



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:47 pm BST

PDB ID : 4JIB
Title : Crystal structure of of PDE2-inhibitor complex
Authors : Pandit, J.
Deposited on : 2013-03-05
Resolution : 1.72 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

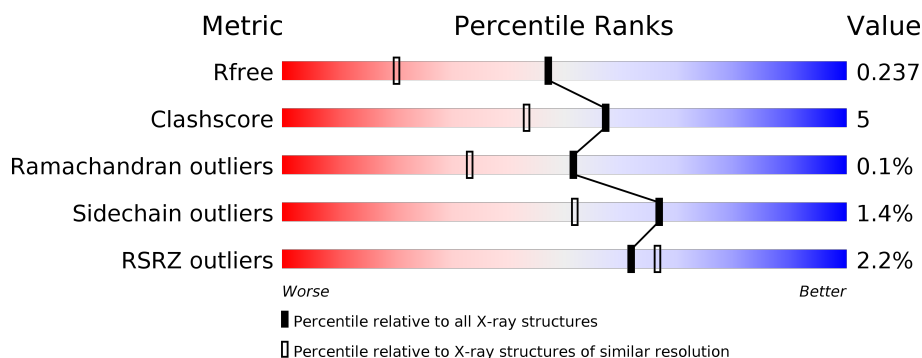
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 on 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	345	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>••</div> </div> </div>
1	B	345	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	345	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>• 5%</div> </div> </div>
1	D	345	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12566 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	11	0
			2794	1779	471	517	27			
1	B	336	Total	C	N	O	S	0	6	0
			2768	1762	472	509	25			
1	C	327	Total	C	N	O	S	0	3	0
			2683	1710	460	487	26			
1	D	335	Total	C	N	O	S	0	6	0
			2754	1753	471	504	26			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	EXPRESSION TAG	UNP O00408
A	576	SER	-	EXPRESSION TAG	UNP O00408
A	577	ALA	-	EXPRESSION TAG	UNP O00408
A	578	MET	-	EXPRESSION TAG	UNP O00408
B	575	GLY	-	EXPRESSION TAG	UNP O00408
B	576	SER	-	EXPRESSION TAG	UNP O00408
B	577	ALA	-	EXPRESSION TAG	UNP O00408
B	578	MET	-	EXPRESSION TAG	UNP O00408
C	575	GLY	-	EXPRESSION TAG	UNP O00408
C	576	SER	-	EXPRESSION TAG	UNP O00408
C	577	ALA	-	EXPRESSION TAG	UNP O00408
C	578	MET	-	EXPRESSION TAG	UNP O00408
D	575	GLY	-	EXPRESSION TAG	UNP O00408
D	576	SER	-	EXPRESSION TAG	UNP O00408
D	577	ALA	-	EXPRESSION TAG	UNP O00408
D	578	MET	-	EXPRESSION TAG	UNP O00408

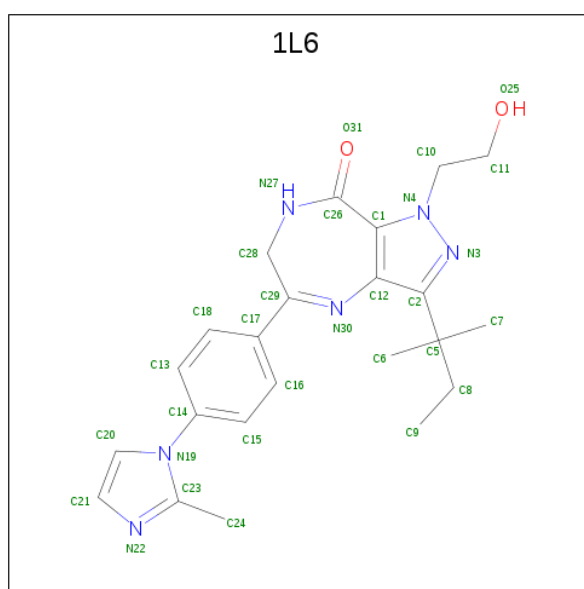
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 1-(2-hydroxyethyl)-3-(2-methylbutan-2-yl)-5-[4-(2-methyl-1H-imidazol-1-yl)phenyl]-6,7-dihydropyrazolo[4,3-e][1,4]diazepin-8(1H)-one (three-letter code: 1L6) (formula: C₂₃H₂₈N₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 31 23 6 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			31	23	6	2		
4	C	1	Total	C	N	O	0	0
			31	23	6	2		
4	D	1	Total	C	N	O	0	0
			31	23	6	2		

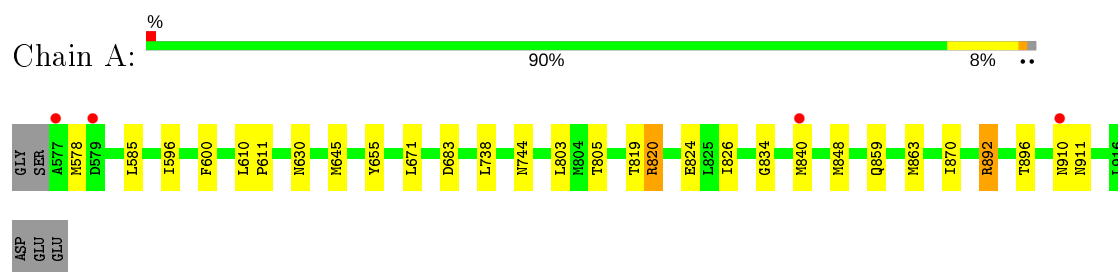
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	381	Total	O	0	0
			381	381		
5	B	361	Total	O	0	0
			361	361		
5	C	333	Total	O	0	0
			333	333		
5	D	360	Total	O	0	0
			360	360		

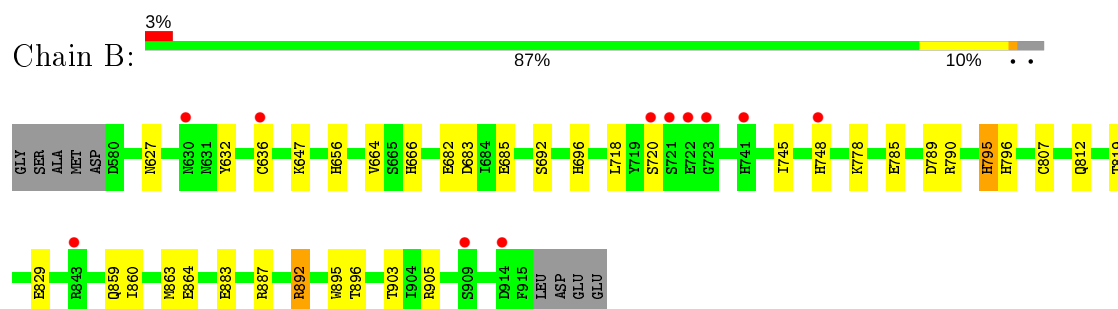
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

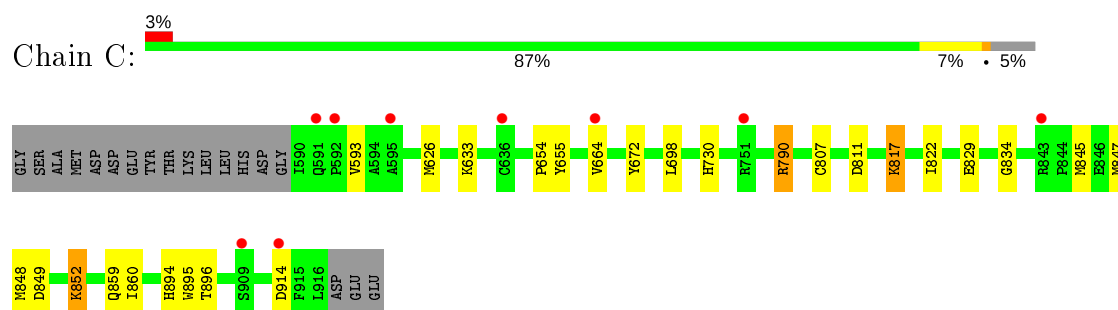
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



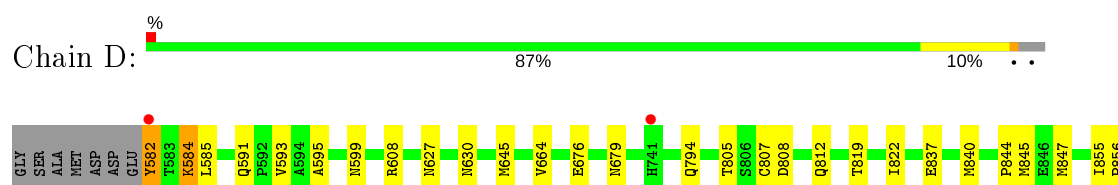
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

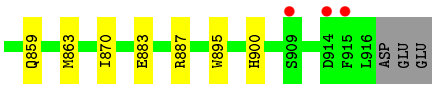


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.88Å 74.13Å 91.80Å 109.67° 88.72° 88.97°	Depositor
Resolution (Å)	50.00 – 1.72 34.77 – 1.72	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-1.72) 96.6 (34.77-1.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.240 0.187 , 0.237	Depositor DCC
R_{free} test set	7141 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12566	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1L6, ZN, MG

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	0/2916	0.67	0/3937
1	B	0.64	0/2865	0.65	0/3867
1	C	0.60	0/2763	0.63	0/3727
1	D	0.63	0/2856	0.66	1/3853 (0.0%)
All	All	0.63	0/11400	0.65	1/15384 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	808	ASP	CB-CG-OD1	7.14	124.73	118.30

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	2794	0	2727	22	0
1	B	2768	0	2709	37	0
1	C	2683	0	2636	16	0
1	D	2754	0	2704	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	28	4	0
4	B	31	0	28	0	0
4	C	31	0	28	0	0
4	D	31	0	28	1	0
5	A	381	0	0	7	0
5	B	361	0	0	10	0
5	C	333	0	0	3	0
5	D	360	0	0	2	0
All	All	12566	0	10888	109	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 5.

All (109) 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:D:584:LYS:HD3	1:D:584:LYS:H	0.99	1.09
1:D:584:LYS:HD3	1:D:584:LYS:N	1.76	1.01
1:A:820:ARG:HH11	1:A:820:ARG:HG2	1.19	1.00
1:B:892:ARG:HH12	1:B:896:THR:HG21	1.23	0.99
1:B:745:ILE:O	1:B:748:HIS:HE1	1.47	0.97
1:B:789:ASP:H	1:B:795:HIS:HD2	1.16	0.92
1:B:745:ILE:O	1:B:748:HIS:CE1	2.23	0.91
1:A:683:ASP:HB2	5:A:1446:HOH:O	1.72	0.90
1:D:584:LYS:H	1:D:584:LYS:CD	1.82	0.88
1:B:892:ARG:NH1	1:B:896:THR:HG21	1.89	0.87
1:D:582:TYR:CE2	1:D:584:LYS:HG2	2.14	0.82
1:B:682:GLU:HG3	5:B:1247:HOH:O	1.80	0.82
1:B:647:LYS:HE3	5:B:1438:HOH:O	1.83	0.78
1:B:656:HIS:HD2	1:B:829:GLU:OE2	1.69	0.75
1:A:819:THR:HG23	5:A:1322:HOH:O	1.86	0.75
1:D:582:TYR:CZ	1:D:584:LYS:HG2	2.23	0.72
1:C:730:HIS:HE1	5:C:1415:HOH:O	1.73	0.72
5:B:1180:HOH:O	1:D:794:GLN:HG3	1.90	0.72
1:B:790:ARG:O	1:B:796:HIS:HE1	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:TYR:HB3	1:B:748:HIS:NE2	2.07	0.69
1:A:578:MET:CG	5:A:1395:HOH:O	2.39	0.69
1:B:812:GLN:OE1	1:B:819[A]:THR:HG23	1.92	0.68
1:B:685:GLU:OE1	1:B:796:HIS:HD2	1.77	0.68
1:C:633:LYS:HE2	5:C:1206:HOH:O	1.95	0.66
1:B:864[A]:GLU:OE2	1:B:892:ARG:NH2	2.27	0.65
1:B:892:ARG:NH1	1:B:896:THR:CG2	2.60	0.65
1:C:698:LEU:O	1:C:730:HIS:HD2	1.80	0.65
1:B:883:GLU:O	1:B:887:ARG:HG3	1.98	0.64
1:B:666:HIS:HD2	5:B:1115:HOH:O	1.81	0.64
4:A:1003:1L6:H29	4:A:1003:1L6:H10	1.81	0.62
1:B:627:ASN:HA	5:B:1203:HOH:O	2.00	0.62
1:D:819:THR:HG22	1:D:895:TRP:HE1	1.64	0.61
1:A:820:ARG:NH1	1:A:820:ARG:HG2	1.97	0.61
1:B:789:ASP:H	1:B:795:HIS:CD2	2.07	0.61
1:D:582:TYR:CE2	1:D:585:LEU:HG	2.35	0.61
1:C:654:PRO:HD2	1:C:829:GLU:HG3	1.83	0.61
1:B:632:TYR:HB3	1:B:748:HIS:CD2	2.36	0.60
1:B:860:ILE:O	1:B:864[A]:GLU:HG3	2.02	0.60
1:D:819:THR:CG2	1:D:895:TRP:HE1	2.15	0.59
1:D:883:GLU:O	1:D:887:ARG:HD2	2.02	0.58
1:B:632:TYR:O	1:B:748:HIS:CG	2.57	0.58
1:D:812:GLN:OE1	1:D:819:THR:HG23	2.03	0.58
1:D:584:LYS:N	1:D:584:LYS:CD	2.54	0.58
1:C:790:ARG:HG3	1:C:790:ARG:O	2.02	0.57
1:D:582:TYR:C	1:D:582:TYR:HD2	2.09	0.56
1:A:820:ARG:CG	1:A:820:ARG:HH11	2.02	0.56
1:C:845[A]:MET:HG3	1:C:847:MET:HG2	1.87	0.56
1:D:900:HIS:HD2	5:D:1378:HOH:O	1.89	0.55
1:A:820:ARG:NH1	1:A:824:GLU:OE2	2.38	0.55
1:A:820:ARG:NH1	1:A:820:ARG:CG	2.67	0.55
1:D:582:TYR:C	1:D:582:TYR:CD2	2.81	0.54
1:D:845:MET:HG3	1:D:847:MET:HG2	1.89	0.54
1:A:645:MET:HG2	5:A:1377:HOH:O	2.08	0.54
1:B:819[A]:THR:CG2	1:B:895:TRP:HE1	2.21	0.54
1:C:849:ASP:OD2	1:C:852:LYS:HD3	2.09	0.53
1:B:887:ARG:HD2	5:B:1155:HOH:O	2.08	0.52
1:A:683:ASP:CB	5:A:1446:HOH:O	2.44	0.52
1:B:859:GLN:O	1:B:863:MET:HG2	2.10	0.52
1:D:859:GLN:HG2	1:D:895:TRP:CE2	2.45	0.52
1:B:819[A]:THR:HG22	1:B:895:TRP:HE1	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676[A]:GLU:OE2	1:D:679:ASN:HB2	2.11	0.50
1:D:837:GLU:OE1	1:D:844:PRO:HB3	2.13	0.49
1:B:903:THR:HB	1:B:905:ARG:HH12	1.78	0.48
1:B:656:HIS:HE1	5:B:1103:HOH:O	1.96	0.48
1:C:894:HIS:HE1	5:C:1222:HOH:O	1.96	0.48
1:C:859:GLN:HG2	1:C:895:TRP:CE2	2.50	0.46
1:A:840[A]:MET:HG2	5:A:1378:HOH:O	2.15	0.46
1:C:811:ASP:HB3	1:C:822:ILE:HG13	1.98	0.46
1:B:778:LYS:HB3	1:B:778:LYS:HE3	1.65	0.46
1:B:692:SER:O	1:B:696:HIS:HB3	2.16	0.45
1:B:778:LYS:HD2	5:B:1320:HOH:O	2.16	0.45
1:B:790:ARG:O	1:B:796:HIS:CE1	2.62	0.45
1:A:805:THR:HG22	1:A:870:ILE:HD13	1.98	0.45
1:D:645:MET:HG2	5:D:1213:HOH:O	2.16	0.45
1:A:671:LEU:HD13	1:A:803:LEU:HD22	1.97	0.45
1:A:738:LEU:O	1:A:744:ASN:HB2	2.17	0.45
1:A:630[B]:ASN:ND2	5:A:1447:HOH:O	2.50	0.44
1:A:892:ARG:NH1	1:A:896:THR:OG1	2.43	0.44
1:D:664:VAL:HG13	1:D:807:CYS:HB3	1.99	0.44
1:B:685:GLU:OE1	1:B:796:HIS:CD2	2.66	0.44
1:D:591:GLN:HG2	1:D:595:ALA:HB3	2.00	0.44
1:D:859:GLN:O	1:D:863:MET:HG3	2.17	0.44
1:C:626:MET:HG2	1:C:672:TYR:CD2	2.53	0.44
1:C:860:ILE:HD13	1:C:896:THR:HG22	2.00	0.44
1:C:834:GLY:HA3	1:C:848:MET:O	2.18	0.43
1:B:664:VAL:HG13	1:B:807:CYS:HB3	2.00	0.43
1:D:840:MET:HB3	1:D:840:MET:HE2	1.91	0.43
4:A:1003:1L6:C24	4:A:1003:1L6:C13	2.96	0.43
1:A:610:LEU:HD12	1:A:611:PRO:HD2	2.00	0.43
1:B:636:CYS:SG	5:B:1437:HOH:O	2.62	0.42
1:B:864[A]:GLU:HG2	1:B:892:ARG:HE	1.83	0.42
1:A:596:ILE:HG21	1:A:600:PHE:CE1	2.55	0.42
1:C:817:LYS:HB3	1:C:817:LYS:HE3	1.76	0.42
1:A:859:GLN:O	1:A:863:MET:HG3	2.19	0.42
1:D:855:ILE:N	1:D:856:PRO:HD2	2.35	0.42
4:A:1003:1L6:H24	4:A:1003:1L6:H15	1.83	0.41
1:C:655:TYR:HE1	1:C:822:ILE:HD12	1.84	0.41
4:D:1003:1L6:H24	4:D:1003:1L6:H15	1.84	0.41
1:D:608:ARG:CZ	1:D:822:ILE:HD11	2.51	0.41
1:B:785[A]:GLU:HG3	5:B:1158:HOH:O	2.21	0.41
1:D:627:ASN:ND2	1:D:630:ASN:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ASN:O	1:A:911:ASN:HB2	2.20	0.41
1:D:591:GLN:HE21	1:D:595:ALA:CB	2.34	0.41
1:D:805:THR:HG22	1:D:870:ILE:HD13	2.03	0.41
1:B:859:GLN:HG2	1:B:895:TRP:CE2	2.56	0.40
4:A:1003:1L6:C24	4:A:1003:1L6:H10	2.49	0.40
1:A:655:TYR:CD2	1:A:826:ILE:HD13	2.56	0.40
1:C:664:VAL:HG13	1:C:807:CYS:HB3	2.04	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	349/345 (101%)	348 (100%)	1 (0%)	0	100	100
1	B	340/345 (99%)	333 (98%)	7 (2%)	0	100	100
1	C	328/345 (95%)	323 (98%)	3 (1%)	2 (1%)	25	10
1	D	340/345 (99%)	338 (99%)	2 (1%)	0	100	100
All	All	1357/1380 (98%)	1342 (99%)	13 (1%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	914[A]	ASP
1	C	914[B]	ASP

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	314/310 (101%)	309 (98%)	5 (2%)	62	47
1	B	309/310 (100%)	304 (98%)	5 (2%)	62	47
1	C	298/310 (96%)	294 (99%)	4 (1%)	69	55
1	D	309/310 (100%)	305 (99%)	4 (1%)	69	55
All	All	1230/1240 (99%)	1212 (98%)	18 (2%)	67	49

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	LEU
1	A	820	ARG
1	A	848[A]	MET
1	A	848[B]	MET
1	A	892	ARG
1	B	683	ASP
1	B	718	LEU
1	B	720	SER
1	B	795	HIS
1	B	892	ARG
1	C	593	VAL
1	C	790	ARG
1	C	817	LYS
1	C	852	LYS
1	D	582	TYR
1	D	584	LYS
1	D	593	VAL
1	D	599	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	656	HIS
1	B	666	HIS
1	B	674	ASN
1	B	741	HIS
1	B	748	HIS
1	B	795	HIS
1	B	796	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	842	ASN
1	B	900	HIS
1	B	911	ASN
1	C	730	HIS
1	C	859	GLN
1	C	865	HIS
1	C	894	HIS
1	D	587	HIS
1	D	591	GLN
1	D	627	ASN
1	D	708	GLN
1	D	739	ASN
1	D	791	ASN
1	D	911	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
4	1L6	D	1003	-	28,34,34	1.73	4 (14%)	31,50,50	2.26	12 (38%)
4	1L6	C	1003	-	28,34,34	1.82	4 (14%)	31,50,50	2.11	13 (41%)
4	1L6	B	1003	-	28,34,34	1.84	4 (14%)	31,50,50	2.29	10 (32%)
4	1L6	A	1003	-	28,34,34	1.78	5 (17%)	31,50,50	2.60	14 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1L6	D	1003	-	-	1/18/33/33	0/3/4/4
4	1L6	C	1003	-	-	3/18/33/33	0/3/4/4
4	1L6	B	1003	-	-	3/18/33/33	0/3/4/4
4	1L6	A	1003	-	-	1/18/33/33	0/3/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	1L6	C14-N19	-6.36	1.36	1.44
4	D	1003	1L6	C14-N19	-6.28	1.36	1.44
4	A	1003	1L6	C14-N19	-6.21	1.36	1.44
4	C	1003	1L6	C14-N19	-5.84	1.36	1.44
4	B	1003	1L6	C20-N19	-5.05	1.34	1.38
4	C	1003	1L6	C20-N19	-4.82	1.34	1.38
4	A	1003	1L6	C20-N19	-4.23	1.34	1.38
4	D	1003	1L6	C20-N19	-3.69	1.35	1.38
4	C	1003	1L6	C29-N30	-3.56	1.25	1.29
4	D	1003	1L6	C29-N30	-3.26	1.26	1.29
4	A	1003	1L6	C26-N27	-2.64	1.31	1.33
4	C	1003	1L6	C12-N30	-2.48	1.38	1.40
4	B	1003	1L6	C2-N3	2.36	1.37	1.34
4	A	1003	1L6	C2-N3	2.34	1.37	1.34
4	A	1003	1L6	C23-N19	-2.28	1.33	1.37
4	D	1003	1L6	C12-N30	-2.27	1.38	1.40
4	B	1003	1L6	C29-N30	-2.22	1.27	1.29

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	1L6	C17-C29-N30	7.45	126.26	118.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	1L6	C17-C29-N30	6.55	125.27	118.04
4	D	1003	1L6	C1-C12-C2	5.16	111.25	107.46
4	C	1003	1L6	C1-C12-C2	4.72	110.92	107.46
4	B	1003	1L6	C15-C14-C13	-4.65	114.44	121.33
4	D	1003	1L6	C15-C14-C13	-4.64	114.46	121.33
4	A	1003	1L6	C13-C14-N19	4.38	124.69	119.41
4	C	1003	1L6	C17-C29-N30	4.34	122.83	118.04
4	C	1003	1L6	C15-C14-C13	-4.33	114.92	121.33
4	D	1003	1L6	C13-C14-N19	4.32	124.62	119.41
4	B	1003	1L6	C15-C14-N19	4.12	124.38	119.41
4	A	1003	1L6	O31-C26-N27	-3.88	118.09	122.18
4	D	1003	1L6	C1-C26-N27	3.88	122.84	117.73
4	A	1003	1L6	C1-C26-N27	3.59	122.47	117.73
4	B	1003	1L6	C5-C2-N3	-3.57	116.76	120.58
4	A	1003	1L6	C15-C14-C13	-3.51	116.12	121.33
4	B	1003	1L6	C28-C29-N30	-3.51	114.84	121.99
4	A	1003	1L6	C5-C2-N3	-3.49	116.84	120.58
4	A	1003	1L6	C16-C15-C14	3.47	124.12	119.07
4	B	1003	1L6	C16-C15-C14	3.47	124.11	119.07
4	D	1003	1L6	C10-N4-C1	3.37	132.77	128.48
4	A	1003	1L6	C16-C17-C29	-3.22	116.92	120.84
4	D	1003	1L6	C16-C15-C14	3.18	123.69	119.07
4	B	1003	1L6	C1-C26-N27	3.15	121.88	117.73
4	A	1003	1L6	C28-C29-C17	-3.13	115.15	120.16
4	D	1003	1L6	C18-C13-C14	2.96	123.38	119.07
4	C	1003	1L6	C18-C13-C14	2.95	123.36	119.07
4	C	1003	1L6	C10-N4-C1	2.93	132.21	128.48
4	C	1003	1L6	C16-C15-C14	2.88	123.26	119.07
4	B	1003	1L6	C1-C12-C2	2.88	109.57	107.46
4	D	1003	1L6	C20-N19-C14	-2.80	121.11	124.18
4	C	1003	1L6	C13-C14-N19	2.80	122.78	119.41
4	A	1003	1L6	C24-C23-N22	2.69	129.47	121.77
4	D	1003	1L6	O31-C26-N27	-2.63	119.40	122.18
4	B	1003	1L6	C18-C13-C14	2.57	122.81	119.07
4	A	1003	1L6	C10-N4-C1	2.55	131.72	128.48
4	C	1003	1L6	C28-C29-N30	-2.53	116.82	121.99
4	D	1003	1L6	C17-C29-N30	2.40	120.69	118.04
4	B	1003	1L6	C5-C2-C12	2.38	135.46	130.69
4	C	1003	1L6	C15-C14-N19	2.38	122.28	119.41
4	C	1003	1L6	C20-N19-C14	-2.27	121.69	124.18
4	C	1003	1L6	C29-C28-N27	2.23	116.20	111.90
4	C	1003	1L6	O31-C26-N27	-2.21	119.85	122.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	1L6	C1-C26-N27	2.20	120.63	117.73
4	A	1003	1L6	C28-C29-N30	-2.19	117.53	121.99
4	D	1003	1L6	C29-C28-N27	2.09	115.93	111.90
4	D	1003	1L6	C6-C5-C2	2.06	115.02	110.11
4	A	1003	1L6	C20-N19-C14	-2.06	121.93	124.18
4	A	1003	1L6	C1-C12-C2	2.05	108.96	107.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	1L6	C12-C2-C5-C7
4	B	1003	1L6	C12-C2-C5-C6
4	C	1003	1L6	C7-C5-C8-C9
4	C	1003	1L6	C6-C5-C8-C9
4	C	1003	1L6	N4-C10-C11-O25
4	A	1003	1L6	N4-C10-C11-O25
4	B	1003	1L6	N4-C10-C11-O25
4	D	1003	1L6	N4-C10-C11-O25

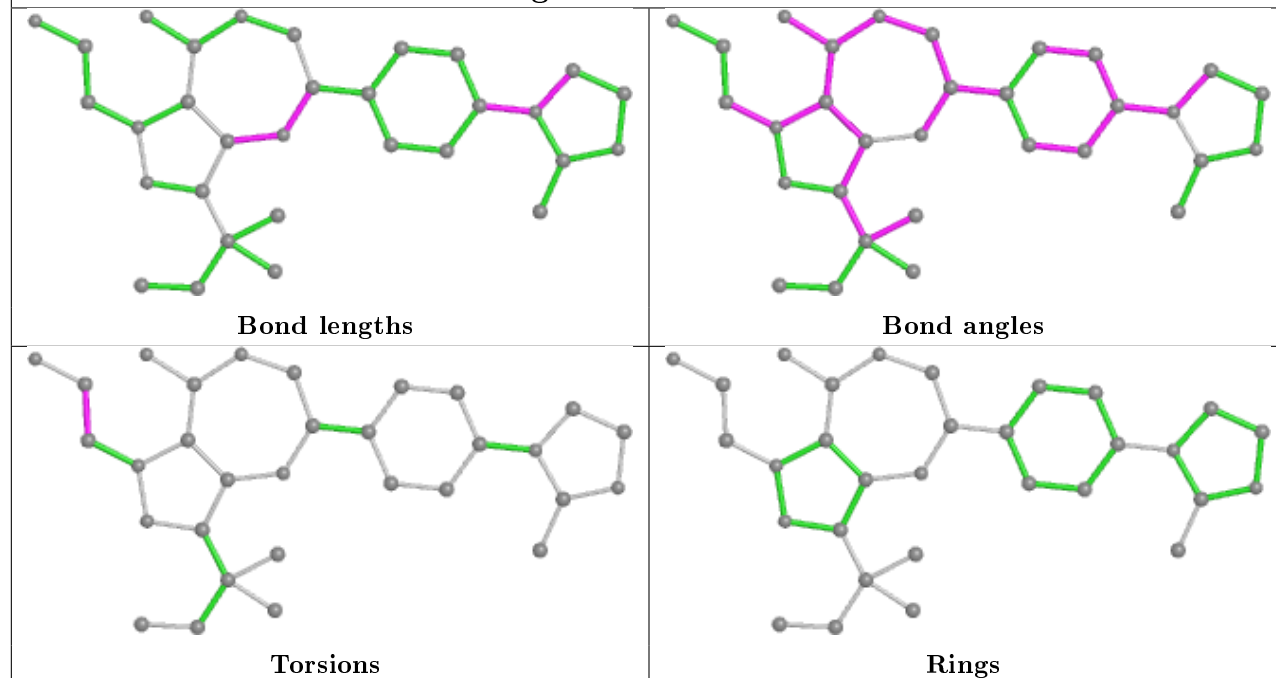
There are no ring outliers.

2 monomers are involved in 5 short contacts:

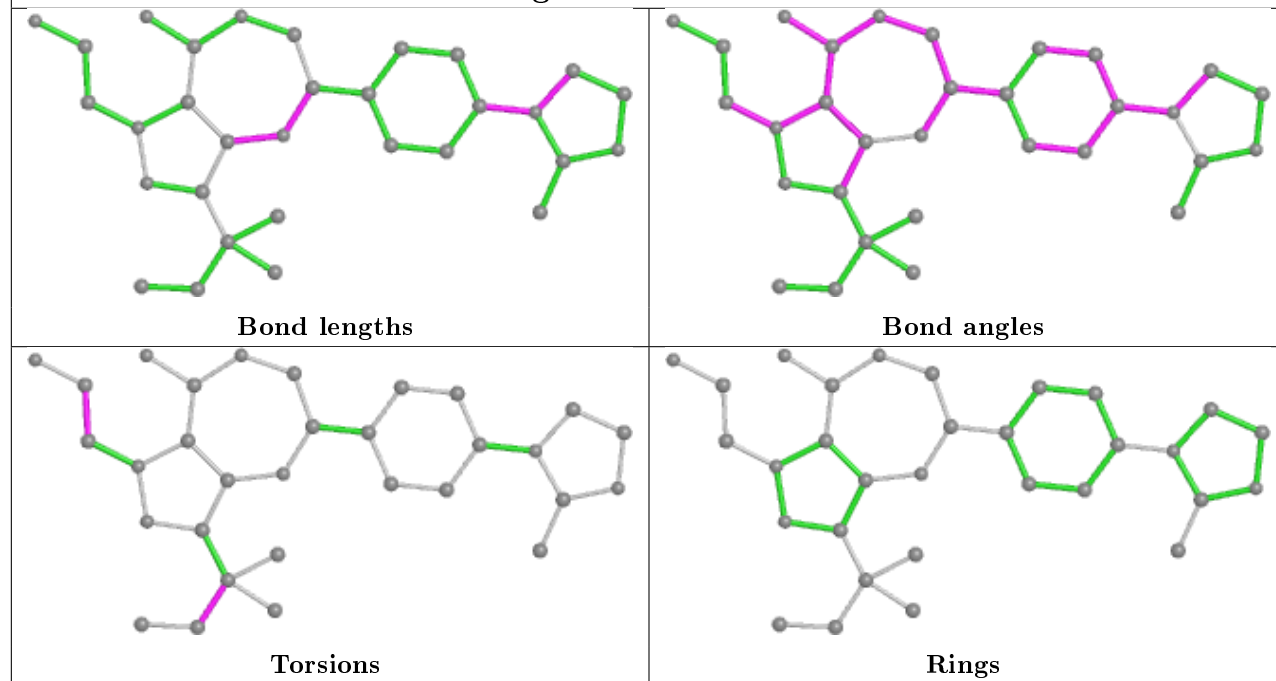
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1003	1L6	1	0
4	A	1003	1L6	4	0

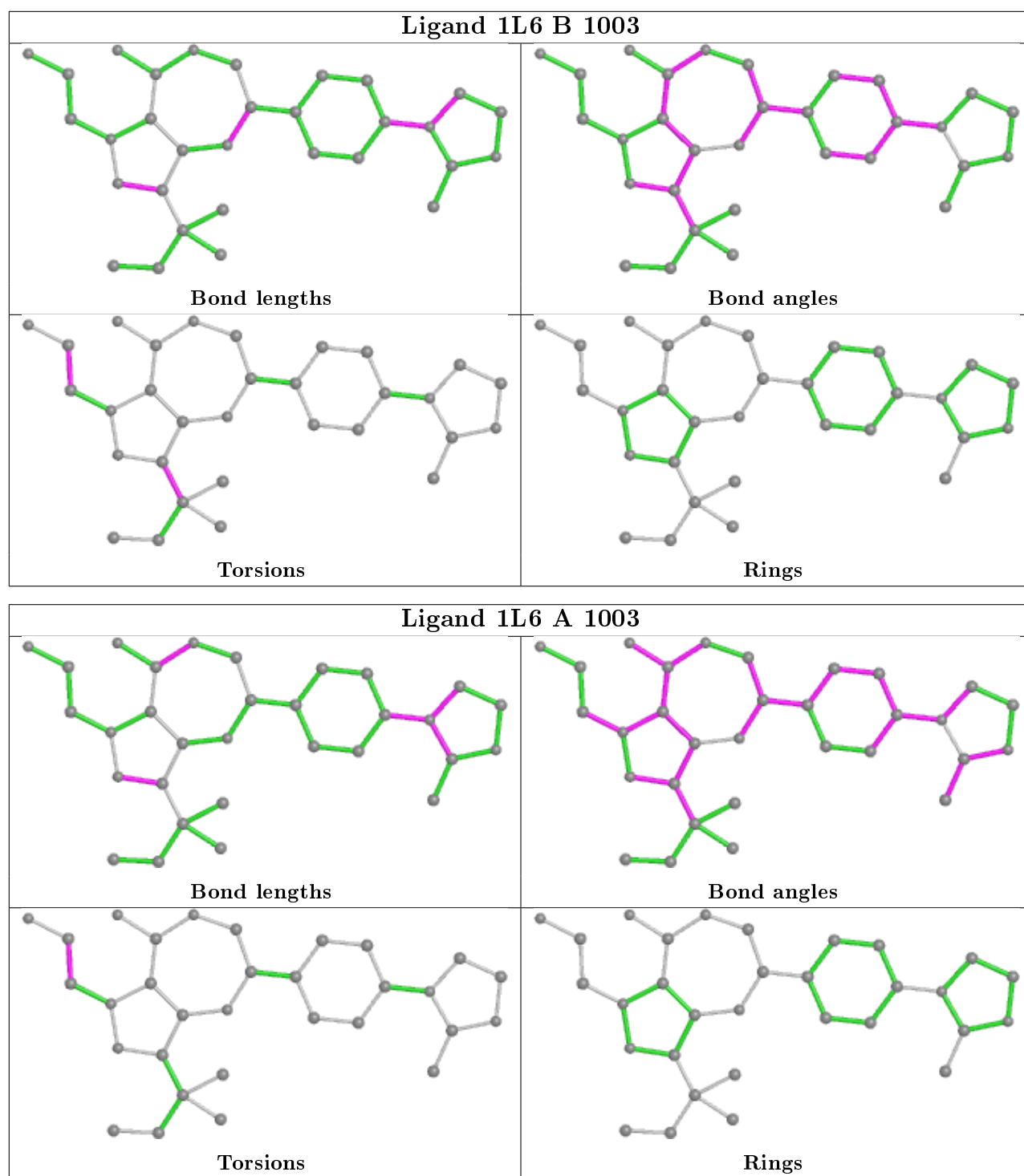
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 1L6 D 1003



Ligand 1L6 C 1003





5.7 Other polymers [i](#)

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	340/345 (98%)	-0.08	4 (1%) 79 83	10, 20, 32, 45	0
1	B	336/345 (97%)	0.07	11 (3%) 46 51	11, 22, 34, 42	0
1	C	327/345 (94%)	0.24	9 (2%) 53 57	12, 24, 37, 46	0
1	D	335/345 (97%)	-0.06	5 (1%) 73 78	12, 21, 32, 38	0
All	All	1338/1380 (96%)	0.04	29 (2%) 62 66	10, 21, 35, 46	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	582	TYR	4.8
1	B	721	SER	4.3
1	B	843	ARG	3.4
1	B	748	HIS	3.2
1	B	722	GLU	3.2
1	B	741	HIS	3.2
1	D	909	SER	3.2
1	C	592	PRO	3.1
1	B	636	CYS	3.0
1	D	914	ASP	2.9
1	C	751	ARG	2.9
1	A	910	ASN	2.9
1	A	577	ALA	2.9
1	B	909	SER	2.7
1	C	664	VAL	2.7
1	C	843	ARG	2.6
1	B	720	SER	2.6
1	C	909	SER	2.5
1	C	636	CYS	2.5
1	D	915	PHE	2.5
1	C	595	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	741	HIS	2.4
1	A	840[A]	MET	2.4
1	B	914	ASP	2.3
1	C	591	GLN	2.2
1	A	579	ASP	2.2
1	B	630	ASN	2.1
1	C	914[A]	ASP	2.1
1	B	723	GLY	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 carbohydrates 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.

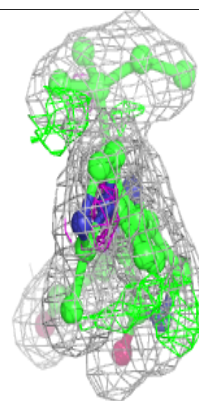
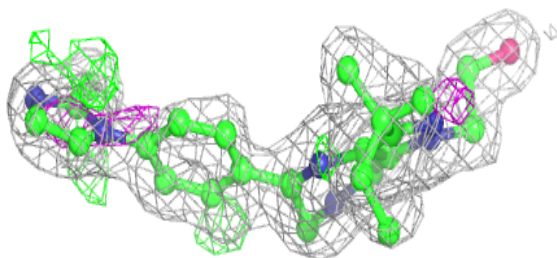
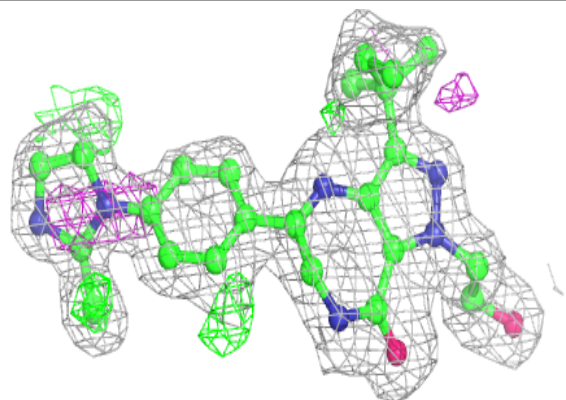
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	1L6	D	1003	31/31	0.81	0.15	21,27,30,31	0
4	1L6	B	1003	31/31	0.82	0.14	20,27,39,39	0
4	1L6	C	1003	31/31	0.88	0.14	20,22,24,25	0
4	1L6	A	1003	31/31	0.90	0.12	15,21,28,28	0
3	MG	C	1002	1/1	0.98	0.15	13,13,13,13	0
3	MG	A	1002	1/1	0.99	0.12	12,12,12,12	0
2	ZN	C	1001	1/1	1.00	0.09	17,17,17,17	0
2	ZN	A	1001	1/1	1.00	0.07	16,16,16,16	0
2	ZN	B	1001	1/1	1.00	0.07	16,16,16,16	0
3	MG	B	1002	1/1	1.00	0.14	12,12,12,12	0
2	ZN	D	1001	1/1	1.00	0.07	18,18,18,18	0
3	MG	D	1002	1/1	1.00	0.13	14,14,14,14	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.

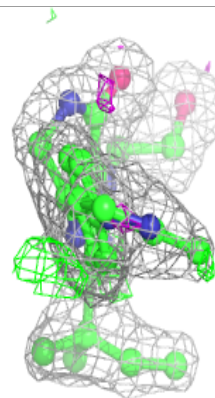
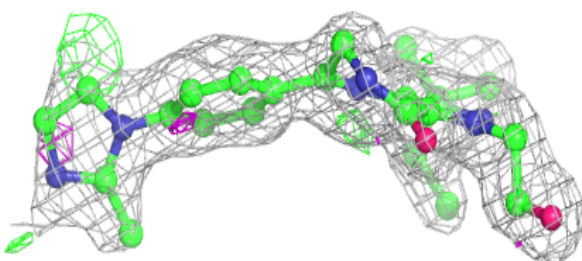
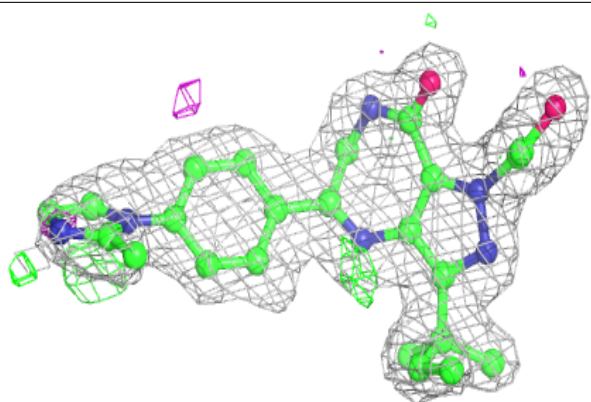
Electron density around 1L6 D 1003:

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



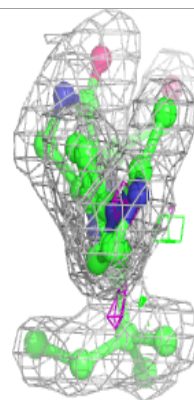
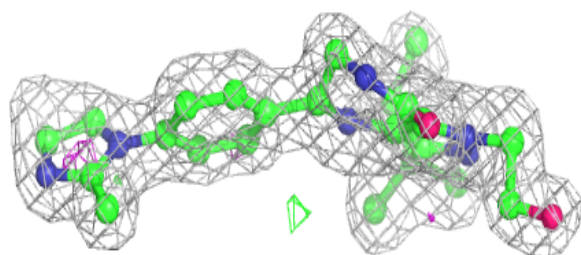
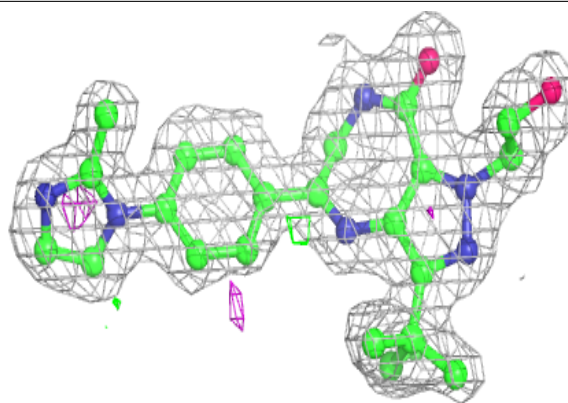
Electron density around 1L6 B 1003:

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

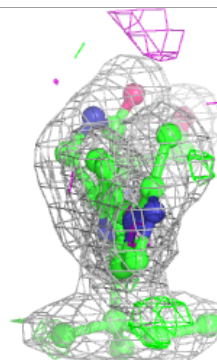
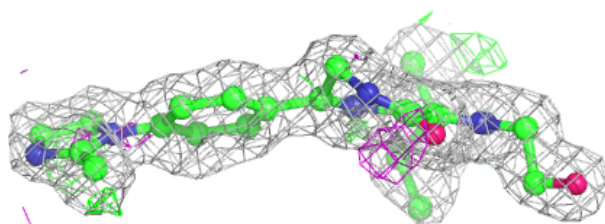
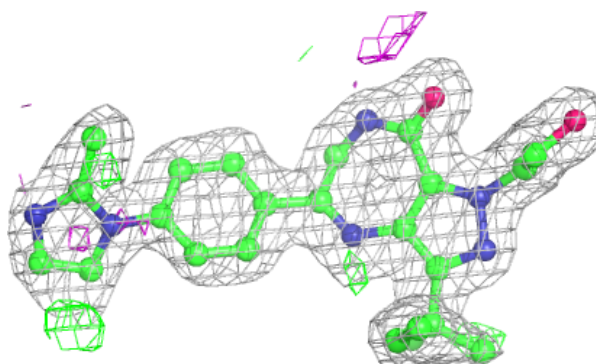


Electron density around 1L6 C 1003:

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

**Electron density around 1L6 A 1003:**

$2mF_o-DF_c$ (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.