



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:52 PM UTC

PDB ID : 9G4C / pdb_00009g4c
Title : 25-phosphosteroid lyase + phosphate + desmost-1,4-diene-3-one
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Deposited on : 2024-07-15
Resolution : 2.50 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

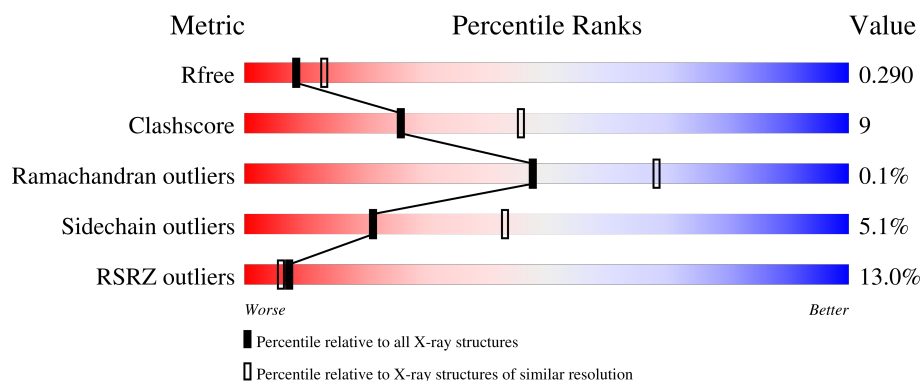
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	362	<div> <div>19%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	B	362	<div> <div>6%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	362	<div> <div>21%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	D	362	<div> <div>6%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23083 atoms, of which 11242 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 25-phosphosteroid lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	H	N	O	S	0	0	0
			5715	1860	2804	501	537	13			
1	B	361	Total	C	H	N	O	S	0	1	0
			5746	1869	2818	505	541	13			
1	C	360	Total	C	H	N	O	S	0	0	0
			5715	1860	2804	501	537	13			
1	D	361	Total	C	H	N	O	S	0	1	0
			5744	1869	2816	504	542	13			

There are 4 discrepancies between the modelled and reference sequences:

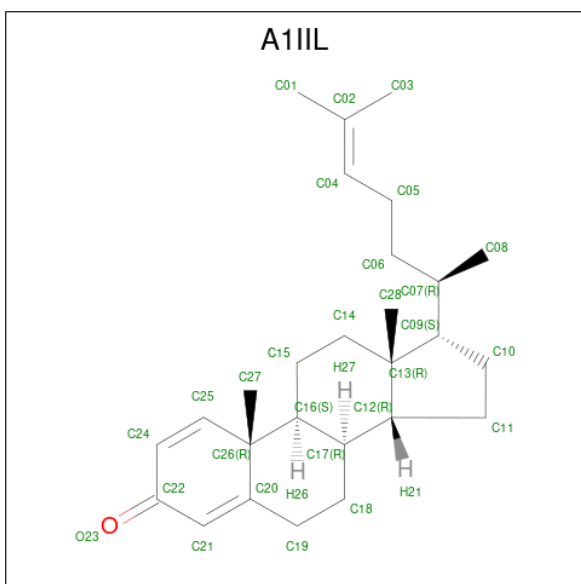
Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ASN	ASP	conflict	UNP A0A7Z7MWD0
B	176	ASN	ASP	conflict	UNP A0A7Z7MWD0
C	176	ASN	ASP	conflict	UNP A0A7Z7MWD0
D	176	ASN	ASP	conflict	UNP A0A7Z7MWD0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is (8 {R},9 {S},10 {R},13 {R},14 {R},17 {S})-10,13-dimethyl-17-[(2 {R})-6-methylhept-5-en-2-yl]-6,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-3-one (CCD ID: A1IIL) (formula: C₂₇H₄₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			28	27	1		
3	D	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	2	Total	Mg	0	1
			3	3		

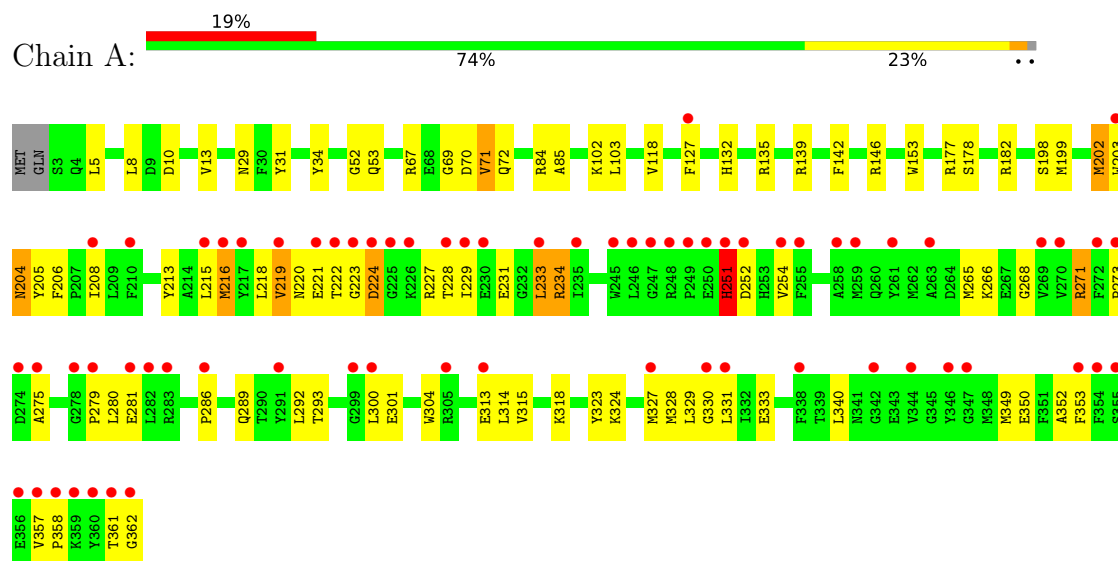
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	1
			17	17		
6	B	22	Total	O	0	1
			23	23		
6	C	17	Total	O	0	1
			18	18		
6	D	22	Total	O	0	0
			22	22		

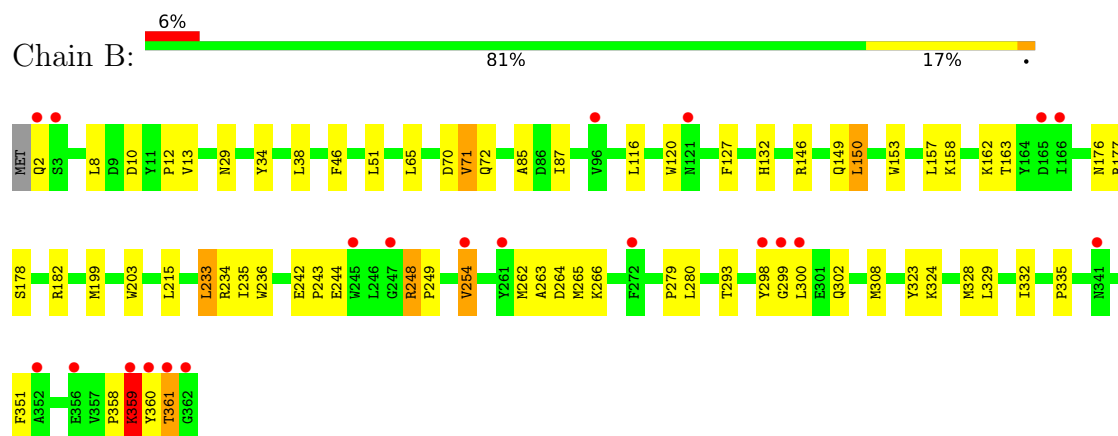
3 Residue-property plots [i](#)

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.

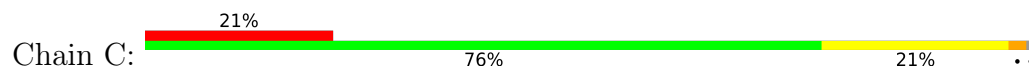
- Molecule 1: 25-phosphosteroid lyase

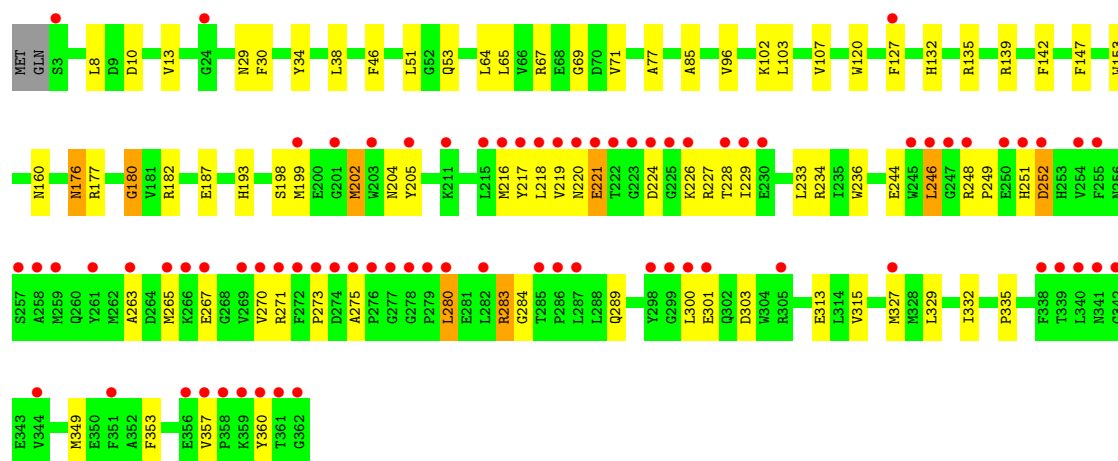


- Molecule 1: 25-phosphosteroid lyase

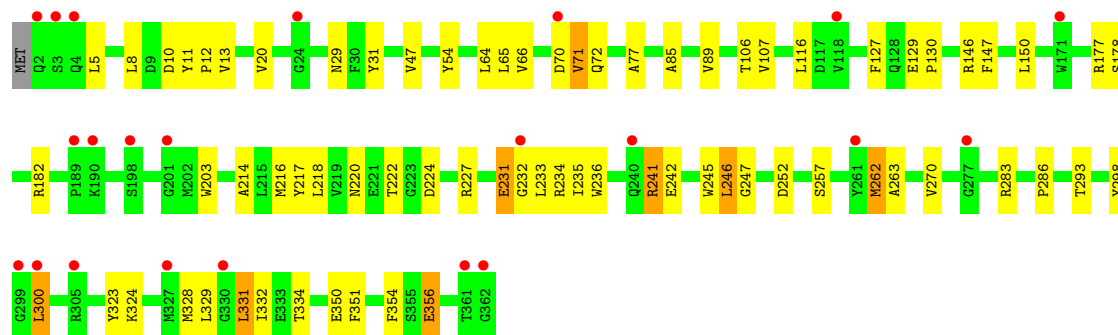
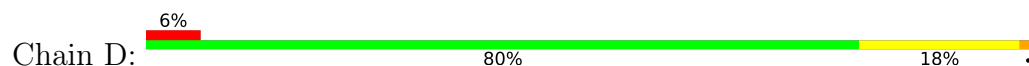


- Molecule 1: 25-phosphosteroid lyase





- Molecule 1: 25-phosphosteroid lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.26Å 155.48Å 96.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.50 48.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.74-2.50) 99.7 (48.74-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.290 0.239 , 0.290	Depositor DCC
R_{free} test set	3759 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23083	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6936e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1IIL, PO4, MG, CL

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	0.65	0/2993	0.90	5/4055 (0.1%)
1	B	0.69	1/3010 (0.0%)	0.86	4/4078 (0.1%)
1	C	0.72	3/2993 (0.1%)	0.91	7/4055 (0.2%)
1	D	0.74	2/3010 (0.1%)	0.88	1/4078 (0.0%)
All	All	0.70	6/12006 (0.0%)	0.89	17/16266 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	283	ARG	C-N	6.79	1.39	1.33
1	C	180	GLY	C-O	-6.70	1.20	1.24
1	D	232	GLY	C-O	-6.53	1.15	1.23
1	C	249	PRO	C-O	-6.20	1.17	1.23
1	B	249	PRO	C-O	-6.18	1.16	1.23
1	D	233	LEU	C-O	-5.18	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	ARG	CA-C-N	6.82	129.08	122.73
1	C	283	ARG	C-N-CA	6.82	129.08	122.73
1	A	251	HIS	CA-CB-CG	6.59	120.39	113.80
1	C	267	GLU	CA-C-N	6.54	126.20	119.92
1	C	267	GLU	C-N-CA	6.54	126.20	119.92
1	C	252	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	219	VAL	O-C-N	-5.96	117.79	122.97
1	A	223	GLY	CA-C-N	5.63	129.62	120.60
1	A	223	GLY	C-N-CA	5.63	129.62	120.60
1	B	248	ARG	N-CA-C	-5.51	99.46	109.44
1	C	252	ASP	CB-CA-C	5.42	119.84	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLY	N-CA-C	5.31	119.02	110.90
1	B	149	GLN	CA-C-N	5.23	130.78	122.94
1	B	149	GLN	C-N-CA	5.23	130.78	122.94
1	C	267	GLU	CA-C-O	-5.15	114.89	120.09
1	D	29	ASN	N-CA-C	5.11	119.23	113.15
1	B	150	LEU	N-CA-C	-5.02	101.22	109.40

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	2911	2804	2803	62	0
1	B	2928	2818	2816	47	0
1	C	2911	2804	2803	61	0
1	D	2928	2816	2814	54	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	B	28	0	0	6	0
3	D	28	0	0	6	0
4	B	1	0	0	0	0
4	C	2	0	0	1	0
5	B	1	0	0	0	0
5	D	3	0	0	0	0
6	A	17	0	0	2	0
6	B	23	0	0	0	0
6	C	18	0	0	0	0
6	D	22	0	0	1	0
All	All	11841	11242	11236	218	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 (218) 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:C:216:MET:HE3	1:C:218:LEU:HD23	1.49	0.94
1:B:176:ASN:ND2	3:B:401:A1IIL:C01	2.41	0.84
1:D:354:PHE:HE1	3:D:401:A1IIL:C27	1.96	0.78
1:C:275:ALA:CB	1:C:280:LEU:HD22	2.12	0.78
1:D:354:PHE:CE1	3:D:401:A1IIL:C27	2.67	0.76
1:B:176:ASN:HD21	3:B:401:A1IIL:C01	1.98	0.75
1:A:132:HIS:HE1	1:A:199:MET:HE2	1.52	0.74
1:A:132:HIS:CD2	1:A:229:ILE:HD11	2.23	0.73
1:A:203:TRP:C	1:A:204:ASN:HD22	2.00	0.70
1:B:358:PRO:HA	1:B:361:THR:O	1.95	0.66
1:A:204:ASN:HB2	1:A:219:VAL:HG12	1.76	0.65
1:A:132:HIS:CE1	1:A:199:MET:HE2	2.32	0.65
1:C:204:ASN:HB2	1:C:219:VAL:HG12	1.80	0.64
1:C:34:TYR:CE2	1:C:177:ARG:HD3	2.34	0.63
1:B:254:VAL:HG22	1:B:266:LYS:HB3	1.81	0.62
1:B:65:LEU:C	1:B:65:LEU:HD23	2.24	0.62
1:D:216:MET:HE2	1:D:218:LEU:HD23	1.82	0.62
1:A:132:HIS:HE1	1:A:199:MET:CE	2.13	0.62
1:A:293:THR:HG21	1:A:330:GLY:HA3	1.82	0.61
1:C:284:GLY:O	1:C:349:MET:HE1	2.00	0.61
1:D:293:THR:HG22	1:D:298:TYR:HB3	1.83	0.61
1:A:265:MET:HE1	1:A:268:GLY:HA2	1.83	0.60
1:C:132:HIS:ND1	1:C:229:ILE:HD11	2.16	0.60
1:A:70:ASP:CG	1:A:324:LYS:HE3	2.27	0.60
1:A:224:ASP:OD1	1:A:224:ASP:N	2.35	0.59
1:D:146:ARG:HG3	1:D:178:SER:HB3	1.83	0.59
1:A:67:ARG:NH1	1:A:69:GLY:O	2.35	0.59
1:D:231:GLU:OE1	1:D:231:GLU:HA	2.02	0.59
1:D:245:TRP:CZ2	1:D:247:GLY:HA2	2.37	0.59
1:C:284:GLY:HA3	1:C:349:MET:HE2	1.84	0.58
1:C:275:ALA:HB3	1:C:280:LEU:HD22	1.85	0.58
1:B:293:THR:HG22	1:B:298:TYR:HB3	1.86	0.58
1:C:8:LEU:HD13	1:D:13:VAL:HG12	1.86	0.58
1:D:129:GLU:OE1	1:D:146:ARG:HD2	2.04	0.57
1:A:202:MET:HG3	1:A:353:PHE:CE1	2.38	0.57
1:D:65:LEU:HD23	1:D:65:LEU:C	2.29	0.57
1:B:132:HIS:HE1	1:B:199:MET:HE2	1.68	0.57
1:A:216:MET:SD	1:A:218:LEU:HD23	2.45	0.57
1:A:358:PRO:HA	1:A:361:THR:HG22	1.87	0.57
1:D:263:ALA:O	1:D:332:ILE:CD1	2.53	0.57
1:C:202:MET:HG3	1:C:353:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HG	1:C:85:ALA:HB2	1.86	0.56
1:B:8:LEU:HG	1:B:85:ALA:HB2	1.87	0.56
1:B:70:ASP:OD2	1:B:324:LYS:HE3	2.06	0.56
1:B:234:ARG:HD3	1:B:236:TRP:CZ2	2.41	0.55
1:D:236:TRP:CD1	1:D:241:ARG:HG2	2.41	0.55
3:B:401:A1IIL:C28	3:B:401:A1IIL:C27	2.84	0.55
1:C:228:THR:HG22	1:C:229:ILE:HG13	1.87	0.55
1:A:265:MET:HE1	1:A:268:GLY:CA	2.36	0.55
1:D:262:MET:HE3	1:D:328:MET:O	2.06	0.55
1:D:8:LEU:HG	1:D:85:ALA:HB2	1.88	0.54
1:C:205:TYR:CE1	1:C:216:MET:HE1	2.41	0.54
3:B:401:A1IIL:C08	3:B:401:A1IIL:C14	2.85	0.54
1:D:203:TRP:O	1:D:351:PHE:HA	2.07	0.54
1:A:213:TYR:OH	1:A:340:LEU:HD23	2.07	0.54
1:A:142:PHE:HE1	1:A:198:SER:HB3	1.72	0.54
3:B:401:A1IIL:C02	2:B:402:PO4:O2	2.56	0.54
1:C:64:LEU:HD22	1:C:107:VAL:HG21	1.90	0.53
1:D:323:TYR:CE1	1:D:328:MET:HE2	2.43	0.53
1:A:31:TYR:CE1	1:A:182:ARG:HG2	2.43	0.53
6:A:504:HOH:O	1:C:193:HIS:HE1	1.92	0.53
1:B:127:PHE:CE1	1:B:235:ILE:HD13	2.44	0.52
1:A:70:ASP:OD2	1:A:324:LYS:HE3	2.09	0.52
1:D:146:ARG:HA	1:D:177:ARG:O	2.10	0.52
1:D:300:LEU:HD21	1:D:329:LEU:CD1	2.39	0.52
1:C:67:ARG:NH1	1:C:69:GLY:O	2.42	0.52
1:D:127:PHE:CE2	1:D:235:ILE:HD13	2.44	0.52
1:B:300:LEU:HD13	1:B:329:LEU:HD12	1.92	0.52
1:C:102:LYS:C	1:C:103:LEU:HD12	2.35	0.52
1:C:217:TYR:CE2	1:C:270:VAL:HG21	2.45	0.51
1:C:142:PHE:HE1	1:C:198:SER:HB3	1.75	0.51
1:D:286:PRO:HB3	1:D:334:THR:HG21	1.91	0.51
1:B:29:ASN:HB3	1:B:182:ARG:O	2.11	0.50
1:A:34:TYR:CE2	1:A:177:ARG:HD3	2.47	0.50
1:D:236:TRP:N	6:D:503:HOH:O	2.44	0.50
1:C:221:GLU:HG3	1:C:227:ARG:HE	1.77	0.50
1:C:228:THR:C	1:C:229:ILE:HG13	2.35	0.50
1:A:275:ALA:HB3	1:A:280:LEU:HD13	1.94	0.50
1:A:329:LEU:HD12	1:A:329:LEU:C	2.36	0.50
1:C:234:ARG:HB2	1:C:246:LEU:HD11	1.93	0.50
1:A:8:LEU:HG	1:A:85:ALA:HB2	1.93	0.50
1:A:8:LEU:HD13	1:B:13:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:C	1:B:51:LEU:HD23	2.37	0.49
1:A:102:LYS:C	1:A:103:LEU:HD12	2.36	0.49
1:C:65:LEU:C	1:C:65:LEU:HD23	2.36	0.49
1:B:38:LEU:HG	1:B:153:TRP:CD1	2.47	0.49
1:B:215:LEU:HD12	1:B:233:LEU:O	2.11	0.49
1:D:242:GLU:CD	1:D:242:GLU:H	2.21	0.49
1:A:254:VAL:HG11	1:A:266:LYS:HD2	1.95	0.49
1:A:204:ASN:HD22	1:A:204:ASN:N	2.11	0.49
1:B:132:HIS:CE1	1:B:199:MET:HE2	2.47	0.49
1:C:300:LEU:HD11	1:C:329:LEU:CD1	2.43	0.48
3:D:401:A1IIL:C08	3:D:401:A1IIL:C14	2.92	0.48
1:A:146:ARG:HG3	1:A:178:SER:HB3	1.96	0.48
1:B:120:TRP:HB2	1:B:153:TRP:CZ3	2.49	0.48
1:A:202:MET:HB2	1:A:357:VAL:HG21	1.94	0.48
1:A:218:LEU:HG	1:A:231:GLU:HB3	1.96	0.47
1:C:176:ASN:C	1:C:176:ASN:HD22	2.22	0.47
1:B:293:THR:HG22	1:B:298:TYR:CB	2.44	0.47
1:C:202:MET:HE3	1:C:360:TYR:CE2	2.50	0.47
1:C:251:HIS:O	1:C:251:HIS:CG	2.67	0.47
1:D:77:ALA:CB	1:D:89:VAL:HG12	2.45	0.47
1:A:314:LEU:HG	1:A:315:VAL:N	2.29	0.47
1:A:327:MET:O	1:A:327:MET:HG3	2.14	0.47
1:C:38:LEU:HG	1:C:153:TRP:CD1	2.50	0.47
1:D:246:LEU:CD1	1:D:246:LEU:N	2.77	0.47
1:D:300:LEU:HD21	1:D:329:LEU:HD11	1.96	0.47
1:A:103:LEU:HD12	1:A:103:LEU:N	2.29	0.47
1:B:71:VAL:CG1	1:B:72:GLN:N	2.77	0.47
1:A:29:ASN:HB3	1:A:182:ARG:O	2.15	0.47
1:B:146:ARG:HG3	1:B:178:SER:HB3	1.97	0.47
1:B:234:ARG:HD3	1:B:236:TRP:CE2	2.50	0.47
1:C:13:VAL:HG12	1:D:8:LEU:HD13	1.97	0.47
1:A:219:VAL:HA	1:A:229:ILE:O	2.15	0.47
1:D:106:THR:HA	1:D:116:LEU:O	2.15	0.47
1:B:34:TYR:CE2	1:B:177:ARG:HD3	2.50	0.46
1:B:242:GLU:HG3	1:B:243:PRO:HD2	1.97	0.46
1:B:298:TYR:CE1	3:B:401:A1IIL:C08	2.98	0.46
1:C:271:ARG:HA	1:C:280:LEU:O	2.15	0.46
1:A:220:ASN:C	1:A:220:ASN:ND2	2.72	0.46
1:B:279:PRO:C	1:B:280:LEU:HD12	2.40	0.46
1:A:13:VAL:HG12	1:B:8:LEU:HD13	1.97	0.46
1:D:71:VAL:CG1	1:D:72:GLN:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:THR:O	1:C:229:ILE:HG13	2.16	0.46
1:C:234:ARG:HD3	1:C:236:TRP:CZ2	2.51	0.46
1:C:30:PHE:HA	1:C:180:GLY:O	2.16	0.45
1:D:356:GLU:N	1:D:356:GLU:OE1	2.49	0.45
1:B:203:TRP:O	1:B:351:PHE:HA	2.17	0.45
1:D:64:LEU:HD22	1:D:107:VAL:HG21	1.98	0.45
1:A:205:TYR:HB3	1:A:350:GLU:HB3	1.98	0.45
1:D:77:ALA:HB1	1:D:89:VAL:HG12	1.98	0.45
1:A:205:TYR:CE1	1:A:216:MET:HE1	2.50	0.45
1:D:70[A]:ASP:OD1	1:D:70[A]:ASP:N	2.41	0.45
1:C:202:MET:HB2	1:C:357:VAL:HG21	1.98	0.45
1:C:233:LEU:HA	1:C:246:LEU:HD12	1.98	0.45
3:D:401:A1IIL:C08	3:D:401:A1IIL:C28	2.93	0.45
1:A:71:VAL:CG1	1:A:72:GLN:N	2.80	0.44
1:A:118:VAL:HG23	1:A:153:TRP:CZ3	2.52	0.44
1:A:84:ARG:O	1:B:12:PRO:HG2	2.17	0.44
1:B:300:LEU:CD1	1:B:329:LEU:HD12	2.47	0.44
1:C:283:ARG:HG2	1:C:283:ARG:NH1	2.32	0.44
1:B:263:ALA:O	1:B:332:ILE:CD1	2.66	0.44
1:A:279:PRO:C	1:A:280:LEU:HD12	2.43	0.44
1:C:147:PHE:CB	1:D:5:LEU:HD11	2.48	0.44
1:B:46:PHE:CD1	1:B:335:PRO:HD3	2.53	0.44
1:C:53:GLN:OE1	1:D:12:PRO:HB2	2.18	0.44
1:D:246:LEU:N	1:D:246:LEU:HD12	2.33	0.44
1:C:120:TRP:HB2	1:C:153:TRP:CZ3	2.52	0.44
1:C:218:LEU:HD12	1:C:218:LEU:C	2.42	0.43
1:B:359:LYS:HD2	1:B:359:LYS:HA	1.74	0.43
1:B:360:TYR:C	1:B:361:THR:HG22	2.42	0.43
1:D:245:TRP:CE2	1:D:247:GLY:HA2	2.53	0.43
1:C:202:MET:O	1:C:220:ASN:HA	2.19	0.43
1:A:304:TRP:HA	6:A:511:HOH:O	2.18	0.43
1:C:127:PHE:HZ	1:C:216:MET:HG2	1.83	0.43
1:B:233:LEU:HD22	1:B:235:ILE:HG13	1.99	0.43
1:C:283:ARG:HG2	1:C:283:ARG:HH11	1.84	0.43
1:D:216:MET:HE2	1:D:218:LEU:HB3	2.00	0.43
1:A:361:THR:HG23	1:A:362:GLY:N	2.34	0.43
1:C:301:GLU:HB3	1:C:303:ASP:OD1	2.18	0.43
1:D:331:LEU:HD21	1:D:350:GLU:HG3	2.00	0.43
1:D:218:LEU:C	1:D:218:LEU:HD12	2.44	0.43
1:A:286:PRO:HB2	1:A:289:GLN:HE21	1.83	0.43
1:A:331:LEU:HD12	1:A:352:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD13	1:B:157:LEU:HD13	2.01	0.43
1:A:8:LEU:HD13	1:B:13:VAL:CG1	2.48	0.42
1:A:206:PHE:CD1	1:A:349:MET:HA	2.54	0.42
1:D:217:TYR:CE2	1:D:270:VAL:HG21	2.54	0.42
1:A:228:THR:O	1:A:228:THR:HG22	2.18	0.42
1:C:218:LEU:HD11	1:C:229:ILE:HG22	1.99	0.42
1:A:361:THR:CG2	1:A:362:GLY:N	2.82	0.42
1:C:327:MET:O	1:C:327:MET:HG3	2.18	0.42
1:C:263:ALA:O	1:C:332:ILE:HD13	2.20	0.42
1:C:289:GLN:HG3	4:C:403:CL:CL	2.57	0.42
1:D:331:LEU:HD13	3:D:401:A1IIL:C28	2.49	0.42
1:A:227:ARG:NH2	1:A:251:HIS:CD2	2.87	0.42
1:B:233:LEU:HD23	1:B:234:ARG:N	2.34	0.42
1:C:34:TYR:CD2	1:C:177:ARG:HD3	2.54	0.42
1:C:46:PHE:CD1	1:C:335:PRO:HD3	2.54	0.42
1:D:234:ARG:HH11	1:D:234:ARG:HG3	1.84	0.42
1:C:176:ASN:ND2	2:C:401:PO4:O2	2.48	0.42
1:D:220:ASN:O	1:D:227:ARG:HA	2.19	0.42
1:A:53:GLN:OE1	1:B:12:PRO:HB2	2.19	0.42
1:A:127:PHE:CE1	1:A:216:MET:HG3	2.55	0.42
1:C:233:LEU:HD12	1:C:244:GLU:O	2.19	0.42
1:A:323:TYR:CD1	1:A:328:MET:HG3	2.55	0.42
1:B:120:TRP:CD1	1:B:120:TRP:C	2.98	0.42
1:B:158:LYS:HG2	1:B:163:THR:HG22	2.01	0.42
1:B:323:TYR:CE1	1:B:328:MET:HE2	2.55	0.42
1:A:233:LEU:HD23	1:A:234:ARG:N	2.35	0.41
1:C:29:ASN:HB3	1:C:182:ARG:O	2.19	0.41
1:D:147:PHE:CZ	1:D:177:ARG:HG3	2.54	0.41
1:A:292:LEU:HD22	1:A:333:GLU:OE2	2.20	0.41
1:D:31:TYR:CE1	1:D:182:ARG:HG2	2.55	0.41
1:D:47:VAL:HG22	1:D:66:VAL:HG22	2.01	0.41
1:D:129:GLU:HB3	1:D:130:PRO:CD	2.50	0.41
1:C:275:ALA:HB1	1:C:280:LEU:HD22	2.00	0.41
1:D:150:LEU:HD23	1:D:214:ALA:HB1	2.02	0.41
1:D:293:THR:HG22	1:D:298:TYR:CB	2.49	0.41
1:B:299:GLY:O	1:B:300:LEU:C	2.62	0.41
1:C:271:ARG:C	1:C:273:PRO:HD3	2.45	0.41
1:C:135:ARG:HA	1:C:139:ARG:O	2.20	0.41
1:D:222:THR:O	1:D:224:ASP:O	2.39	0.41
1:A:208:ILE:HD12	1:A:215:LEU:HD22	2.03	0.41
1:A:271:ARG:C	1:A:273:PRO:HD3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TYR:CD1	1:D:54:TYR:N	2.89	0.41
1:B:302:GLN:O	1:B:308:MET:HE1	2.19	0.41
1:C:77:ALA:HA	1:C:315:VAL:O	2.21	0.41
1:C:96:VAL:HG11	1:D:11:TYR:CE1	2.55	0.41
1:D:298:TYR:CD1	3:D:401:A1IIL:C08	3.03	0.41
1:B:87:ILE:O	1:B:87:ILE:HG22	2.21	0.41
1:C:51:LEU:C	1:C:51:LEU:HD23	2.46	0.41
1:C:176:ASN:C	1:C:176:ASN:ND2	2.78	0.41
1:A:218:LEU:HD12	1:A:218:LEU:C	2.46	0.40
1:A:135:ARG:HA	1:A:139:ARG:O	2.21	0.40
1:C:147:PHE:HB2	1:D:5:LEU:HD11	2.02	0.40
1:B:233:LEU:HD23	1:B:244:GLU:O	2.22	0.40
1:A:331:LEU:HD11	1:A:350:GLU:CG	2.52	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	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
1	B	360/362 (99%)	345 (96%)	14 (4%)	1 (0%)	36	55
1	C	358/362 (99%)	343 (96%)	15 (4%)	0	100	100
1	D	360/362 (99%)	348 (97%)	12 (3%)	0	100	100
All	All	1436/1448 (99%)	1381 (96%)	54 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	359	LYS

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	306/308 (99%)	287 (94%)	19 (6%)	16	34
1	B	308/308 (100%)	295 (96%)	13 (4%)	26	52
1	C	306/308 (99%)	290 (95%)	16 (5%)	21	42
1	D	308/308 (100%)	294 (96%)	14 (4%)	24	49
All	All	1228/1232 (100%)	1166 (95%)	62 (5%)	21	44

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	ASP
1	A	71	VAL
1	A	202	MET
1	A	204	ASN
1	A	216	MET
1	A	221	GLU
1	A	222	THR
1	A	224	ASP
1	A	233	LEU
1	A	234	ARG
1	A	251	HIS
1	A	252	ASP
1	A	271	ARG
1	A	281	GLU
1	A	300	LEU
1	A	301	GLU
1	A	313	GLU
1	A	318	LYS
1	B	2	GLN
1	B	10	ASP
1	B	71	VAL
1	B	150	LEU
1	B	162	LYS

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Mol	Chain	Res	Type
1	B	233	LEU
1	B	248	ARG
1	B	254	VAL
1	B	262	MET
1	B	264	ASP
1	B	265	MET
1	B	359	LYS
1	B	361	THR
1	C	10	ASP
1	C	71	VAL
1	C	160	ASN
1	C	176	ASN
1	C	187	GLU
1	C	199	MET
1	C	202	MET
1	C	221	GLU
1	C	224	ASP
1	C	226	LYS
1	C	246	LEU
1	C	248	ARG
1	C	252	ASP
1	C	265	MET
1	C	280	LEU
1	C	313	GLU
1	D	10	ASP
1	D	20	VAL
1	D	71	VAL
1	D	231	GLU
1	D	241	ARG
1	D	246	LEU
1	D	252	ASP
1	D	257	SER
1	D	262	MET
1	D	283	ARG
1	D	300	LEU
1	D	324	LYS
1	D	331	LEU
1	D	356	GLU

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	132	HIS
1	A	137	HIS
1	A	193	HIS
1	A	204	ASN
1	A	220	ASN
1	A	306	HIS
1	B	137	HIS
1	B	204	ASN
1	B	220	ASN
1	B	256	ASN
1	C	22	HIS
1	C	110	ASN
1	C	121	ASN
1	C	137	HIS
1	C	176	ASN
1	C	193	HIS
1	C	220	ASN
1	D	137	HIS

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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
3	A1IIL	B	401	-	31,31,31	2.50	11 (35%)	48,48,48	5.74	35 (72%)
2	PO4	C	401	-	4,4,4	1.19	0	6,6,6	0.78	0
2	PO4	B	402	-	4,4,4	1.30	0	6,6,6	0.96	0
2	PO4	A	401	-	4,4,4	1.20	1 (25%)	6,6,6	0.60	0
3	A1IIL	D	401	-	31,31,31	2.36	5 (16%)	48,48,48	6.06	33 (68%)
2	PO4	D	402	-	4,4,4	1.40	0	6,6,6	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1IIL	B	401	-	-	1/10/68/68	0/4/4/4
3	A1IIL	D	401	-	-	3/10/68/68	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	A1IIL	C26-C16	7.88	1.68	1.57
3	B	401	A1IIL	C15-C16	5.34	1.62	1.53
3	B	401	A1IIL	C13-C09	-5.25	1.45	1.55
3	D	401	A1IIL	C18-C17	-5.09	1.44	1.53
3	D	401	A1IIL	C13-C09	-4.81	1.46	1.55
3	B	401	A1IIL	C13-C12	-4.69	1.46	1.55
3	B	401	A1IIL	C19-C20	-4.61	1.42	1.50
3	B	401	A1IIL	C14-C13	-4.35	1.46	1.54
3	D	401	A1IIL	C13-C12	-4.20	1.47	1.55
3	D	401	A1IIL	C15-C16	3.31	1.59	1.53
3	B	401	A1IIL	C11-C12	-3.15	1.48	1.54
3	B	401	A1IIL	C06-C07	-3.08	1.46	1.54
3	B	401	A1IIL	C24-C22	2.69	1.52	1.46
3	B	401	A1IIL	C18-C17	-2.69	1.48	1.53
3	B	401	A1IIL	C10-C09	-2.67	1.48	1.54
3	B	401	A1IIL	C26-C20	-2.30	1.49	1.51
2	A	401	PO4	P-O1	2.18	1.55	1.50

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	A1IIL	C19-C20-C26	22.38	133.48	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	A1IIL	C26-C16-C17	-19.28	97.03	112.07
3	B	401	A1IIL	C19-C20-C26	18.61	130.52	115.86
3	B	401	A1IIL	C26-C16-C17	-12.73	102.14	112.07
3	B	401	A1IIL	C14-C13-C12	-12.05	89.21	107.25
3	B	401	A1IIL	C08-C07-C09	-11.92	94.99	112.88
3	D	401	A1IIL	C27-C26-C16	-10.02	103.55	111.73
3	B	401	A1IIL	C27-C26-C16	-9.48	103.99	111.73
3	D	401	A1IIL	C18-C17-C16	8.44	120.63	110.52
3	B	401	A1IIL	C28-C13-C12	8.35	126.83	111.68
3	D	401	A1IIL	C19-C20-C21	-8.29	107.61	120.86
3	D	401	A1IIL	C25-C26-C20	8.20	119.73	111.76
3	B	401	A1IIL	C14-C13-C09	-8.02	104.78	116.60
3	B	401	A1IIL	C25-C26-C20	7.85	119.39	111.76
3	B	401	A1IIL	C19-C20-C21	-7.80	108.39	120.86
3	D	401	A1IIL	C28-C13-C12	7.47	125.23	111.68
3	B	401	A1IIL	C15-C16-C26	7.20	120.31	113.55
3	D	401	A1IIL	C28-C13-C14	-7.17	100.04	110.61
3	B	401	A1IIL	C13-C12-C17	-7.02	104.44	114.41
3	D	401	A1IIL	C14-C13-C12	-6.96	96.82	107.25
3	D	401	A1IIL	C19-C18-C17	-6.45	100.34	111.64
3	D	401	A1IIL	C06-C05-C04	-6.03	96.32	112.16
3	B	401	A1IIL	C10-C09-C13	5.76	110.62	103.84
3	D	401	A1IIL	C13-C12-C17	-5.72	106.30	114.41
3	B	401	A1IIL	C27-C26-C25	-5.60	89.93	107.75
3	D	401	A1IIL	C26-C20-C21	-5.28	118.85	122.32
3	B	401	A1IIL	C18-C17-C12	5.05	120.47	112.08
3	D	401	A1IIL	C13-C09-C07	-4.99	111.79	119.50
3	B	401	A1IIL	C15-C16-C17	-4.97	104.84	111.78
3	B	401	A1IIL	C28-C13-C09	4.72	120.23	111.68
3	D	401	A1IIL	C03-C02-C01	4.61	125.21	114.59
3	B	401	A1IIL	C16-C26-C20	4.56	112.06	107.49
3	B	401	A1IIL	C11-C12-C13	4.51	109.14	103.84
3	D	401	A1IIL	C11-C12-C13	4.43	109.05	103.84
3	D	401	A1IIL	C10-C09-C13	4.23	108.82	103.84
3	D	401	A1IIL	C27-C26-C25	-4.20	94.38	107.75
3	B	401	A1IIL	C16-C17-C12	4.19	114.56	109.09
3	D	401	A1IIL	C18-C19-C20	-4.13	104.36	111.93
3	D	401	A1IIL	C15-C16-C26	4.07	117.38	113.55
3	D	401	A1IIL	C05-C04-C02	-4.03	114.21	127.64
3	D	401	A1IIL	C25-C24-C22	-3.99	118.12	121.49
3	B	401	A1IIL	C18-C19-C20	-3.98	104.63	111.93
3	B	401	A1IIL	C14-C15-C16	3.77	119.54	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	A1IIL	C18-C17-C12	-3.70	105.93	112.08
3	D	401	A1IIL	C28-C13-C09	3.49	118.01	111.68
3	D	401	A1IIL	C24-C22-C21	3.47	120.64	117.12
3	D	401	A1IIL	C11-C10-C09	-3.37	98.54	105.14
3	D	401	A1IIL	C08-C07-C06	-3.19	105.40	110.34
3	B	401	A1IIL	C08-C07-C06	-3.18	105.41	110.34
3	B	401	A1IIL	C06-C05-C04	-3.14	103.91	112.16
3	B	401	A1IIL	C20-C21-C22	-3.13	119.88	122.72
3	B	401	A1IIL	C16-C26-C25	3.05	119.82	110.46
3	D	401	A1IIL	C16-C26-C25	3.04	119.78	110.46
3	B	401	A1IIL	C10-C09-C07	2.88	116.54	112.18
3	B	401	A1IIL	C13-C09-C07	-2.70	115.32	119.50
3	B	401	A1IIL	C06-C07-C09	-2.69	104.75	110.33
3	B	401	A1IIL	C26-C25-C24	-2.68	120.15	124.28
3	D	401	A1IIL	C10-C09-C07	2.53	116.00	112.18
3	D	401	A1IIL	C27-C26-C20	2.49	111.76	108.66
3	D	401	A1IIL	C05-C06-C07	-2.37	109.77	114.58
3	B	401	A1IIL	C24-C22-C21	2.35	119.50	117.12
3	B	401	A1IIL	C25-C24-C22	-2.26	119.58	121.49
3	B	401	A1IIL	C19-C18-C17	-2.26	107.68	111.64
3	B	401	A1IIL	C05-C04-C02	-2.25	120.14	127.64
3	D	401	A1IIL	C06-C07-C09	-2.19	105.79	110.33
3	D	401	A1IIL	C03-C02-C04	-2.14	116.25	122.66
3	B	401	A1IIL	O23-C22-C21	-2.03	118.54	121.43
3	B	401	A1IIL	C26-C20-C21	-2.01	121.00	122.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	A1IIL	C04-C05-C06-C07
3	B	401	A1IIL	C04-C05-C06-C07
3	D	401	A1IIL	C06-C07-C09-C10
3	D	401	A1IIL	C06-C07-C09-C13

There are no ring outliers.

4 monomers are involved in 13 short contacts:

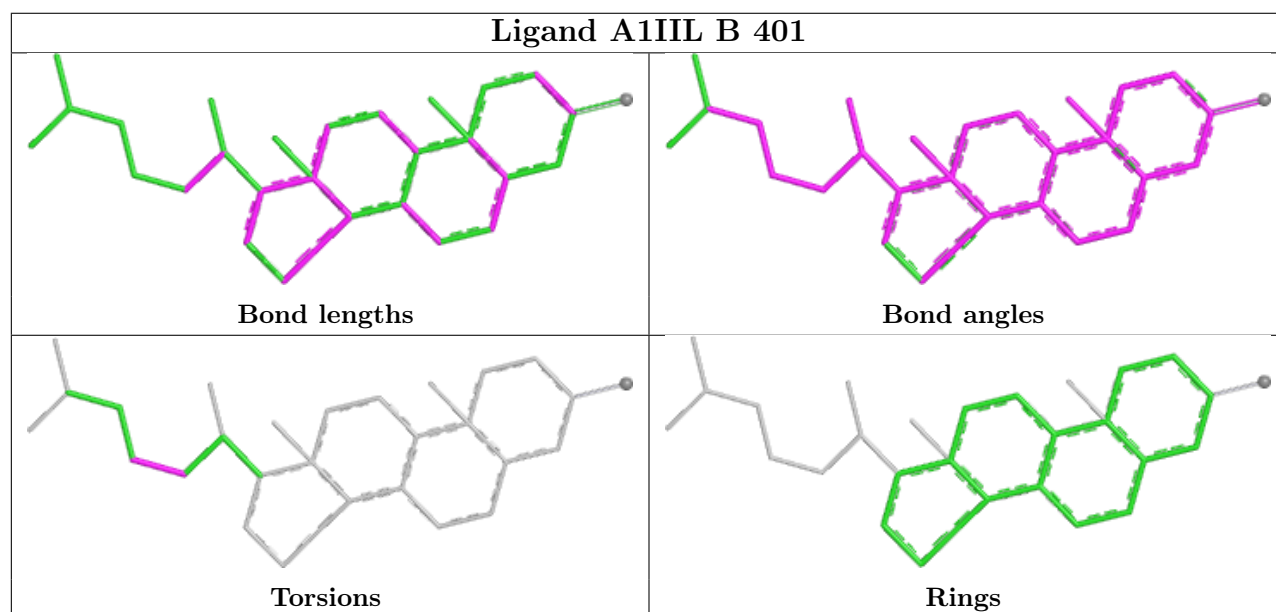
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	A1IIL	6	0
2	C	401	PO4	1	0

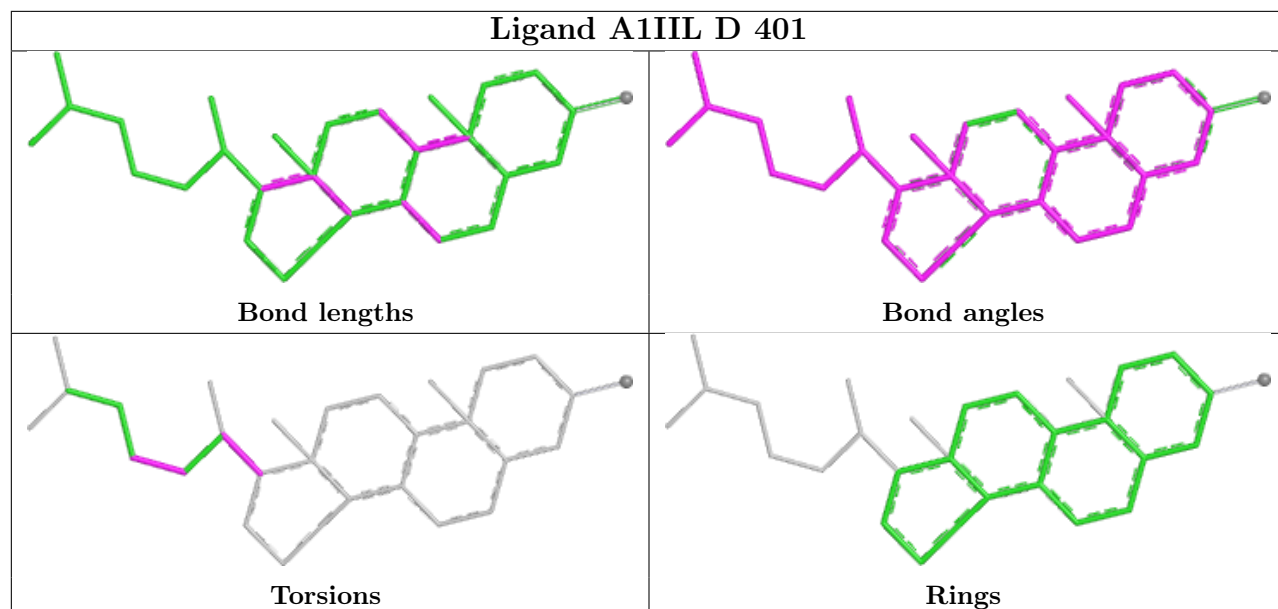
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	PO4	1	0
3	D	401	A1IIL	6	0

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 [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	360/362 (99%)	0.92	68 (18%) 3 2	46, 77, 138, 157	0
1	B	361/362 (99%)	0.56	21 (5%) 29 25	34, 68, 98, 120	1 (0%)
1	C	360/362 (99%)	0.98	76 (21%) 2 2	48, 78, 136, 157	0
1	D	361/362 (99%)	0.60	22 (6%) 27 23	41, 65, 93, 117	1 (0%)
All	All	1442/1448 (99%)	0.76	187 (12%) 7 6	34, 70, 126, 157	2 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	GLY	5.4
1	B	3	SER	5.2
1	C	222	THR	5.1
1	B	359	LYS	5.0
1	C	285	THR	4.9
1	A	361	THR	4.7
1	B	121[A]	ASN	4.6
1	D	300	LEU	4.6
1	A	357	VAL	4.6
1	A	360	TYR	4.6
1	C	300	LEU	4.5
1	A	228	THR	4.5
1	C	273	PRO	4.4
1	D	361	THR	4.3
1	C	226	LYS	4.3
1	C	201	GLY	4.2
1	A	222	THR	4.2
1	C	269	VAL	4.2
1	A	300	LEU	4.2
1	A	362	GLY	4.1
1	A	273	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	300	LEU	4.1
1	B	247	GLY	4.0
1	C	221	GLU	4.0
1	C	228	THR	4.0
1	C	279	PRO	3.9
1	C	245	TRP	3.8
1	A	225	GLY	3.8
1	B	299	GLY	3.7
1	C	276	PRO	3.7
1	A	272	PHE	3.7
1	D	3	SER	3.6
1	A	299	GLY	3.6
1	D	362	GLY	3.6
1	A	254	VAL	3.6
1	C	223	GLY	3.6
1	C	361	THR	3.6
1	A	358	PRO	3.6
1	A	252	ASP	3.6
1	A	279	PRO	3.5
1	A	247	GLY	3.5
1	C	252	ASP	3.5
1	A	344	VAL	3.5
1	C	247	GLY	3.4
1	A	224	ASP	3.3
1	C	224	ASP	3.3
1	C	356	GLU	3.3
1	A	251	HIS	3.3
1	C	298	TYR	3.2
1	C	250	GLU	3.2
1	C	287	LEU	3.2
1	A	261	TYR	3.2
1	C	299	GLY	3.2
1	C	272	PHE	3.2
1	C	217	TYR	3.2
1	A	355	SER	3.1
1	A	245	TRP	3.1
1	C	270	VAL	3.1
1	C	261	TYR	3.1
1	A	263	ALA	3.1
1	C	282	LEU	3.1
1	A	269	VAL	3.1
1	C	248	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	261	TYR	3.0
1	C	259	MET	3.0
1	C	278	GLY	3.0
1	C	254	VAL	3.0
1	C	3	SER	3.0
1	C	203	TRP	2.9
1	A	226	LYS	2.9
1	C	246	LEU	2.9
1	D	70[A]	ASP	2.9
1	D	4	GLN	2.9
1	A	229	ILE	2.9
1	B	96	VAL	2.9
1	A	342	GLY	2.9
1	C	216	MET	2.9
1	C	220	ASN	2.9
1	C	342	GLY	2.9
1	C	359	LYS	2.9
1	A	274	ASP	2.9
1	C	257	SER	2.8
1	A	208	ILE	2.8
1	A	359	LYS	2.8
1	D	330	GLY	2.8
1	A	210	PHE	2.8
1	B	362	GLY	2.7
1	C	286	PRO	2.7
1	A	230	GLU	2.7
1	C	274	ASP	2.7
1	C	271	ARG	2.7
1	C	230	GLU	2.7
1	C	251	HIS	2.7
1	C	341	ASN	2.7
1	A	216	MET	2.7
1	A	221	GLU	2.7
1	A	313	GLU	2.7
1	A	305	ARG	2.7
1	A	356	GLU	2.7
1	C	266	LYS	2.6
1	D	190	LYS	2.6
1	C	215	LEU	2.6
1	C	275	ALA	2.6
1	B	298	TYR	2.6
1	A	283	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	127	PHE	2.6
1	C	218	LEU	2.6
1	A	258	ALA	2.6
1	B	361	THR	2.6
1	A	347	GLY	2.6
1	C	255	PHE	2.6
1	C	267	GLU	2.6
1	C	219	VAL	2.6
1	D	305	ARG	2.5
1	B	356	GLU	2.5
1	C	280	LEU	2.5
1	D	2	GLN	2.5
1	A	219	VAL	2.5
1	C	344	VAL	2.5
1	C	362	GLY	2.5
1	A	282	LEU	2.5
1	A	338	PHE	2.5
1	C	263	ALA	2.5
1	C	265	MET	2.5
1	A	217	TYR	2.5
1	A	215	LEU	2.5
1	A	275	ALA	2.5
1	D	277	GLY	2.4
1	A	353	PHE	2.4
1	A	330	GLY	2.4
1	C	340	LEU	2.4
1	D	118	VAL	2.4
1	A	278	GLY	2.4
1	B	165	ASP	2.4
1	C	327	MET	2.4
1	C	357	VAL	2.4
1	C	277	GLY	2.3
1	D	299	GLY	2.3
1	A	248	ARG	2.3
1	A	354	PHE	2.3
1	C	360	TYR	2.3
1	A	203	TRP	2.3
1	D	24	GLY	2.3
1	A	246	LEU	2.3
1	B	254	VAL	2.3
1	B	360	TYR	2.3
1	A	235	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	261	TYR	2.3
1	C	258	ALA	2.3
1	B	2	GLN	2.3
1	C	225	GLY	2.3
1	C	229	ILE	2.3
1	C	301	GLU	2.3
1	C	338	PHE	2.3
1	A	255	PHE	2.2
1	A	286	PRO	2.2
1	A	259	MET	2.2
1	D	327	MET	2.2
1	C	305	ARG	2.2
1	C	205	TYR	2.2
1	C	211	LYS	2.2
1	A	327	MET	2.2
1	A	331	LEU	2.2
1	D	189	PRO	2.2
1	B	341	ASN	2.2
1	C	24	GLY	2.2
1	A	270	VAL	2.1
1	D	201	GLY	2.1
1	A	127	PHE	2.1
1	B	245	TRP	2.1
1	A	291	TYR	2.1
1	C	358	PRO	2.1
1	A	250	GLU	2.1
1	A	281	GLU	2.1
1	A	346	TYR	2.1
1	B	272	PHE	2.0
1	B	352	ALA	2.0
1	A	233	LEU	2.0
1	D	232	GLY	2.0
1	A	249	PRO	2.0
1	C	199	MET	2.0
1	D	198	SER	2.0
1	D	240	GLN	2.0
1	C	351	PHE	2.0
1	B	166	ILE	2.0
1	C	339	THR	2.0
1	D	171	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

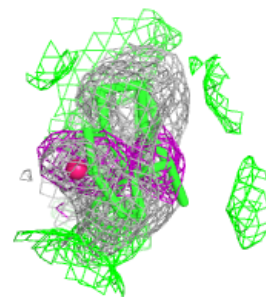
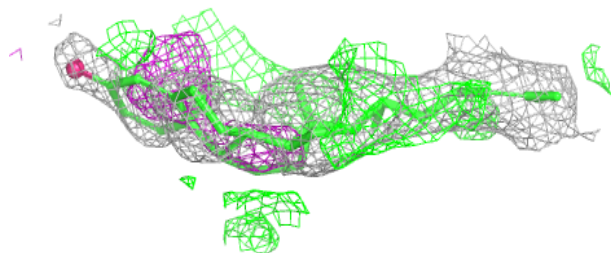
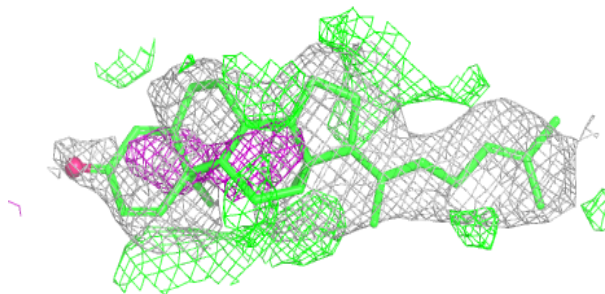
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1IIL	B	401	28/28	0.63	0.32	53,77,87,96	0
3	A1IIL	D	401	28/28	0.76	0.29	57,88,99,100	0
5	MG	D	404	1/1	0.76	0.29	75,75,75,75	0
4	CL	C	403	1/1	0.79	0.15	89,89,89,89	0
5	MG	B	404	1/1	0.80	0.22	82,82,82,82	0
2	PO4	C	401	5/5	0.80	0.19	64,70,77,78	0
4	CL	B	403	1/1	0.85	0.19	84,84,84,84	0
4	CL	C	402	1/1	0.87	0.16	90,90,90,90	0
2	PO4	A	401	5/5	0.88	0.18	57,61,71,72	0
2	PO4	B	402	5/5	0.90	0.18	56,64,71,74	0
2	PO4	D	402	5/5	0.91	0.15	64,66,70,72	0
5	MG	D	403[B]	1/1	0.95	0.42	46,46,46,46	1
5	MG	D	403[A]	1/1	0.95	0.42	37,37,37,37	1

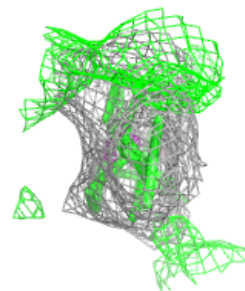
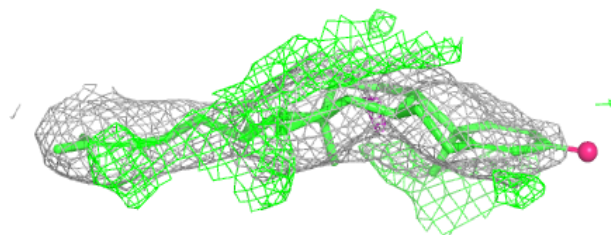
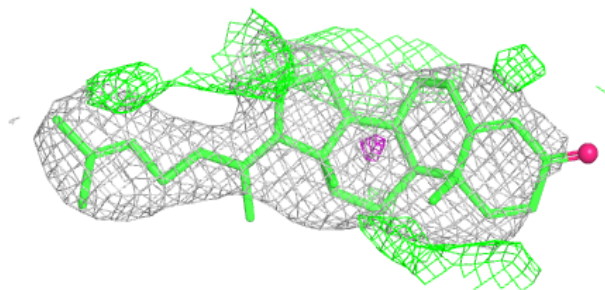
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IIL B 401:

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

**Electron density around A1IIL D 401:**

$2mF_o-DF_c$ (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.