



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:32 AM UTC

PDB ID : 9JK1 / pdb_00009jk1
Title : Crystal structure of CDK12/Cyclin K in complex with covalent inhibitor YJZ5118
Authors : Huang, W.X.; Zhang, P.J.; Yang, J.Z.; Ding, K.
Deposited on : 2024-09-14
Resolution : 2.72 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 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

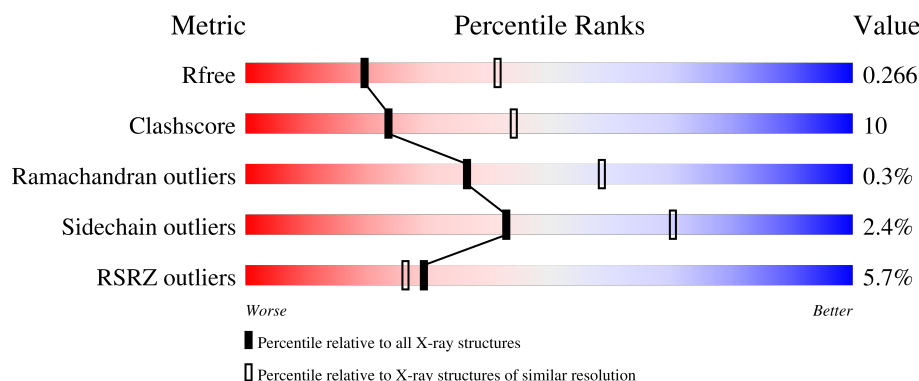
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	6% 70% 20% 9%
1	B	340	10% 66% 25% 7%
2	C	269	0% 71% 16% 13%
2	D	269	2% 68% 18% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8709 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 Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	P	S	0	0	0
			2406	1552	393	443	1	17			
1	B	315	Total	C	N	O	P	S	0	0	0
			2386	1539	387	442	1	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	GLY	-	expression tag	UNP Q9NYV4
A	714	ALA	-	expression tag	UNP Q9NYV4
B	713	GLY	-	expression tag	UNP Q9NYV4
B	714	ALA	-	expression tag	UNP Q9NYV4

- Molecule 2 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	238	Total	C	N	O	S	0	0	0
			1916	1253	306	346	11			
2	C	235	Total	C	N	O	S	0	0	0
			1888	1234	306	337	11			

There are 4 discrepancies between the modelled and reference sequences:

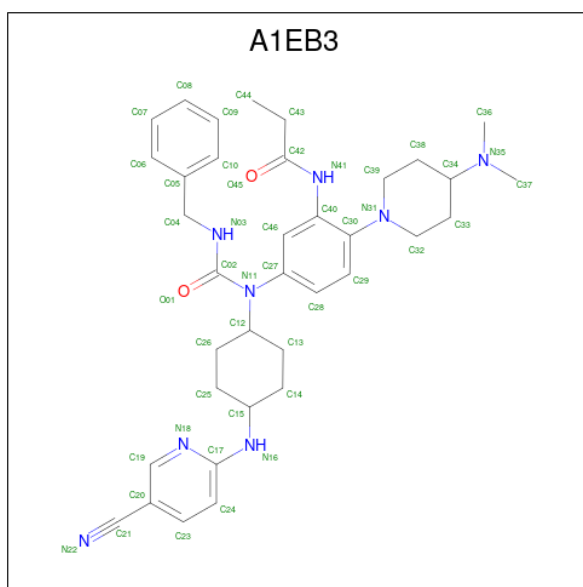
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP O75909
D	0	ALA	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ALA	-	expression tag	UNP O75909

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	D	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is N-[5-[[4-[(5-cyanopyridin-2-yl)amino]cyclohexyl]-[(phenylmethyl)carbamoyl]amino]-2-[4-(dimethylamino)piperidin-1-yl]phenyl]propanamide (CCD ID: A1EB3) (formula: C₃₆H₄₆N₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			46	36	8	2		

Continued on next page...

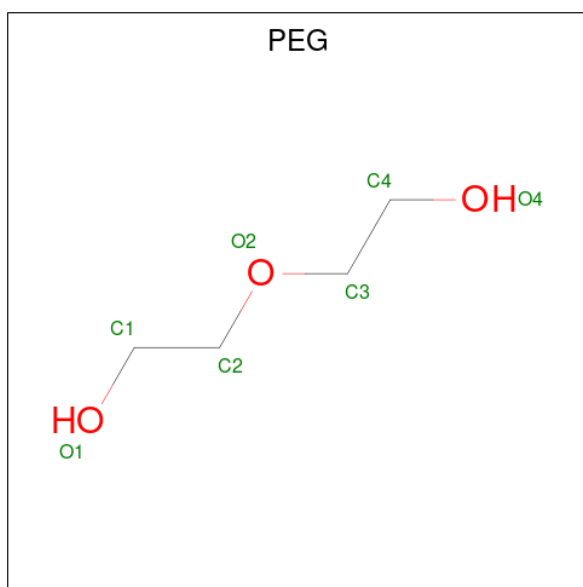
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			46	36	8	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

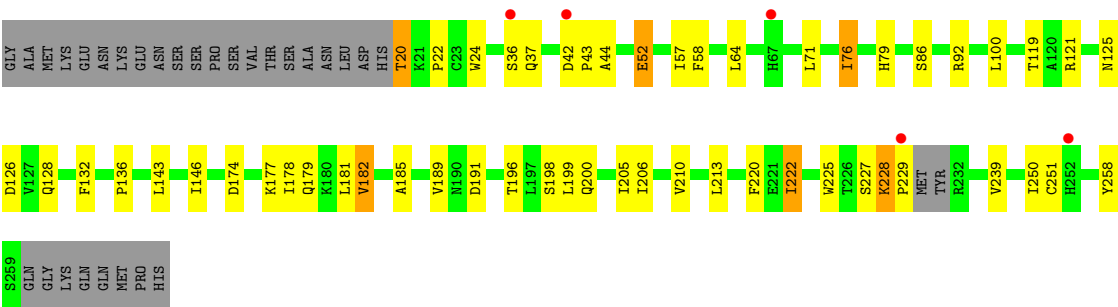
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



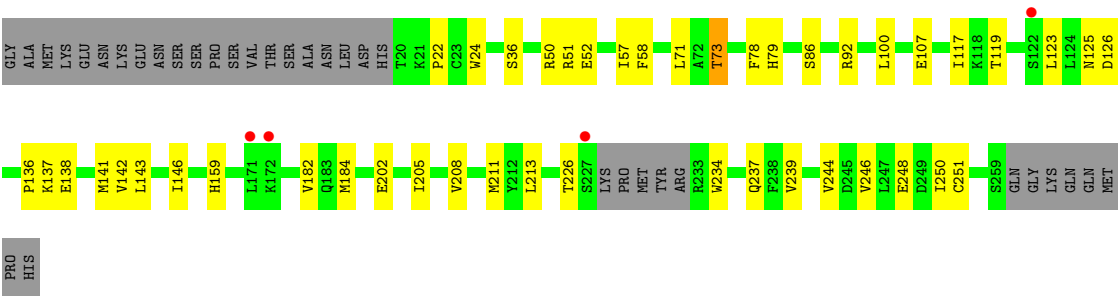
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	B	2	Total	O	0	0
			2	2		



● Molecule 2: Cyclin-K



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.20Å 77.19Å 91.46Å 75.88° 85.63° 77.92°	Depositor
Resolution (Å)	29.56 – 2.72 29.56 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.56-2.72) 97.4 (29.56-2.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.248 , 0.267 0.249 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (5.72%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8709	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.02% 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: EDO, TPO, PEG, A1EB3, 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	0.17	0/2450	0.37	0/3327
1	B	0.21	0/2428	0.45	2/3304 (0.1%)
2	C	0.17	0/1940	0.34	0/2641
2	D	0.15	0/1969	0.34	0/2679
All	All	0.18	0/8787	0.38	2/11951 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	765	GLU	N-CA-C	6.89	121.36	112.26
1	B	761	ASP	N-CA-C	-6.39	100.43	109.96

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	2406	0	2292	47	0
1	B	2386	0	2242	69	0
2	C	1888	0	1797	24	0
2	D	1916	0	1829	32	0
3	A	4	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	6	0	0
4	A	46	0	0	1	0
4	B	46	0	0	2	0
5	A	1	0	0	0	0
6	C	7	0	10	1	0
7	A	3	0	0	0	0
7	B	2	0	0	1	0
All	All	8709	0	8182	172	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 10.

All (172) 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:B:760:LEU:HD23	1:B:809:PHE:CD2	1.61	1.34
1:B:760:LEU:CD2	1:B:809:PHE:CD2	2.45	0.99
2:D:228:LYS:HB3	2:D:229:PRO:HD2	1.43	0.97
1:B:760:LEU:CD2	1:B:809:PHE:CE2	2.51	0.93
1:A:956:CYS:HB3	1:A:977:GLN:HE22	1.34	0.89
1:B:760:LEU:HD23	1:B:809:PHE:HD2	1.05	0.88
1:A:858:ARG:HH11	1:A:882:ARG:HB2	1.44	0.83
1:B:760:LEU:HD23	1:B:809:PHE:CE2	2.11	0.82
1:B:718:ASP:HA	1:B:791:GLU:HA	1.69	0.75
2:D:57:ILE:HG23	2:D:100:LEU:HB2	1.70	0.74
1:B:926:LEU:HD12	1:B:997:LEU:HD13	1.71	0.72
1:A:818:HIS:HA	4:A:1202:A1EB3:O01	1.90	0.72
1:B:1015:LEU:CD2	1:B:1020:LEU:HD13	2.21	0.70
2:C:58:PHE:HA	2:C:71:LEU:HD23	1.74	0.70
1:A:858:ARG:NH1	1:A:882:ARG:HB2	2.08	0.69
1:B:1010:THR:HG22	1:B:1012:GLU:H	1.57	0.68
1:A:1010:THR:HG22	1:A:1012:GLU:H	1.57	0.68
1:A:956:CYS:HB3	1:A:977:GLN:NE2	2.09	0.67
1:A:858:ARG:HH21	1:A:896:VAL:HG11	1.61	0.65
2:C:57:ILE:HG23	2:C:100:LEU:HB2	1.79	0.65
2:C:208:VAL:HA	2:C:211:MET:HE3	1.79	0.64
1:B:841:LYS:HG2	1:B:1025:LEU:HD11	1.78	0.64
1:B:759:ARG:C	1:B:761:ASP:H	2.04	0.63
1:B:823:LEU:HB3	1:B:829:VAL:HG11	1.80	0.63
1:A:842:GLN:HG2	1:A:1025:LEU:HD21	1.82	0.62
1:B:903:PRO:HG2	1:B:906:LEU:HG	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:LYS:HB3	2:D:229:PRO:CD	2.24	0.61
2:C:36:SER:HA	2:C:86:SER:HB2	1.84	0.60
1:B:858:ARG:NH1	1:B:913:TYR:OH	2.35	0.60
1:B:1015:LEU:HD23	1:B:1020:LEU:CD1	2.32	0.59
1:A:793:VAL:HG23	1:A:810:TYR:HB2	1.85	0.59
1:B:760:LEU:HD12	1:B:760:LEU:O	2.03	0.59
1:B:773:ARG:O	1:B:777:ILE:HG12	2.03	0.58
1:A:830:HIS:O	1:A:830:HIS:ND1	2.36	0.58
2:D:191:ASP:OD2	2:D:258:TYR:OH	2.22	0.57
1:A:980:ARG:HH22	1:A:1002:THR:HA	1.69	0.57
1:B:760:LEU:HD12	1:B:760:LEU:C	2.29	0.57
2:C:213:LEU:HD13	2:C:251:CYS:HB3	1.86	0.57
1:B:760:LEU:CD2	1:B:809:PHE:HE2	2.14	0.57
2:D:132:PHE:HB3	2:D:136:PRO:HB3	1.87	0.56
2:D:36:SER:HA	2:D:86:SER:HB2	1.88	0.56
1:B:823:LEU:HD23	1:B:831:PHE:HZ	1.70	0.56
2:C:52:GLU:OE1	2:C:92:ARG:NH1	2.39	0.56
1:A:841:LYS:HD3	1:A:1023:VAL:HG13	1.87	0.55
1:B:774:GLU:HB2	1:B:879:GLY:HA2	1.89	0.55
1:B:1015:LEU:HD23	1:B:1020:LEU:HD13	1.89	0.55
1:B:1038:ASP:OD1	1:B:1038:ASP:N	2.35	0.55
2:D:121:ARG:NH2	2:D:126:ASP:OD1	2.34	0.54
2:D:185:ALA:HB1	2:D:210:VAL:HG23	1.90	0.54
2:C:117:ILE:HD13	2:C:136:PRO:HB2	1.89	0.54
4:B:1101:A1EB3:C25	4:B:1101:A1EB3:C24	2.85	0.54
1:A:838:SER:O	1:A:842:GLN:HG3	2.07	0.54
2:D:177:LYS:HG2	2:D:220:PHE:CZ	2.43	0.54
2:C:137:LYS:O	2:C:141:MET:HG2	2.07	0.53
1:A:775:ILE:O	1:A:779:ARG:HG3	2.08	0.53
1:B:1036:TRP:HA	7:B:1202:HOH:O	2.07	0.53
1:A:949:SER:HB3	1:A:954:SER:HA	1.89	0.53
2:D:52:GLU:OE1	2:D:92:ARG:NH1	2.42	0.53
1:B:854:ASN:O	1:B:883:LEU:HD23	2.09	0.53
2:D:174:ASP:HB3	2:D:177:LYS:HB2	1.90	0.53
1:B:898:THR:HG23	1:B:901:TYR:HD1	1.74	0.52
1:B:925:ILE:O	1:B:929:LEU:HG	2.10	0.52
2:D:37:GLN:HE22	2:D:43:PRO:HA	1.75	0.52
1:B:927:GLY:C	1:B:935:ILE:HD11	2.35	0.52
1:B:931:THR:OG1	1:B:933:LYS:O	2.28	0.51
2:D:213:LEU:HD13	2:D:251:CYS:HB3	1.91	0.51
1:A:773:ARG:O	1:A:777:ILE:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1101:A1EB3:C39	4:B:1101:A1EB3:N41	2.73	0.51
2:D:181:LEU:HD21	2:D:222:ILE:HD13	1.93	0.51
1:B:818:HIS:HB3	1:B:823:LEU:HD11	1.92	0.51
1:B:861:LYS:HD3	1:B:898:THR:HG21	1.92	0.50
1:A:847:LEU:HD21	1:A:918:ASP:HB3	1.93	0.50
1:A:777:ILE:HD12	1:A:855:PHE:CE1	2.46	0.50
1:A:916:ALA:HA	1:A:919:VAL:HG22	1.93	0.50
1:B:795:ASP:N	1:B:795:ASP:OD1	2.42	0.50
2:C:205:ILE:HD13	2:C:239:VAL:HG11	1.94	0.50
1:A:882:ARG:HD3	1:A:883:LEU:O	2.11	0.50
1:B:840:MET:HE3	1:B:926:LEU:HA	1.93	0.49
2:C:73:THR:HG23	2:C:159:HIS:NE2	2.27	0.49
1:B:936:PHE:HB3	1:B:944:GLN:NE2	2.28	0.49
1:A:899:LEU:O	1:A:944:GLN:NE2	2.46	0.49
2:D:206:ILE:HD13	2:D:250:ILE:HD13	1.95	0.49
2:D:227:SER:O	2:D:228:LYS:HB2	2.12	0.49
1:B:724:VAL:CG1	1:B:795:ASP:HB3	2.42	0.49
2:D:64:LEU:HD21	2:D:119:THR:OG1	2.12	0.49
1:A:733:ILE:N	1:A:741:VAL:O	2.43	0.49
1:B:759:ARG:C	1:B:761:ASP:N	2.64	0.48
2:D:196:THR:O	2:D:200:GLN:HG3	2.13	0.48
1:A:829:VAL:HG12	1:A:1034:PRO:HD3	1.94	0.48
1:B:844:MET:HB2	1:B:1015:LEU:HD21	1.95	0.48
1:B:861:LYS:O	1:B:865:ILE:HG12	2.13	0.48
2:D:22:PRO:HG2	2:D:24:TRP:NE1	2.29	0.48
1:B:983:ARG:HA	1:B:994:LEU:HD21	1.96	0.48
1:B:841:LYS:HB2	1:B:1020:LEU:HD22	1.96	0.47
2:C:226:THR:HG21	2:C:234:TRP:HB2	1.96	0.47
1:A:732:ILE:HG12	1:A:742:TYR:HE1	1.80	0.47
1:B:838:SER:O	1:B:842:GLN:HG3	2.14	0.47
2:C:244:VAL:O	2:C:248:GLU:HG2	2.15	0.47
1:A:774:GLU:HB2	1:A:879:GLY:HA2	1.96	0.47
1:B:847:LEU:HD21	1:B:918:ASP:HB3	1.95	0.47
2:C:50:ARG:HB3	2:C:79:HIS:HE1	1.80	0.47
2:C:125:ASN:CG	2:C:126:ASP:N	2.73	0.47
1:A:1010:THR:HB	1:A:1013:GLN:HG2	1.96	0.47
2:D:125:ASN:H	2:D:128:GLN:HB2	1.80	0.46
2:C:50:ARG:HB3	2:C:79:HIS:CE1	2.50	0.46
2:C:50:ARG:HA	2:C:78:PHE:HE1	1.79	0.46
1:B:885:ASN:ND2	1:B:892:TYR:OH	2.48	0.46
1:A:823:LEU:HD22	1:A:829:VAL:HG11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:MET:HG3	1:A:926:LEU:HD13	1.98	0.46
1:B:956:CYS:HB3	1:B:977:GLN:OE1	2.15	0.46
1:B:724:VAL:HG12	1:B:795:ASP:HB3	1.97	0.46
1:A:719:TRP:CZ3	1:A:779:ARG:HD2	2.51	0.46
1:B:844:MET:HE1	1:B:922:CYS:SG	2.56	0.46
1:A:923:GLY:HA2	1:A:1000:MET:HE3	1.98	0.46
2:C:119:THR:O	2:C:123:LEU:HD13	2.15	0.46
1:B:821:MET:O	1:B:825:GLU:HG2	2.16	0.45
1:B:993:ALA:HB2	1:B:1019:PHE:CE1	2.52	0.45
2:D:79:HIS:HB3	2:D:199:LEU:HD11	1.98	0.45
1:B:841:LYS:HA	1:B:1020:LEU:HD13	1.99	0.45
1:B:980:ARG:NH2	1:B:998:ASP:OD1	2.47	0.45
2:C:246:VAL:O	2:C:250:ILE:HG13	2.16	0.45
1:A:903:PRO:HD2	1:A:906:LEU:HD22	1.99	0.45
1:B:778:LEU:HD13	1:B:813:PHE:HE1	1.82	0.45
2:C:138:GLU:O	2:C:142:VAL:HG22	2.17	0.45
1:A:733:ILE:HD13	1:A:733:ILE:HA	1.80	0.44
1:A:821:MET:O	1:A:825:GLU:HG2	2.17	0.44
1:B:900:TRP:CZ3	1:B:934:PRO:HG2	2.53	0.44
2:D:42:ASP:OD1	2:D:44:ALA:N	2.51	0.44
2:D:143:LEU:HD12	2:D:146:ILE:HB	1.99	0.44
2:D:76:ILE:HD13	2:D:198:SER:HB3	2.00	0.44
1:B:986:PHE:O	1:B:989:ILE:HG12	2.17	0.44
1:B:1000:MET:HG2	1:B:1009:CYS:HB2	1.99	0.43
2:D:205:ILE:HD13	2:D:239:VAL:HG11	2.00	0.43
1:B:1015:LEU:HD23	1:B:1020:LEU:HD12	1.99	0.43
1:B:900:TRP:CE3	1:B:934:PRO:HG2	2.53	0.43
2:D:185:ALA:O	2:D:189:VAL:HG23	2.18	0.43
1:B:820:LEU:HD13	1:B:929:LEU:HD21	2.00	0.43
1:A:1037:GLN:O	1:A:1039:CYS:N	2.49	0.43
1:A:844:MET:HE2	1:A:1014:THR:HG21	2.00	0.43
1:B:984:GLU:HA	1:B:987:SER:HB3	2.00	0.43
1:B:760:LEU:HD22	1:B:809:PHE:HE2	1.81	0.43
1:B:821:MET:HE2	1:B:821:MET:HB3	1.83	0.43
1:A:1010:THR:O	1:A:1014:THR:HG23	2.18	0.43
2:D:181:LEU:HD22	2:D:225:TRP:HZ3	1.84	0.43
2:C:143:LEU:HD12	2:C:146:ILE:HB	2.01	0.43
2:C:107:GLU:O	6:C:301:PEG:H21	2.19	0.42
1:A:795:ASP:N	1:A:795:ASP:OD1	2.51	0.42
1:A:843:LEU:CD2	1:A:925:ILE:HD11	2.49	0.42
1:B:914:THR:HG23	1:B:916:ALA:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ARG:NH2	1:A:995:ASP:OD1	2.50	0.42
2:D:179:GLN:OE1	1:B:959:VAL:HA	2.19	0.42
1:A:794:THR:OG1	1:A:795:ASP:N	2.52	0.42
1:A:925:ILE:O	1:A:929:LEU:HG	2.20	0.42
1:B:840:MET:HG3	1:B:926:LEU:HD23	2.01	0.42
1:B:916:ALA:HA	1:B:919:VAL:HG22	2.00	0.42
1:A:772:ILE:O	1:A:776:LYS:HG2	2.20	0.42
1:B:982:LEU:HD11	1:B:1001:LEU:HD12	2.02	0.41
2:C:22:PRO:HG2	2:C:24:TRP:NE1	2.36	0.41
2:C:226:THR:HB	2:C:237:GLN:OE1	2.20	0.41
1:A:717:SER:HA	2:D:20:THR:O	2.21	0.41
2:D:76:ILE:CD1	2:D:198:SER:HB3	2.50	0.41
1:B:840:MET:HB2	1:B:1020:LEU:HD21	2.02	0.41
1:B:819:ASP:O	1:B:823:LEU:HD13	2.20	0.41
1:B:856:LEU:HD22	1:B:915:PRO:HA	2.02	0.41
1:B:1010:THR:HB	1:B:1013:GLN:HG2	2.03	0.40
1:A:927:GLY:O	1:A:931:THR:HG23	2.21	0.40
1:A:944:GLN:O	1:A:948:ILE:HD12	2.21	0.40
1:A:956:CYS:SG	1:A:959:VAL:HG22	2.61	0.40
1:A:732:ILE:HG12	1:A:742:TYR:CE1	2.57	0.40
2:D:178:ILE:O	2:D:182:VAL:HG13	2.21	0.40
2:C:50:ARG:HA	2:C:78:PHE:CE1	2.56	0.40
2:D:58:PHE:HA	2:D:71:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/340 (89%)	287 (94%)	17 (6%)	0	100	100
1	B	310/340 (91%)	289 (93%)	19 (6%)	2 (1%)	21	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	231/269 (86%)	227 (98%)	4 (2%)	0	100	100
2	D	234/269 (87%)	228 (97%)	5 (2%)	1 (0%)	30	52
All	All	1079/1218 (89%)	1031 (96%)	45 (4%)	3 (0%)	36	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	228	LYS
1	B	762	ASN
1	B	763	GLU

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	247/305 (81%)	242 (98%)	5 (2%)	48	74
1	B	238/305 (78%)	232 (98%)	6 (2%)	42	69
2	C	194/241 (80%)	189 (97%)	5 (3%)	40	69
2	D	199/241 (83%)	194 (98%)	5 (2%)	42	69
All	All	878/1092 (80%)	857 (98%)	21 (2%)	43	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	733	ILE
1	A	738	TYR
1	A	874	LYS
1	A	882	ARG
1	A	906	LEU
2	D	20	THR
2	D	52	GLU
2	D	76	ILE
2	D	182	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	222	ILE
1	B	718	ASP
1	B	866	LEU
1	B	883	LEU
1	B	926	LEU
1	B	996	LEU
1	B	1038	ASP
2	C	51	ARG
2	C	73	THR
2	C	182	VAL
2	C	184	MET
2	C	202	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	780	GLN
1	A	944	GLN
1	A	977	GLN
1	A	1013	GLN
2	D	37	GLN
2	D	125	ASN
2	D	149	GLN
2	D	200	GLN
1	B	835	HIS
1	B	842	GLN
1	B	864	ASN
1	B	885	ASN
1	B	937	GLN
1	B	977	GLN
1	B	1013	GLN
2	C	67	HIS
2	C	170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	893	1	8,10,11	1.10	0	10,14,16	1.82	1 (10%)
1	TPO	B	893	1	8,10,11	1.16	0	10,14,16	1.86	1 (10%)

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
1	TPO	A	893	1	-	0/9/11/13	-
1	TPO	B	893	1	-	0/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	893	TPO	P-OG1-CB	-5.24	109.09	123.33
1	A	893	TPO	P-OG1-CB	-5.06	109.59	123.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	A1EB3	B	1101	1	49,50,50	0.50	1 (2%)	63,68,68	1.09	5 (7%)
3	EDO	D	301	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	A	1201	-	3,3,3	0.42	0	2,2,2	0.40	0
6	PEG	C	301	-	6,6,6	0.36	0	5,5,5	0.22	0
4	A1EB3	A	1202	1	49,50,50	0.42	0	63,68,68	1.97	12 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1EB3	B	1101	1	-	11/37/57/57	0/5/5/5
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	A	1201	-	-	0/1/1/1	-
6	PEG	C	301	-	-	3/4/4/4	-
4	A1EB3	A	1202	1	-	11/37/57/57	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	A1EB3	C02-N11	-2.46	1.34	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1202	A1EB3	N03-C02-N11	6.52	126.25	115.53
4	A	1202	A1EB3	C05-C04-N03	-6.18	100.04	113.07
4	A	1202	A1EB3	C04-N03-C02	5.27	126.50	120.79
4	A	1202	A1EB3	C39-N31-C32	5.20	123.28	111.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1202	A1EB3	C27-N11-C12	-5.08	113.01	119.25
4	B	1101	A1EB3	C27-N11-C12	-3.53	114.92	119.25
4	B	1101	A1EB3	C29-C30-N31	-3.45	117.02	122.42
4	A	1202	A1EB3	O01-C02-N11	-3.16	116.99	121.38
4	B	1101	A1EB3	C39-N31-C30	3.00	123.30	116.19
4	A	1202	A1EB3	O01-C02-N03	-2.99	115.59	123.35
4	A	1202	A1EB3	C29-C30-C40	-2.91	116.03	119.59
4	A	1202	A1EB3	C39-C38-C34	2.90	116.08	110.78
4	B	1101	A1EB3	C28-C27-N11	-2.82	117.05	120.14
4	B	1101	A1EB3	C39-N31-C32	2.44	117.05	111.57
4	A	1202	A1EB3	C29-C30-N31	-2.42	118.63	122.42
4	A	1202	A1EB3	C46-C40-C30	2.41	122.44	119.80
4	A	1202	A1EB3	C32-N31-C30	2.34	121.74	116.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1202	A1EB3	O01-C02-N03-C04
4	A	1202	A1EB3	N11-C02-N03-C04
4	A	1202	A1EB3	C25-C15-N16-C17
4	A	1202	A1EB3	C24-C17-N16-C15
4	A	1202	A1EB3	C33-C34-N35-C36
4	A	1202	A1EB3	C43-C42-N41-C40
4	B	1101	A1EB3	C13-C12-N11-C27
4	B	1101	A1EB3	N18-C17-N16-C15
4	B	1101	A1EB3	C38-C34-N35-C36
4	A	1202	A1EB3	O45-C42-N41-C40
4	B	1101	A1EB3	C43-C42-N41-C40
4	B	1101	A1EB3	O45-C42-N41-C40
6	C	301	PEG	O1-C1-C2-O2
4	B	1101	A1EB3	N41-C42-C43-C44
4	A	1202	A1EB3	C29-C30-N31-C32
4	B	1101	A1EB3	C40-C30-N31-C39
4	B	1101	A1EB3	O45-C42-C43-C44
4	B	1101	A1EB3	C29-C30-N31-C39
4	B	1101	A1EB3	C24-C17-N16-C15
4	A	1202	A1EB3	N18-C17-N16-C15
6	C	301	PEG	O2-C3-C4-O4
4	A	1202	A1EB3	C40-C30-N31-C32
6	C	301	PEG	C4-C3-O2-C2
4	B	1101	A1EB3	C38-C34-N35-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1202	A1EB3	C29-C30-N31-C39

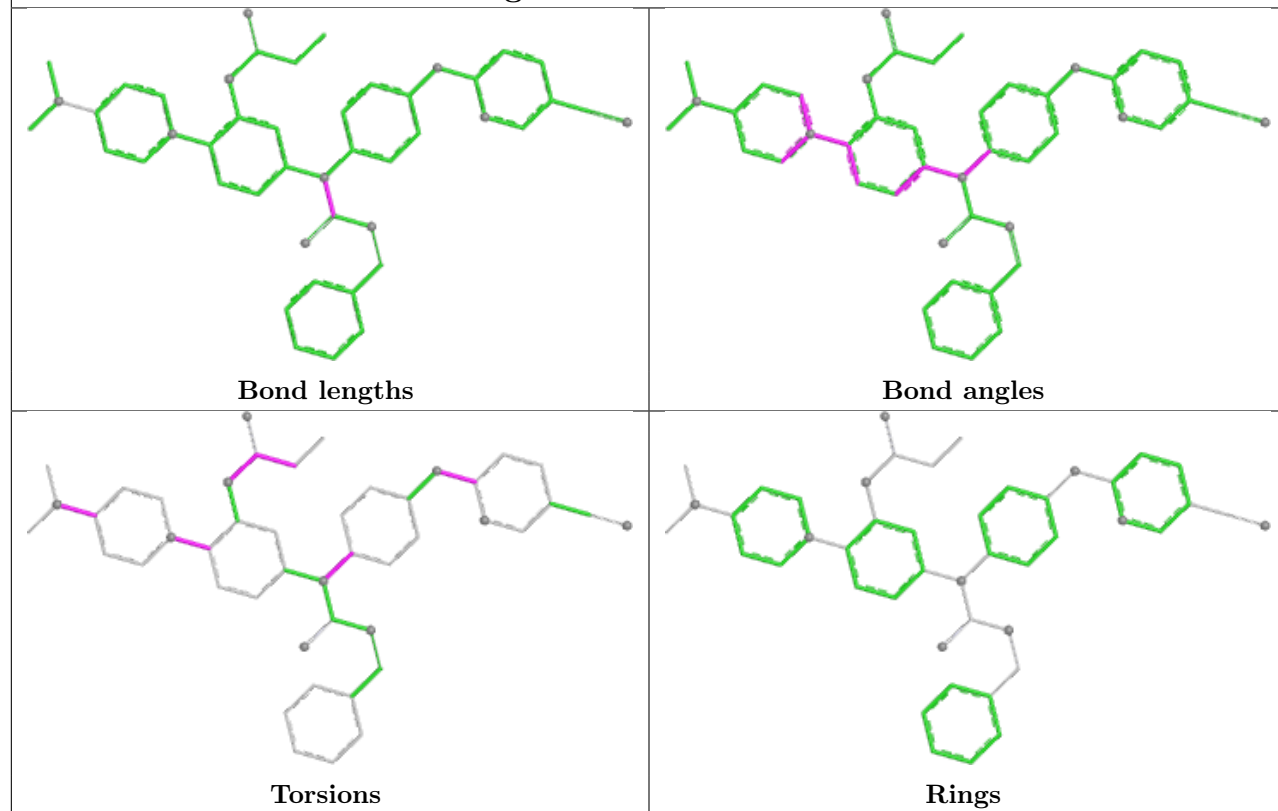
There are no ring outliers.

3 monomers are involved in 4 short contacts:

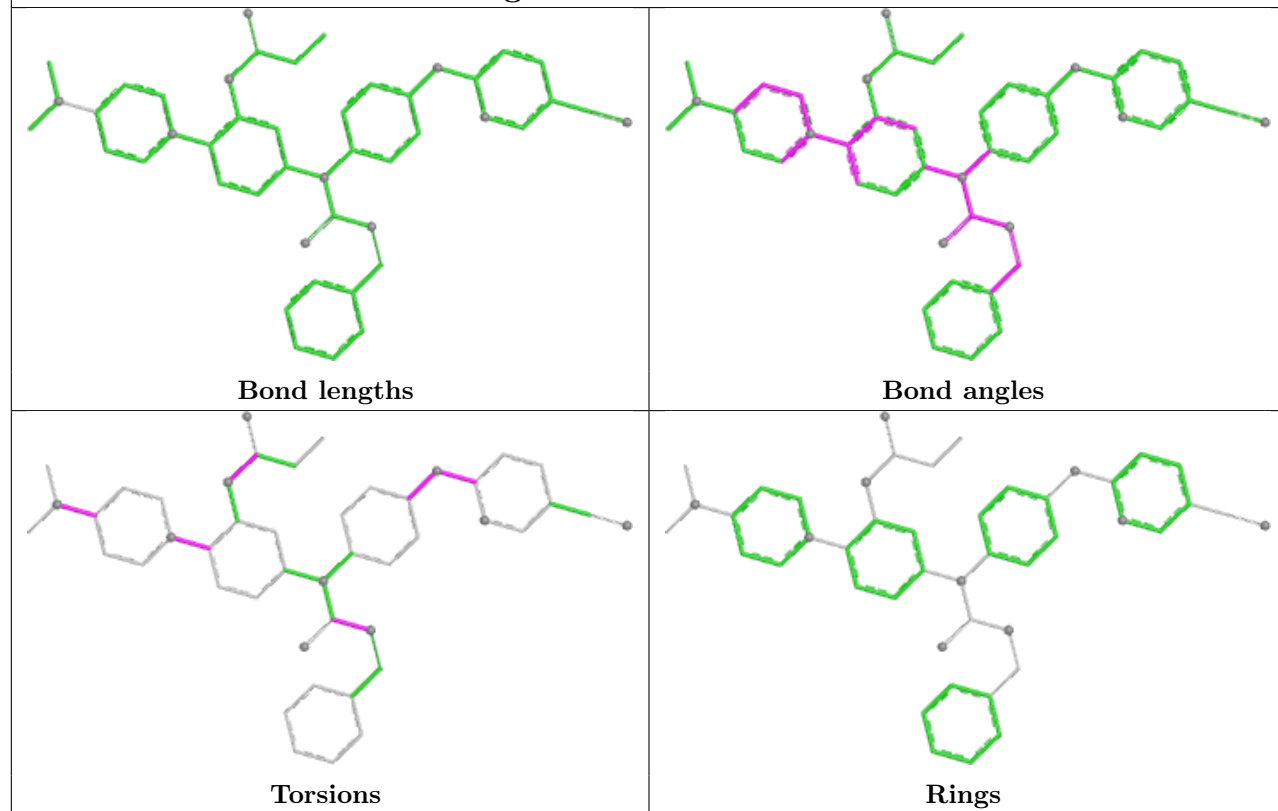
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1101	A1EB3	2	0
6	C	301	PEG	1	0
4	A	1202	A1EB3	1	0

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

Ligand A1EB3 B 1101



Ligand A1EB3 A 1202



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/340 (91%)	0.74	21 (6%) 23 21	45, 67, 96, 112	0
1	B	314/340 (92%)	1.08	33 (10%) 11 10	57, 81, 108, 122	0
2	C	235/269 (87%)	0.60	4 (1%) 69 66	42, 66, 90, 115	0
2	D	238/269 (88%)	0.34	5 (2%) 63 60	33, 52, 76, 92	0
All	All	1097/1218 (90%)	0.72	63 (5%) 29 26	33, 68, 98, 122	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	824	LEU	4.1
1	B	891	PRO	3.8
1	A	896	VAL	3.5
1	A	982	LEU	3.5
1	B	733	ILE	3.3
1	B	749	THR	3.3
1	B	952	CYS	3.2
1	A	972	MET	3.2
1	B	717	SER	3.2
1	B	719	TRP	3.2
2	C	171	LEU	3.1
1	A	891	PRO	3.1
1	B	993	ALA	3.1
1	B	879	GLY	3.0
1	A	1032	ASP	2.9
1	B	730	ILE	2.9
2	C	227	SER	2.9
1	A	749	THR	2.8
1	B	982	LEU	2.8
1	A	881	ALA	2.8
1	A	964	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	122	SER	2.7
1	B	887	GLU	2.6
1	B	884	TYR	2.6
1	B	1031	PRO	2.6
1	A	895	LYS	2.6
1	A	717	SER	2.6
1	B	972	MET	2.6
1	A	887	GLU	2.6
1	B	738	TYR	2.5
1	B	718	ASP	2.5
1	A	965	LYS	2.5
1	A	973	LYS	2.5
2	C	172	LYS	2.5
1	B	923	GLY	2.5
2	D	42	ASP	2.5
2	D	67	HIS	2.4
2	D	36	SER	2.4
1	B	986	PHE	2.4
1	B	984	GLU	2.3
1	A	1022	ASP	2.3
1	A	1036	TRP	2.3
1	B	888	GLU	2.3
1	B	949	SER	2.3
1	A	929	LEU	2.3
1	A	796	LYS	2.2
1	B	748	ASP	2.2
1	B	1023	VAL	2.2
1	B	892	TYR	2.1
1	B	750	GLY	2.1
1	A	963	VAL	2.1
1	A	788	ASN	2.1
2	D	252	HIS	2.1
1	B	810	TYR	2.1
1	A	1029	ALA	2.1
1	B	716	GLU	2.1
1	B	1015	LEU	2.1
1	B	728	ASP	2.0
1	B	933	LYS	2.0
1	B	1010	THR	2.0
2	D	229	PRO	2.0
1	B	964	ILE	2.0
1	A	762	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	A	893	11/12	0.74	0.13	97,99,109,120	0
1	TPO	B	893	11/12	0.78	0.13	68,92,96,108	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

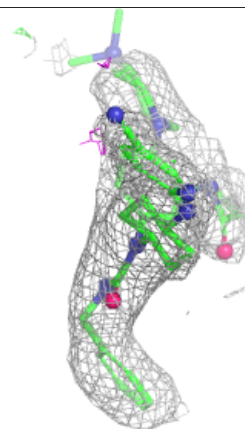
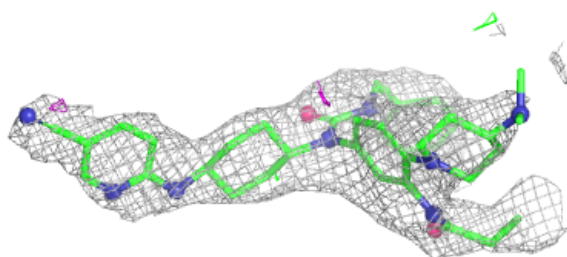
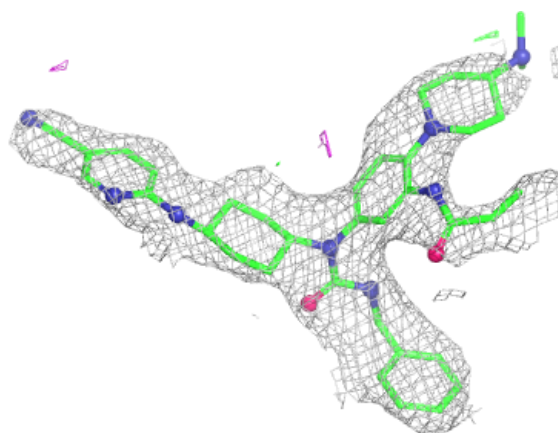
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	1201	4/4	0.30	0.29	88,93,93,98	0
5	MG	A	1203	1/1	0.51	0.15	87,87,87,87	0
3	EDO	D	301	4/4	0.59	0.20	137,138,145,150	0
4	A1EB3	B	1101	46/46	0.79	0.16	59,79,103,107	0
6	PEG	C	301	7/7	0.79	0.14	89,89,89,89	0
4	A1EB3	A	1202	46/46	0.87	0.13	36,63,85,91	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.

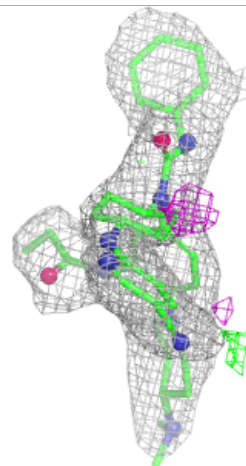
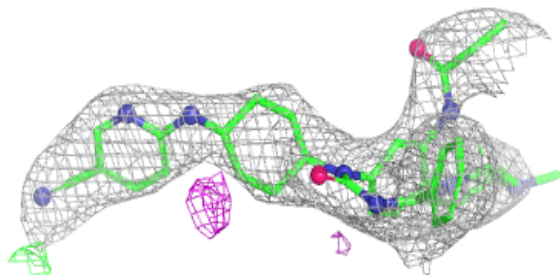
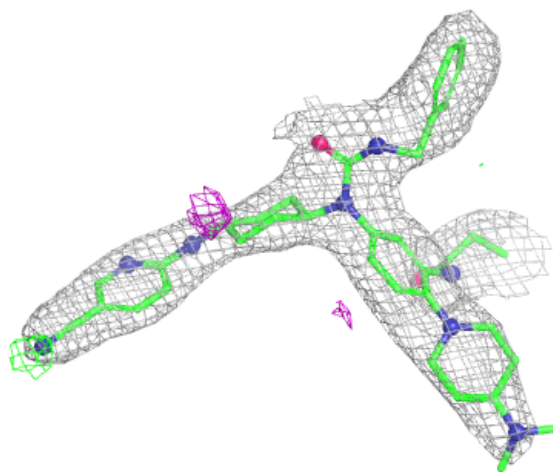
Electron density around A1EB3 B 1101:

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



Electron density around A1EB3 A 1202:

$2mF_o-DF_c$ (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.