26	LEU	3.6
2	B	133	THR	3.6
2	B	586	GLN	3.6
2	B	323	LEU	3.6
2	B	581	LEU	3.6
1	A	674	THR	3.6
1	A	601	LEU	3.6
2	B	403	ARG	3.5
1	A	603	GLY	3.5
1	A	632	VAL	3.5
2	B	52	ASP	3.5
2	B	355	ARG	3.5
1	A	366	ARG	3.5
1	A	591	LEU	3.4
1	A	602	LEU	3.4
2	B	584	LEU	3.4
2	B	229	ALA	3.4
2	B	99	ASN	3.4
2	B	151	PHE	3.4
1	A	742	GLY	3.3
1	A	347	PRO	3.3
1	A	635	ARG	3.3
1	A	531	PHE	3.3
2	B	158	LEU	3.2
2	B	245	SER	3.2
1	A	481	TYR	3.2
2	B	179	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	579	ARG	3.2
2	B	262	LEU	3.2
2	B	51	SER	3.2
1	A	697	ALA	3.2
2	B	143	ALA	3.2
2	B	96	ARG	3.2
2	B	300	THR	3.2
1	A	510	ALA	3.2
1	A	478	VAL	3.2
2	B	150	LEU	3.2
2	B	344	GLU	3.2
2	B	117	ILE	3.2
1	A	399	PHE	3.2
1	A	474	LEU	3.1
2	B	342	GLY	3.1
2	B	291	ALA	3.1
1	A	326	LEU	3.1
2	B	77	LEU	3.1
1	A	580	GLY	3.1
3	C	54	TYR	3.1
2	B	241	GLN	3.1
2	B	62	ALA	3.1
2	B	270	VAL	3.1
2	B	155	PRO	3.1
2	B	248	GLY	3.1
2	B	299	THR	3.1
2	B	319	GLY	3.1
2	B	238	ILE	3.1
1	A	598	GLY	3.0
2	B	152	VAL	3.0
1	A	424	SER	3.0
1	A	358	LEU	3.0
2	B	167	LEU	3.0
1	A	467	ASP	3.0
1	A	455	ALA	3.0
1	A	513	PHE	3.0
1	A	364	ALA	3.0
2	B	494	ALA	3.0
1	A	609	SER	2.9
2	B	34	GLY	2.9
2	B	263	THR	2.9
1	A	597	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	31	SER	2.9
1	A	604	ILE	2.9
2	B	521	ILE	2.9
2	B	59	TRP	2.9
1	A	462	TYR	2.9
2	B	136	ILE	2.9
3	C	108	TYR	2.9
1	A	325	PRO	2.8
1	A	547	ARG	2.8
2	B	267	GLN	2.8
1	A	417	GLY	2.8
1	A	550	VAL	2.8
2	B	107	PRO	2.8
2	B	216	ARG	2.8
2	B	292	ASP	2.8
2	B	38	LEU	2.8
2	B	141	LEU	2.8
1	A	487	VAL	2.8
2	B	286	PRO	2.8
2	B	161	LEU	2.8
2	B	293	LEU	2.8
1	A	362	ALA	2.8
2	B	36	VAL	2.8
1	A	889	ARG	2.8
2	B	129	VAL	2.8
1	A	533	ARG	2.8
1	A	430	LEU	2.7
2	B	60	LEU	2.7
2	B	366	SER	2.7
1	A	324	ALA	2.7
1	A	577	VAL	2.7
2	B	74	THR	2.7
2	B	119	ALA	2.7
2	B	142	PRO	2.7
1	A	346	ALA	2.7
2	B	583	VAL	2.7
1	A	633	ARG	2.7
3	C	56	TYR	2.6
1	A	582	MET	2.6
1	A	345	LEU	2.6
2	B	135	LEU	2.6
2	B	130	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	425	ALA	2.6
2	B	244	PHE	2.6
2	B	371	THR	2.6
2	B	171	LEU	2.6
2	B	73	ASN	2.6
2	B	294	ALA	2.6
2	B	4	THR	2.6
2	B	253	ILE	2.6
2	B	362	ILE	2.6
2	B	39	ILE	2.6
1	A	472	LEU	2.6
1	A	349	VAL	2.6
1	A	670	ILE	2.5
2	B	37	LEU	2.5
2	B	370	LYS	2.5
2	B	363	VAL	2.5
1	A	476	ILE	2.5
1	A	413	ARG	2.5
3	C	80	TYR	2.5
1	A	610	GLY	2.5
1	A	631	VAL	2.5
2	B	94	ALA	2.5
1	A	426	SER	2.5
1	A	696	LEU	2.5
2	B	210	ARG	2.5
3	C	109	ASP	2.5
2	B	50	PRO	2.5
2	B	329	ALA	2.5
3	C	1	GLN	2.5
2	B	375	SER	2.5
2	B	295	PRO	2.5
2	B	46	PHE	2.5
1	A	552	LYS	2.4
3	C	105	ARG	2.4
2	B	41	LEU	2.4
1	A	651	PRO	2.4
2	B	160	ALA	2.4
2	B	289	ALA	2.4
2	B	373	ILE	2.4
3	C	70	ILE	2.4
3	C	107	SER	2.4
1	A	567	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	26	GLY	2.4
1	A	549	PHE	2.4
1	A	789	ALA	2.4
2	B	23	LEU	2.4
2	B	48	ASP	2.4
1	A	506	MET	2.4
1	A	605	GLY	2.4
2	B	522	VAL	2.4
2	B	43	ALA	2.4
2	B	103	SER	2.4
2	B	401	GLU	2.4
1	A	573	GLY	2.4
2	B	269	GLY	2.4
1	A	483	VAL	2.4
2	B	242	VAL	2.4
2	B	374	LEU	2.3
2	B	529	ILE	2.3
1	A	480	VAL	2.3
2	B	32	ALA	2.3
2	B	65	LEU	2.3
1	A	446	ILE	2.3
1	A	363	GLU	2.3
2	B	27	SER	2.3
2	B	314	PRO	2.3
2	B	356	PRO	2.3
1	A	420	THR	2.3
2	B	61	THR	2.3
1	A	882	ARG	2.3
2	B	11	ALA	2.2
3	C	71	SER	2.2
3	C	103	GLN	2.2
1	A	464	PHE	2.2
2	B	255	PHE	2.2
1	A	658	ARG	2.2
3	C	100	ASP	2.2
2	B	124	LEU	2.2
1	A	571	VAL	2.2
1	A	783	VAL	2.2
2	B	524	HIS	2.2
2	B	296	ALA	2.2
2	B	78	GLY	2.2
2	B	257	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	433	ASP	2.2
1	A	615	MET	2.2
1	A	496	ILE	2.2
2	B	20	TYR	2.2
2	B	308	GLN	2.2
2	B	57	LEU	2.2
1	A	412	SER	2.2
1	A	378	ILE	2.2
1	A	590	PHE	2.2
1	A	786	ALA	2.1
2	B	235	THR	2.1
1	A	589	PRO	2.1
2	B	297	LEU	2.1
2	B	126	GLY	2.1
1	A	611	ILE	2.1
2	B	405	ALA	2.1
1	A	521	ARG	2.1
1	A	664	ARG	2.1
2	B	218	GLN	2.1
2	B	131	LEU	2.1
2	B	341	TYR	2.1
1	A	585	VAL	2.1
1	A	475	PHE	2.1
1	A	579	THR	2.1
1	A	432	GLN	2.1
1	A	656	LEU	2.1
2	B	163	GLY	2.1
2	B	531	HIS	2.1
3	C	-2	GLY	2.1
2	B	290	ILE	2.1
1	A	421	ARG	2.1
1	A	509	GLU	2.1
2	B	44	ALA	2.1
3	C	44	GLU	2.1
1	A	428	LYS	2.1
2	B	134	PRO	2.1
1	A	351	LEU	2.1
1	A	482	LEU	2.1
2	B	29	LEU	2.1
3	C	11	LEU	2.1
2	B	357	GLY	2.1
1	A	865	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	377	ILE	2.1
2	B	22	VAL	2.1
3	C	45	ARG	2.0
1	A	484	LEU	2.0
2	B	128	VAL	2.0
2	B	393	VAL	2.0
1	A	532	ARG	2.0
1	A	671	ARG	2.0
2	B	320	ARG	2.0
1	A	318	ALA	2.0
2	B	56	TRP	2.0
1	A	777	PRO	2.0
1	A	429	GLN	2.0
1	A	321	ARG	2.0
2	B	535	VAL	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](#)

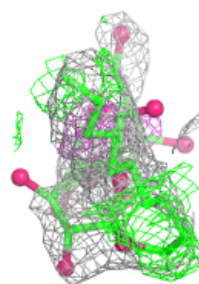
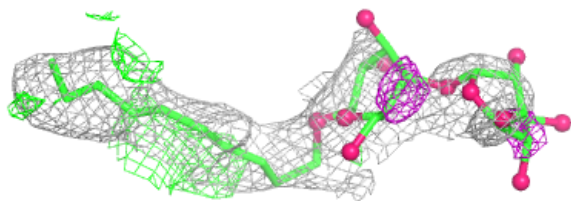
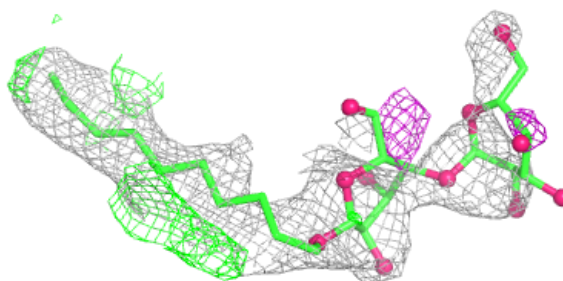
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	DMU	B	601	33/33	0.49	0.30	46,139,153,157	0
4	NI	A	1001	1/1	0.96	0.14	89,89,89,89	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 DMU B 601:

$2mF_o-DF_c$ (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.