Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 05:50 AM EDT

PDB ID	:	6TEJ
Title	:	Structure of apo IrtAB devoid SID in complex with sybody Syb_NL5
Authors	:	Gonda, I.; Arnold, F.M.; Hutter, C.A.J.; Weber, M.S.; Seeger, M.A.; Hurlimann, 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 (i) 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 (i)) were used in the production of this report:

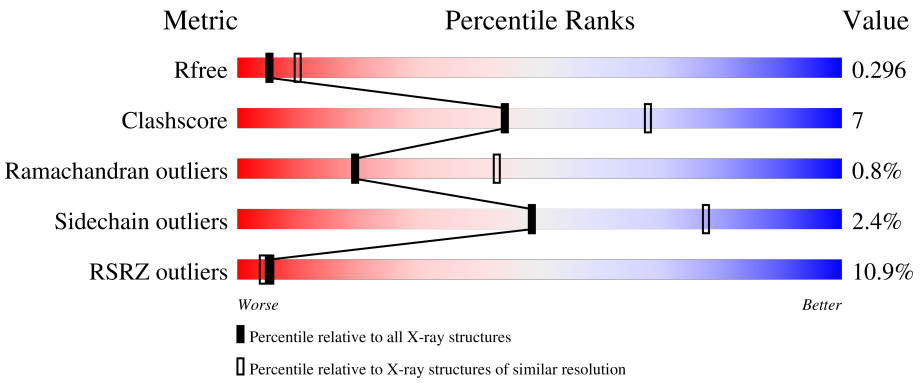
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	5%, 52%, 9%, •, 38%
2	B	586	16%, 81%, 18%, •
3	C	124	2%, 89%, 10%, •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMU	B	601	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	561	4179	2747	671	753	8	0	0	0

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

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

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

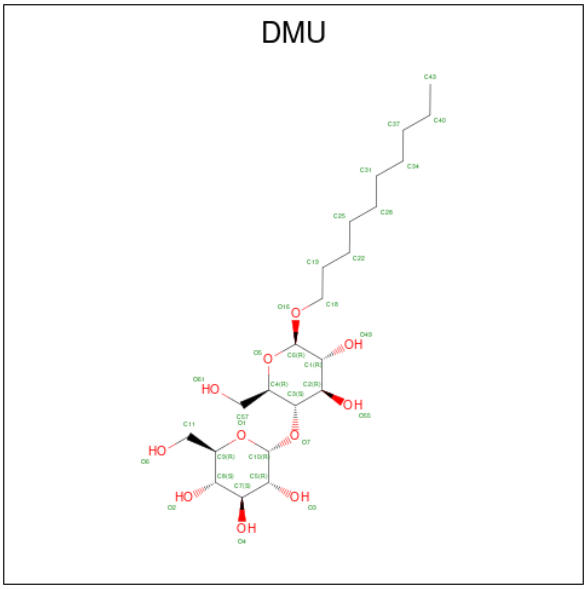
- Molecule 3 is a protein called Syb_NL5.

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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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



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

- Molecule 6 is water.

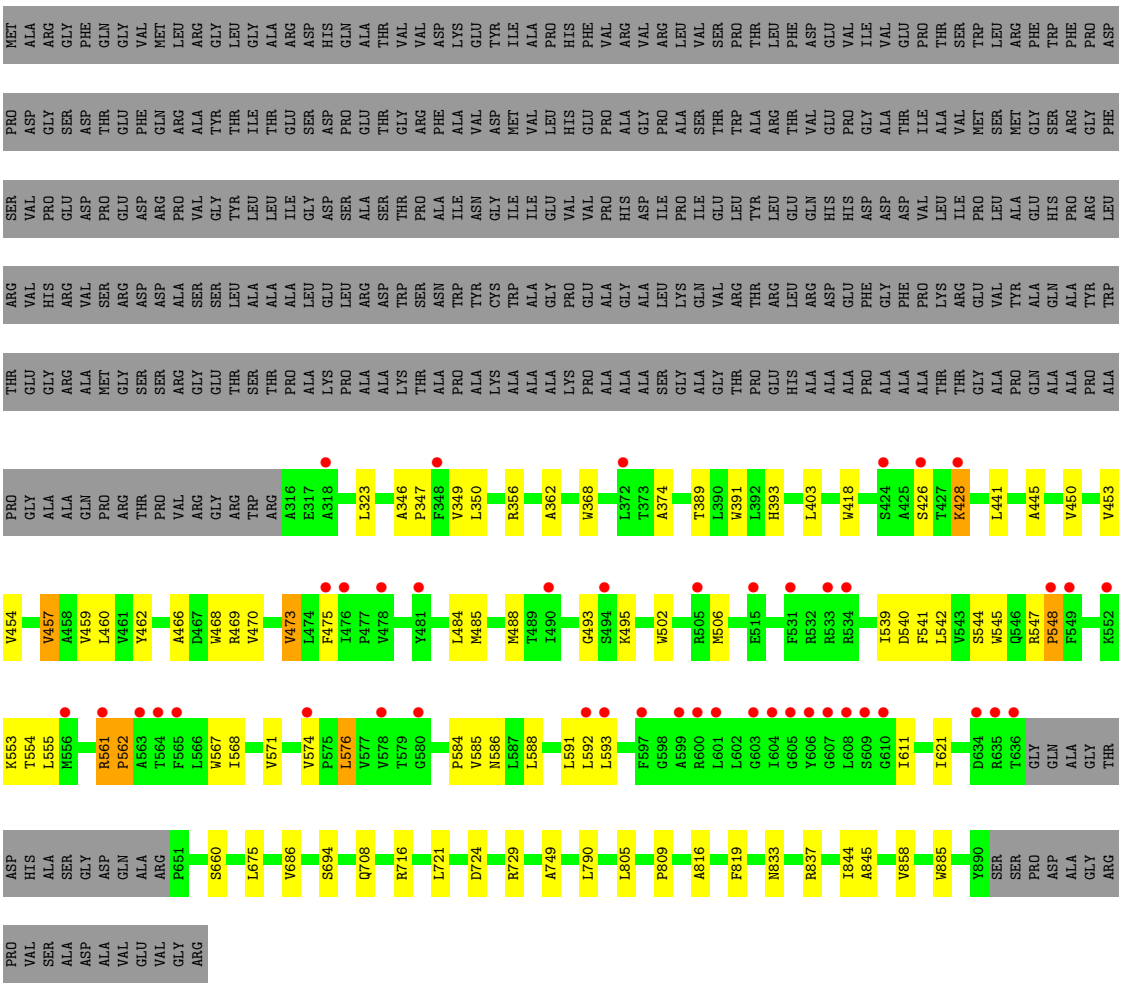
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	27	27	27	0	0
			Total	O		
6	B	22	22	22	0	0
			Total	O		
6	C	5	5	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

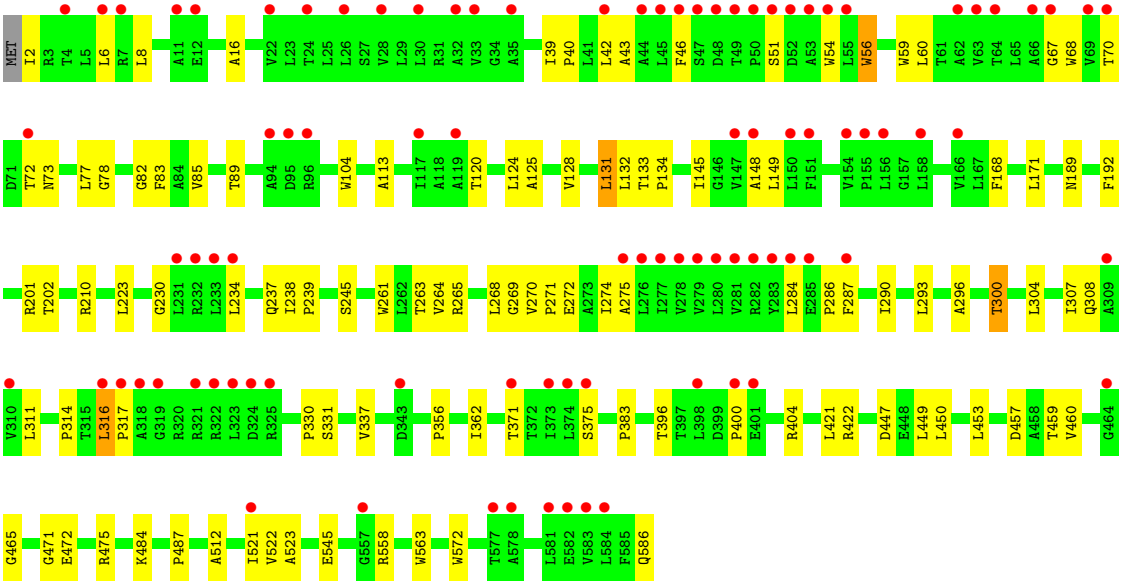
• Molecule 1: Drug ABC transporter ATP-binding protein

Chain A:



• Molecule 2: Drug ABC transporter ATP-binding protein

Chain B:



- Molecule 3: Syb_NL5

Chain C:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.59 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.264 , 0.296 0.264 , 0.296	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)	0.25 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.28	0/4248	0.48	0/5760
2	B	0.29	0/4292	0.48	0/5850
3	C	0.32	0/946	0.53	0/1275
All	All	0.29	0/9486	0.48	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 (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	4179	0	4233	52	0
2	B	4227	0	4242	70	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	123	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 (123) 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: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:716:ARG:HG2	1:A:721:LEU:HD21	1.88	0.56
1:A:426:SER:HB2	1:A:428:LYS:HG2	1.89	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:MET:HE1	1:A:554:THR:HG22	1.91	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: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
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: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:263:THR:C	2:B:265:ARG:H	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:131:LEU:C	2:B:134:PRO:HD2	2.39	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
1:A:541:PHE:O	1:A:544:SER:OG	2.27	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
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:447:ASP:N	2:B:447:ASP:OD1	2.53	0.42
2:B:145:ILE:HA	2:B:148:ALA:HB3	2.02	0.41
1:A:488:MET:HE3	1:A:488:MET:HB2	1.98	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
2:B:308:GLN:O	2:B:311:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	557/908 (61%)	524 (94%)	26 (5%)	7 (1%)	12	30
2	B	583/586 (100%)	548 (94%)	33 (6%)	2 (0%)	41	66
3	C	122/124 (98%)	117 (96%)	4 (3%)	1 (1%)	19	43
All	All	1262/1618 (78%)	1189 (94%)	63 (5%)	10 (1%)	19	43

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 (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	447/711 (63%)	438 (98%)	9 (2%)	55	81
2	B	438/439 (100%)	425 (97%)	13 (3%)	41	70
3	C	101/101 (100%)	99 (98%)	2 (2%)	55	81
All	All	986/1251 (79%)	962 (98%)	24 (2%)	49	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	ARG
1	A	428	LYS
1	A	457	VAL
1	A	460	LEU
1	A	473	VAL
1	A	475	PHE
1	A	586	ASN
1	A	724	ASP
1	A	790	LEU
2	B	2	ILE
2	B	6	LEU
2	B	42	LEU
2	B	56	TRP
2	B	73	ASN
2	B	131	LEU
2	B	168	PHE
2	B	171	LEU
2	B	210	ARG
2	B	245	SER
2	B	300	THR
2	B	316	LEU
2	B	586	GLN
3	C	57	TYR
3	C	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1.52	8 (23%)	45,45,45	1.49	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	-	-	6/19/59/59	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	4.22	1.54	1.44
5	B	601	DMU	C7-C5	-2.90	1.44	1.52
5	B	601	DMU	C11-C9	-2.83	1.42	1.51
5	B	601	DMU	O1-C10	2.39	1.47	1.41
5	B	601	DMU	O3-C5	2.37	1.48	1.43
5	B	601	DMU	O4-C7	2.37	1.48	1.43
5	B	601	DMU	C8-C9	2.15	1.57	1.53
5	B	601	DMU	O5-C6	2.07	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	DMU	C1-C2-C3	3.64	118.00	109.68
5	B	601	DMU	C7-C8-C9	3.60	116.67	110.24
5	B	601	DMU	C10-O7-C3	-3.20	110.05	117.96
5	B	601	DMU	C10-O1-C9	2.81	119.20	113.69
5	B	601	DMU	O1-C9-C8	2.70	114.59	109.69
5	B	601	DMU	C2-C3-C4	2.62	116.92	110.93
5	B	601	DMU	O16-C6-C1	2.39	112.03	108.30
5	B	601	DMU	C6-O5-C4	-2.33	109.11	113.69

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	DMU	C19-C18-O16-C6
5	B	601	DMU	C18-C19-C22-C25
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

There are no ring outliers.

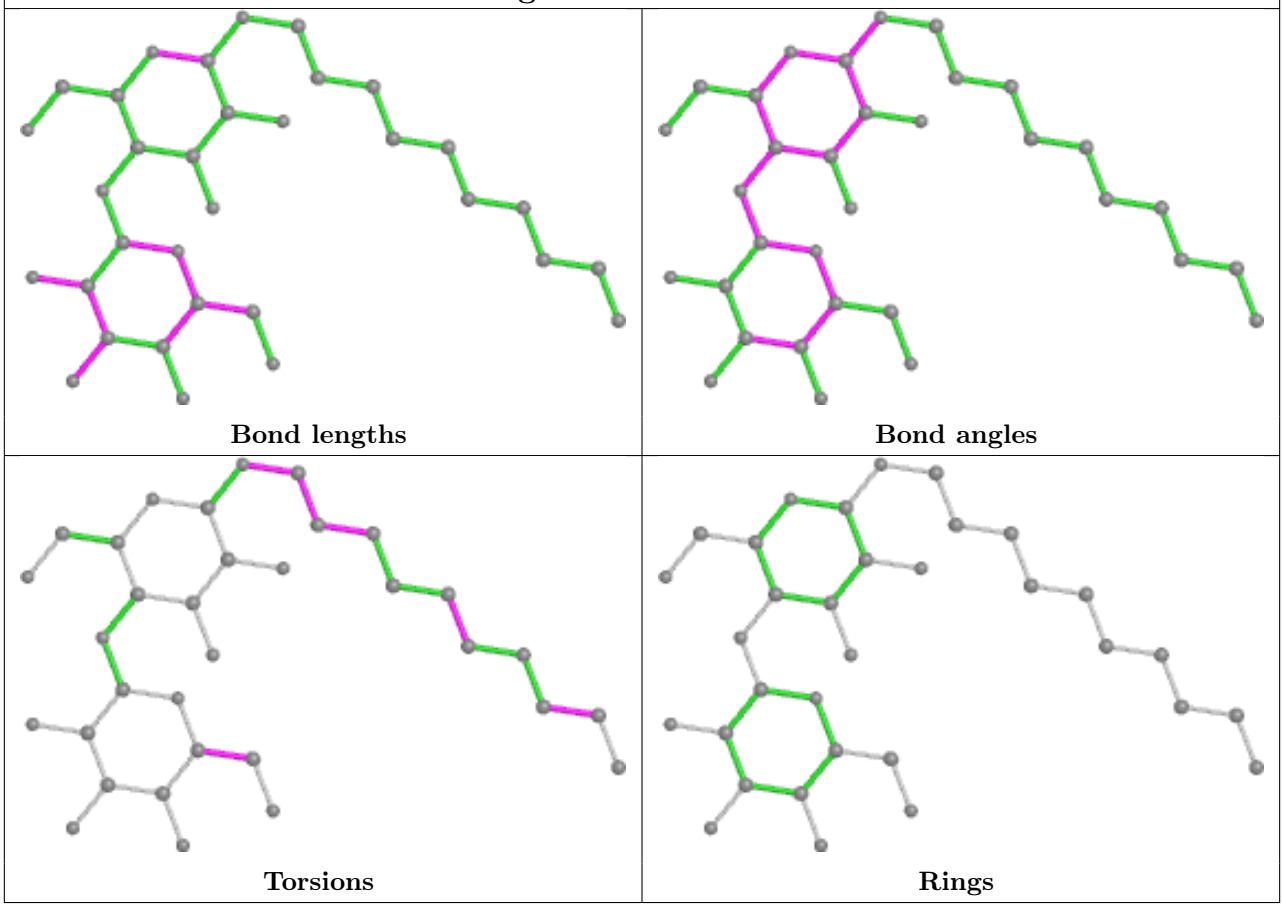
1 monomer is involved in 2 short contacts:

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 then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DMU B 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.35	45 (8%) 12 10	39, 80, 150, 171	0
2	B	585/586 (99%)	0.78	92 (15%) 2 1	37, 97, 156, 183	0
3	C	124/124 (100%)	0.20	2 (1%) 72 74	44, 70, 111, 132	0
All	All	1270/1618 (78%)	0.53	139 (10%) 5 4	37, 84, 153, 183	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	318	ALA	9.8
2	B	53	ALA	9.0
2	B	319	GLY	8.6
1	A	556	MET	8.1
1	A	608	LEU	8.0
1	A	605	GLY	7.8
2	B	321	ARG	7.6
2	B	147	VAL	7.6
2	B	158	LEU	7.3
2	B	323	LEU	7.3
2	B	578	ALA	7.1
2	B	54	TRP	6.7
2	B	284	LEU	6.5
2	B	33	VAL	6.4
2	B	48	ASP	6.3
1	A	424	SER	6.2
2	B	151	PHE	6.2
2	B	150	LEU	6.1
2	B	279	VAL	6.0
2	B	281	VAL	5.8
2	B	46	PHE	5.7
1	A	606	TYR	5.6
2	B	47	SER	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	232	ARG	5.5
2	B	155	PRO	5.5
2	B	55	LEU	5.2
2	B	280	LEU	5.1
2	B	309	ALA	4.9
2	B	42	LEU	4.9
2	B	45	LEU	4.8
1	A	552	LYS	4.8
2	B	66	ALA	4.8
1	A	549	PHE	4.8
2	B	324	ASP	4.8
2	B	343	ASP	4.6
2	B	11	ALA	4.6
2	B	156	LEU	4.4
1	A	565	PHE	4.3
2	B	283	TYR	4.3
2	B	69	VAL	4.2
2	B	154	VAL	4.2
2	B	26	LEU	4.2
2	B	52	ASP	4.2
1	A	533	ARG	4.1
1	A	607	GLY	4.1
2	B	310	VAL	4.0
2	B	70	THR	3.9
2	B	62	ALA	3.9
1	A	634	ASP	3.9
2	B	325	ARG	3.8
2	B	317	PRO	3.8
2	B	50	PRO	3.8
2	B	285	GLU	3.7
1	A	490	ILE	3.7
2	B	12	GLU	3.6
2	B	51	SER	3.5
2	B	557	GLY	3.5
1	A	635	ARG	3.5
2	B	282	ARG	3.5
2	B	166	VAL	3.4
1	A	636	THR	3.3
2	B	316	LEU	3.3
1	A	564	THR	3.3
1	A	593	LEU	3.3
2	B	287	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	603	GLY	3.2
2	B	278	VAL	3.1
2	B	44	ALA	3.1
3	C	121	ALA	3.1
1	A	478	VAL	3.0
2	B	63	VAL	3.0
2	B	581	LEU	3.0
2	B	35	ALA	2.9
1	A	548	PRO	2.9
2	B	96	ARG	2.9
1	A	609	SER	2.8
2	B	322	ARG	2.8
1	A	515	GLU	2.8
2	B	233	LEU	2.8
2	B	64	THR	2.8
1	A	531	PHE	2.8
2	B	49	THR	2.8
1	A	600	ARG	2.8
1	A	597	PHE	2.8
2	B	577	THR	2.8
1	A	601	LEU	2.8
2	B	72	THR	2.8
2	B	464	GLY	2.7
1	A	494	SER	2.7
2	B	30	LEU	2.6
2	B	117	ILE	2.6
2	B	398	LEU	2.6
1	A	561	ARG	2.6
2	B	95	ASP	2.5
1	A	610	GLY	2.5
2	B	6	LEU	2.5
1	A	534	ARG	2.5
2	B	28	VAL	2.5
2	B	4	THR	2.5
1	A	505	ARG	2.5
2	B	400	PRO	2.5
1	A	476	ILE	2.5
1	A	428	LYS	2.5
1	A	481	TYR	2.4
1	A	580	GLY	2.4
2	B	275	ALA	2.4
2	B	276	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	584	LEU	2.4
1	A	604	ILE	2.4
1	A	563	ALA	2.4
2	B	22	VAL	2.4
2	B	32	ALA	2.3
1	A	574	VAL	2.3
2	B	375	SER	2.3
2	B	7	ARG	2.2
1	A	475	PHE	2.2
1	A	426	SER	2.2
1	A	592	LEU	2.2
2	B	94	ALA	2.2
2	B	401	GLU	2.1
1	A	372	LEU	2.1
1	A	599	ALA	2.1
2	B	24	THR	2.1
2	B	231	LEU	2.1
2	B	277	ILE	2.1
2	B	521	ILE	2.1
1	A	348	PHE	2.1
2	B	582	GLU	2.1
2	B	119	ALA	2.1
2	B	67	GLY	2.1
1	A	578	VAL	2.1
1	A	318	ALA	2.1
2	B	371	THR	2.1
2	B	373	ILE	2.0
3	C	120	SER	2.0
2	B	374	LEU	2.0
2	B	148	ALA	2.0
2	B	234	LEU	2.0
2	B	583	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 monosaccharides in this entry.

6.4 Ligands (i)

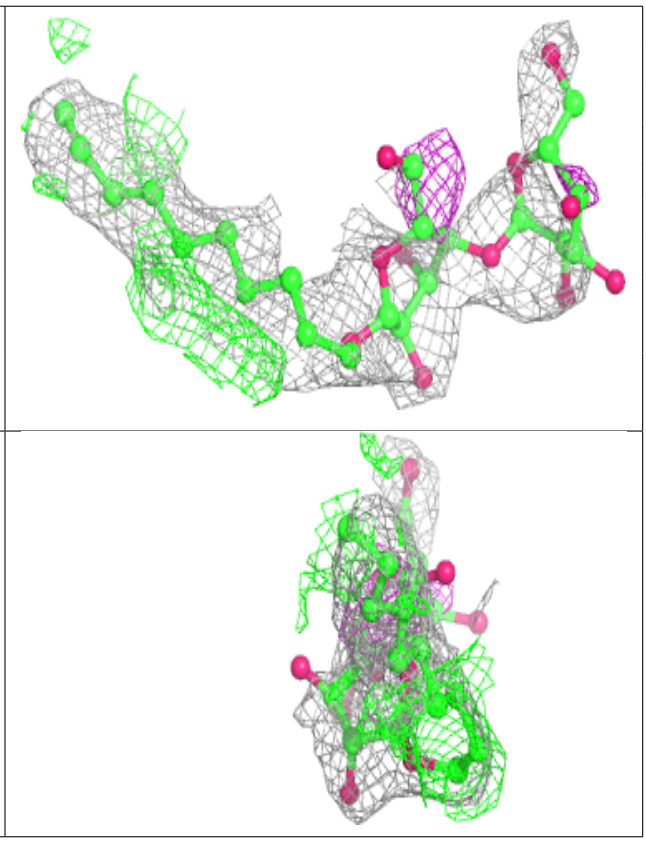
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

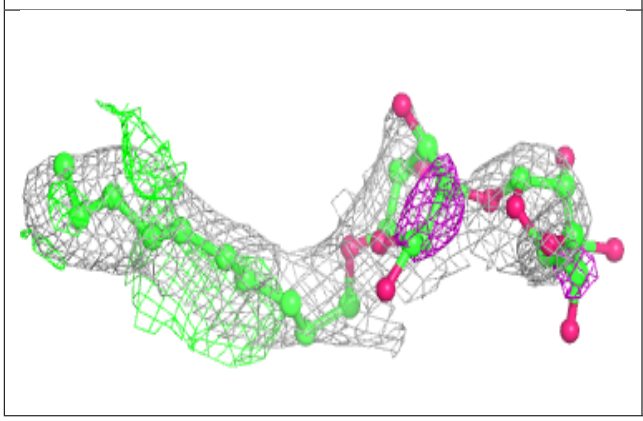
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMU	B	601	33/33	0.57	0.46	46,139,153,157	0
4	NI	A	1001	1/1	0.96	0.21	89,89,89,89	0

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.