Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 10:09 AM EDT

PDB ID	:	9D0V / pdb_00009d0v
Title	:	Crystal structure of CDK2/CyclinE1 in complex with Cpd 2
Authors	:	Kwiatkowski, N.; Liang, T.; Sha, Z.; Collier, P.N.; Yang, A.; Sathappa, M.; Paul, A.; Su, L.; Zheng, X.; Aversa, R.; Li, K.; Mehovic, R.; Breitkopf, S.B.; Chen, D.; Howarth, C.L.; Yuan, K.; Jo, H.; Growney, J.D.; Weiss, M.; Williams, J.
Deposited on	:	2024-08-07
Resolution	:	2.54 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 (1)) were used in the production of this report:

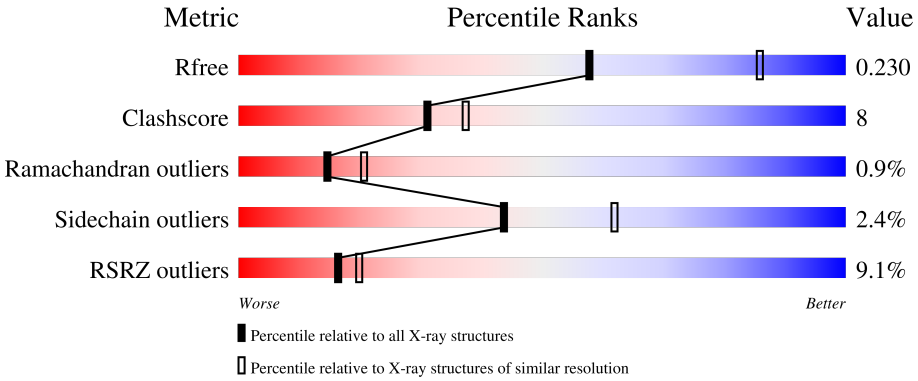
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	298	16% 71% 27%
2	B	286	2% 86% 10%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4873 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 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	2	0
			2344	1520	393	421	1	9			

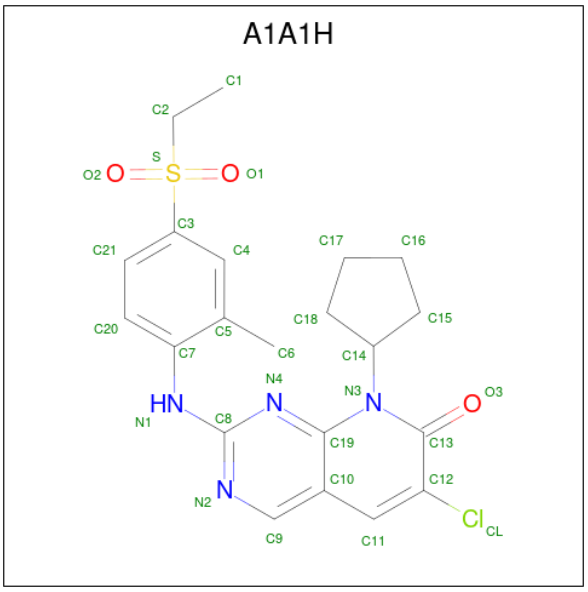
- Molecule 2 is a protein called G1/S-specific cyclin-E1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	P	S	0	1	0
			2289	1484	378	409	1	17			

There are 3 discrepancies between the modelled and reference sequences:

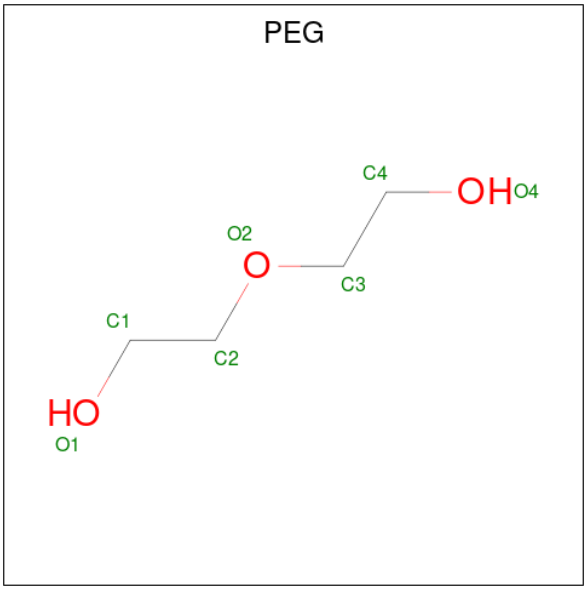
Chain	Residue	Modelled	Actual	Comment	Reference
B	78	SER	-	expression tag	UNP P24864
B	79	GLY	-	expression tag	UNP P24864
B	80	SER	-	expression tag	UNP P24864

- Molecule 3 is 6-chloro-8-cyclopentyl-2-[4-(ethanesulfonyl)-2-methylanilino]pyrido[2,3-d]pyrimidin-7(8H)-one (CCD ID: A1A1H) (formula: $C_{21}H_{23}ClN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



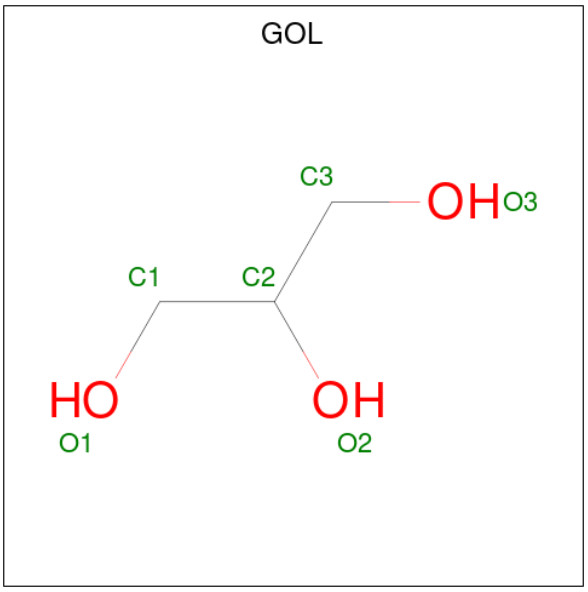
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			30	21	1	4	3	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



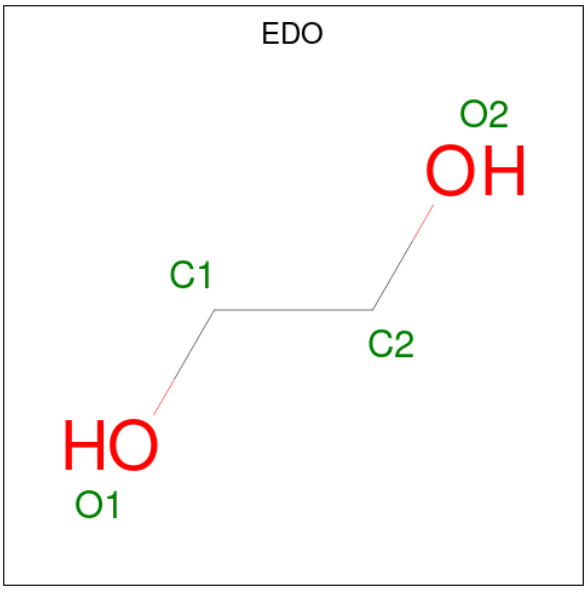
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O		0	0
			7	4	3			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

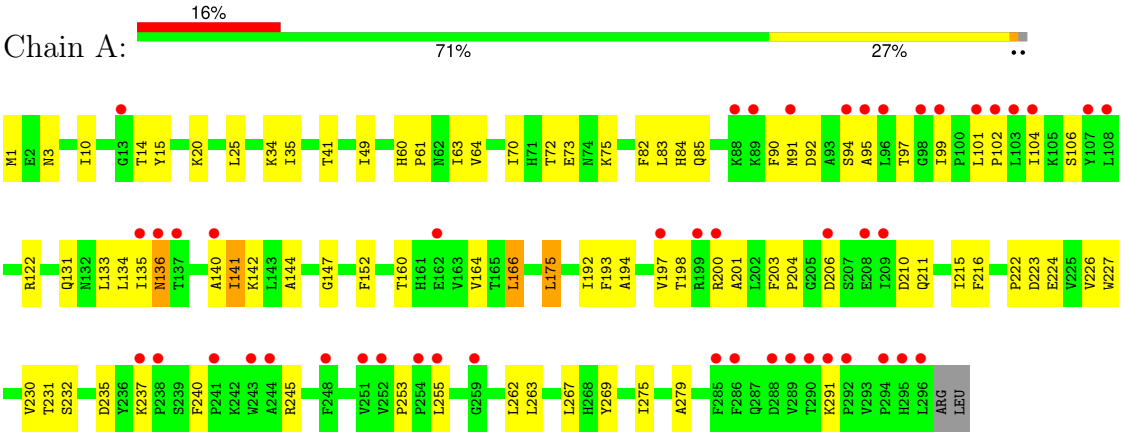
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	50	Total O 50 50	0	0
7	B	123	Total O 123 123	0	0

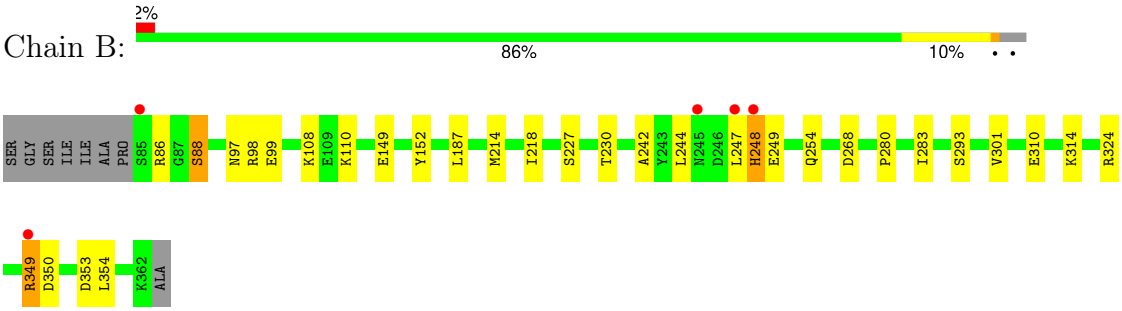
3 Residue-property plots (i)

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

• Molecule 1: Cyclin-dependent kinase 2



• Molecule 2: G1/S-specific cyclin-E1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	76.39Å 76.39Å 257.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.89 – 2.54 24.89 – 2.54	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.89-2.54) 99.9 (24.89-2.54)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.231 0.193 , 0.230	Depositor DCC
R_{free} test set	1519 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4873	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, TPO, GOL, A1A1H, SEP, PEG

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	0.57	0/2397	0.86	0/3259
2	B	0.66	0/2337	0.80	0/3165
All	All	0.62	0/4734	0.83	0/6424

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2344	0	2322	53	0
2	B	2289	0	2297	22	0
3	A	30	0	0	0	0
4	B	7	0	10	0	0
5	B	18	0	24	2	0
6	B	12	0	18	1	0
7	A	50	0	0	0	0
7	B	123	0	0	3	0
All	All	4873	0	4671	76	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 8.

All (76) 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:A:198:THR:HG22	1:A:200:ARG:HB3	1.64	0.80
1:A:135:ILE:HA	1:A:141:ILE:HA	1.71	0.71
1:A:14:THR:HG21	1:A:147:GLY:HA3	1.73	0.71
5:B:403:GOL:H31	7:B:559:HOH:O	1.91	0.70
1:A:175:LEU:HA	1:A:235:ASP:HB2	1.76	0.68
1:A:140:ALA:O	1:A:141:ILE:HG22	1.97	0.64
2:B:214:MET:HE3	2:B:214:MET:O	1.99	0.62
2:B:214:MET:CE	2:B:218:ILE:HG13	2.30	0.62
1:A:197:VAL:HG23	1:A:198:THR:H	1.65	0.61
1:A:14:THR:HG23	1:A:15:TYR:HD1	1.67	0.60
1:A:14:THR:HG23	1:A:15:TYR:CD1	2.40	0.57
1:A:91:MET:HA	1:A:99:ILE:HD11	1.87	0.57
1:A:237:LYS:HB2	1:A:240:PHE:CE1	2.41	0.56
1:A:72:THR:HG22	1:A:73:GLU:H	1.71	0.55
1:A:122:ARG:HA	1:A:152:PHE:CE2	2.43	0.54
2:B:244:LEU:HD22	2:B:248:HIS:HA	1.89	0.54
1:A:90:PHE:CE2	1:A:99:ILE:HD13	2.43	0.54
1:A:203:PHE:CE1	1:A:215:ILE:HA	2.43	0.54
1:A:223:ASP:H	1:A:226:VAL:HG12	1.73	0.54
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.89	0.53
1:A:101:LEU:HA	1:A:104:ILE:HG12	1.90	0.52
1:A:197:VAL:HG23	1:A:198:THR:N	2.23	0.52
2:B:280:PRO:HG2	2:B:283:ILE:HD12	1.91	0.52
1:A:194:ALA:HA	1:A:197:VAL:HG22	1.92	0.52
2:B:244:LEU:HD23	2:B:254:GLN:HE22	1.75	0.52
2:B:214:MET:HE3	2:B:218:ILE:HG13	1.90	0.52
2:B:152:TYR:HB3	2:B:230:THR:HB	1.93	0.51
1:A:206:ASP:OD2	1:A:210:ASP:OD2	2.29	0.51
1:A:131:GLN:OE1	1:A:131:GLN:N	2.35	0.50
1:A:101:LEU:N	1:A:102:PRO:HD2	2.28	0.49
2:B:214:MET:HE2	2:B:218:ILE:HG13	1.92	0.49
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.95	0.48
1:A:15:TYR:HE2	1:A:35:ILE:HD11	1.79	0.47
1:A:3:ASN:HD21	1:A:25:LEU:HB2	1.79	0.47
1:A:216:PHE:HE2	1:A:240:PHE:CD2	2.33	0.47
2:B:88:SEP:HB3	2:B:98:ARG:HH22	1.79	0.47
2:B:353:ASP:OD1	2:B:354:LEU:N	2.47	0.47
1:A:84:HIS:ND1	1:A:136:ASN:HA	2.30	0.47
1:A:222:PRO:HD3	1:A:269:TYR:CZ	2.49	0.47
2:B:108:LYS:NZ	7:B:501:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ALA:HB2	2:B:301:VAL:HG11	1.96	0.46
1:A:263:LEU:O	1:A:267:LEU:HD23	2.15	0.46
1:A:263:LEU:HG	1:A:267:LEU:HD23	1.98	0.46
1:A:134:LEU:O	1:A:141:ILE:HA	2.16	0.45
1:A:201:ALA:O	1:A:204:PRO:HD3	2.16	0.45
1:A:10:ILE:HG13	1:A:20:LYS:N	2.31	0.45
2:B:108:LYS:HE2	2:B:227:SER:O	2.17	0.45
2:B:247:LEU:HB3	2:B:249:GLU:HG3	1.99	0.44
2:B:324:ARG:HA	2:B:324:ARG:HD2	1.80	0.44
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.67	0.43
2:B:268:ASP:OD2	2:B:349:ARG:NH1	2.52	0.43
5:B:403:GOL:H32	7:B:558:HOH:O	2.18	0.43
1:A:34:LYS:CE	1:A:75:LYS:NZ	2.83	0.42
1:A:85:GLN:HE21	1:A:90:PHE:HB2	1.85	0.42
1:A:64:VAL:CG2	1:A:144:ALA:HB2	2.50	0.42
2:B:97:ASN:OD1	2:B:99:GLU:HB2	2.20	0.42
1:A:90:PHE:HE2	1:A:99:ILE:HD13	1.82	0.41
1:A:227:TRP:O	1:A:230:VAL:HG22	2.20	0.41
2:B:149:GLU:HG2	6:B:407:EDO:H22	2.02	0.41
1:A:166:LEU:HD22	1:A:211:GLN:HG2	2.03	0.41
1:A:253:PRO:O	1:A:255:LEU:N	2.53	0.41
1:A:275:ILE:HG12	1:A:279:ALA:HB3	2.03	0.41
1:A:82:PHE:C	1:A:83:LEU:HD12	2.41	0.41
2:B:310:GLU:O	2:B:314:LYS:HG2	2.20	0.41
1:A:1[B]:MET:HG3	1:A:70:ILE:HG21	2.03	0.41
1:A:92:ASP:HA	1:A:95:ALA:HB2	2.02	0.41
1:A:201:ALA:HB3	1:A:204:PRO:HB3	2.02	0.41
2:B:110:LYS:HE3	2:B:110:LYS:HB3	1.82	0.41
1:A:193:PHE:CE2	1:A:262:LEU:HD23	2.55	0.41
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.35	0.41
2:B:244:LEU:HA	2:B:254:GLN:NE2	2.36	0.40
1:A:49:ILE:HG22	2:B:187:LEU:HD21	2.03	0.40
1:A:60:HIS:HB3	1:A:63:ILE:HD12	2.03	0.40
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.87	0.40
1:A:61:PRO:O	1:A:142:LYS:NZ	2.47	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	294/298 (99%)	263 (90%)	27 (9%)	4 (1%)	9 12
2	B	276/286 (96%)	274 (99%)	1 (0%)	1 (0%)	30 40
All	All	570/584 (98%)	537 (94%)	28 (5%)	5 (1%)	14 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	141	ILE
1	A	164	VAL
1	A	245	ARG
2	B	293	SER

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	248/262 (95%)	240 (97%)	8 (3%)	34 49
2	B	250/255 (98%)	246 (98%)	4 (2%)	58 75
All	All	498/517 (96%)	486 (98%)	12 (2%)	44 62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR

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Mol	Chain	Res	Type
1	A	94	SER
1	A	97	THR
1	A	106	SER
1	A	166	LEU
1	A	175	LEU
1	A	232	SER
1	A	291	LYS
2	B	86	ARG
2	B	248	HIS
2	B	349	ARG
2	B	350	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	85	GLN
1	A	268	HIS
1	A	272	ASN
2	B	291	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)

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	160	1	8,10,11	1.62	2 (25%)	10,14,16	1.31	2 (20%)
2	SEP	B	88	2	8,9,10	1.68	2 (25%)	7,12,14	2.14	1 (14%)

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	160	1	-	1/9/11/13	-
2	SEP	B	88	2	-	5/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	88	SEP	P-O1P	3.64	1.61	1.50
1	A	160	TPO	P-OG1	3.25	1.65	1.59
1	A	160	TPO	P-O3P	2.10	1.62	1.54
2	B	88	SEP	P-O2P	2.03	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	88	SEP	OG-CB-CA	5.35	113.35	108.14
1	A	160	TPO	CG2-CB-CA	-2.29	108.81	113.26
1	A	160	TPO	P-OG1-CB	-2.23	117.27	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	88	SEP	N-CA-CB-OG
2	B	88	SEP	CB-OG-P-O2P
2	B	88	SEP	CB-OG-P-O3P
2	B	88	SEP	CB-OG-P-O1P
2	B	88	SEP	CA-CB-OG-P
1	A	160	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	88	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
5	GOL	B	404	-	5,5,5	1.47	1 (20%)	5,5,5	1.26	1 (20%)
3	A1A1H	A	301	-	32,33,33	1.07	2 (6%)	39,49,49	2.65	14 (35%)
4	PEG	B	401	-	6,6,6	0.20	0	5,5,5	0.17	0
5	GOL	B	403	-	5,5,5	1.06	1 (20%)	5,5,5	1.14	0
6	EDO	B	405	-	3,3,3	0.51	0	2,2,2	0.54	0
6	EDO	B	407	-	3,3,3	0.65	0	2,2,2	0.12	0
5	GOL	B	402	-	5,5,5	1.39	0	5,5,5	1.03	0
6	EDO	B	406	-	3,3,3	0.77	0	2,2,2	0.32	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
5	GOL	B	404	-	-	2/4/4/4	-
3	A1A1H	A	301	-	-	7/17/24/24	0/4/4/4
4	PEG	B	401	-	-	2/4/4/4	-
5	GOL	B	403	-	-	0/4/4/4	-
6	EDO	B	405	-	-	0/1/1/1	-
6	EDO	B	407	-	-	1/1/1/1	-
5	GOL	B	402	-	-	2/4/4/4	-
6	EDO	B	406	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	A1A1H	C19-N3	-3.08	1.37	1.39
3	A	301	A1A1H	C19-N4	-2.59	1.30	1.34
5	B	404	GOL	C3-C2	2.52	1.61	1.51
5	B	403	GOL	C1-C2	2.23	1.60	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	A1A1H	O2-S-C3	-10.54	98.24	108.33
3	A	301	A1A1H	C9-C10-C19	5.18	119.12	114.55
3	A	301	A1A1H	C14-N3-C13	4.43	124.00	117.69
3	A	301	A1A1H	N2-C8-N4	-4.02	122.53	126.42
3	A	301	A1A1H	C9-N2-C8	3.96	121.24	115.81
3	A	301	A1A1H	O3-C13-C12	-3.78	117.39	124.83
3	A	301	A1A1H	O2-S-C2	3.57	115.22	108.31
3	A	301	A1A1H	C4-C3-S	2.60	121.52	118.88
3	A	301	A1A1H	C10-C19-N4	-2.47	118.73	122.95
3	A	301	A1A1H	C10-C11-C12	-2.46	116.73	122.37
3	A	301	A1A1H	C6-C5-C7	-2.36	118.55	121.23
3	A	301	A1A1H	O1-S-C3	-2.35	106.08	108.33
3	A	301	A1A1H	C8-N4-C19	2.16	120.92	113.99
3	A	301	A1A1H	O2-S-O1	2.11	120.71	118.45
5	B	404	GOL	C3-C2-C1	-2.11	104.07	111.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	A1A1H	C1-C2-S-C3
3	A	301	A1A1H	C1-C2-S-O2
5	B	404	GOL	C1-C2-C3-O3
3	A	301	A1A1H	C21-C3-S-O2
3	A	301	A1A1H	C4-C3-S-O2
3	A	301	A1A1H	C4-C3-S-C2
3	A	301	A1A1H	C21-C3-S-C2
5	B	402	GOL	C1-C2-C3-O3
5	B	404	GOL	O2-C2-C3-O3
4	B	401	PEG	O1-C1-C2-O2
4	B	401	PEG	O2-C3-C4-O4
3	A	301	A1A1H	C1-C2-S-O1
5	B	402	GOL	O1-C1-C2-C3
6	B	406	EDO	O1-C1-C2-O2
6	B	407	EDO	O1-C1-C2-O2

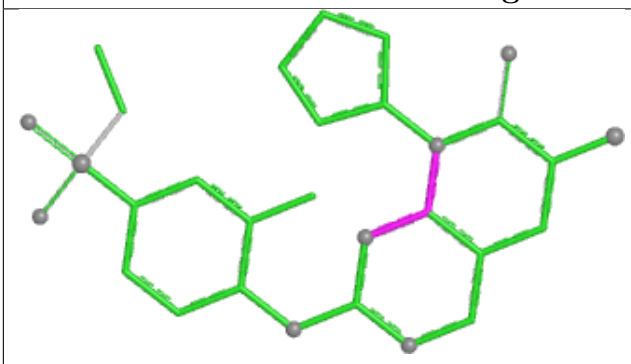
There are no ring outliers.

2 monomers are involved in 3 short contacts:

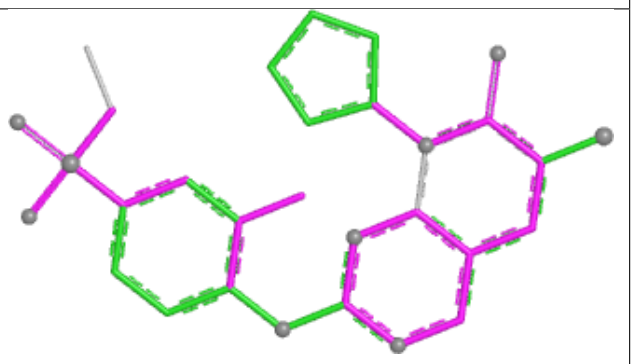
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	GOL	2	0
6	B	407	EDO	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

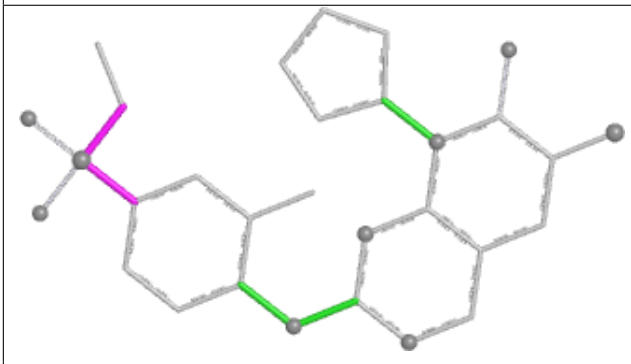
Ligand A1A1H A 301



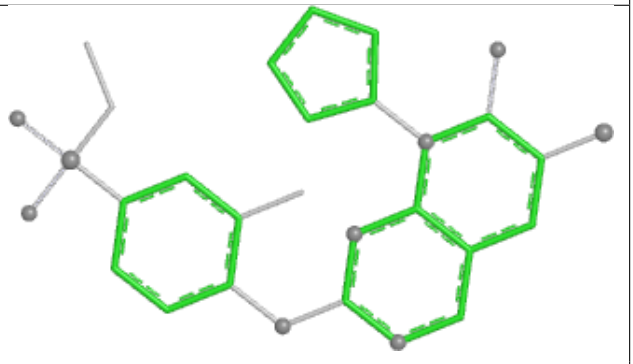
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	295/298 (98%)	0.69	47 (15%) 6 7	29, 73, 119, 136	2 (0%)
2	B	277/286 (96%)	-0.58	5 (1%) 67 71	25, 41, 73, 99	1 (0%)
All	All	572/584 (97%)	0.07	52 (9%) 16 20	25, 54, 106, 136	3 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	VAL	5.6
1	A	103	LEU	5.5
1	A	290	THR	5.1
1	A	251	VAL	4.7
1	A	296	LEU	4.5
1	A	259	GLY	4.3
1	A	104	ILE	4.3
2	B	85	SER	3.7
2	B	349	ARG	3.6
1	A	209	ILE	3.4
1	A	243	TRP	3.2
1	A	199	ARG	3.2
1	A	295	HIS	3.2
1	A	99	ILE	3.1
1	A	241	PRO	3.1
1	A	294	PRO	3.1
1	A	238	PRO	3.0
1	A	95	ALA	2.9
1	A	107	TYR	2.9
1	A	292	PRO	2.9
1	A	140	ALA	2.9
1	A	288	ASP	2.9
1	A	137	THR	2.8
1	A	135	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	197	VAL	2.8
1	A	136	ASN	2.8
1	A	88	LYS	2.7
1	A	291	LYS	2.6
1	A	98	GLY	2.6
2	B	248	HIS	2.6
1	A	162	GLU	2.5
1	A	248	PHE	2.5
1	A	255	LEU	2.5
1	A	244	ALA	2.5
1	A	94	SER	2.4
1	A	285	PHE	2.4
1	A	96	LEU	2.3
1	A	101	LEU	2.3
1	A	89	LYS	2.3
1	A	108	LEU	2.3
2	B	245	ASN	2.2
1	A	254	PRO	2.2
1	A	208	GLU	2.2
1	A	206	ASP	2.1
1	A	237	LYS	2.1
1	A	13	GLY	2.1
2	B	247	LEU	2.1
1	A	200	ARG	2.1
1	A	102	PRO	2.1
1	A	91	MET	2.1
1	A	252	VAL	2.0
1	A	286	PHE	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, 95^{th} 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
2	SEP	B	88	10/11	0.84	0.13	64,80,104,112	0
1	TPO	A	160	11/12	0.96	0.08	41,48,51,56	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

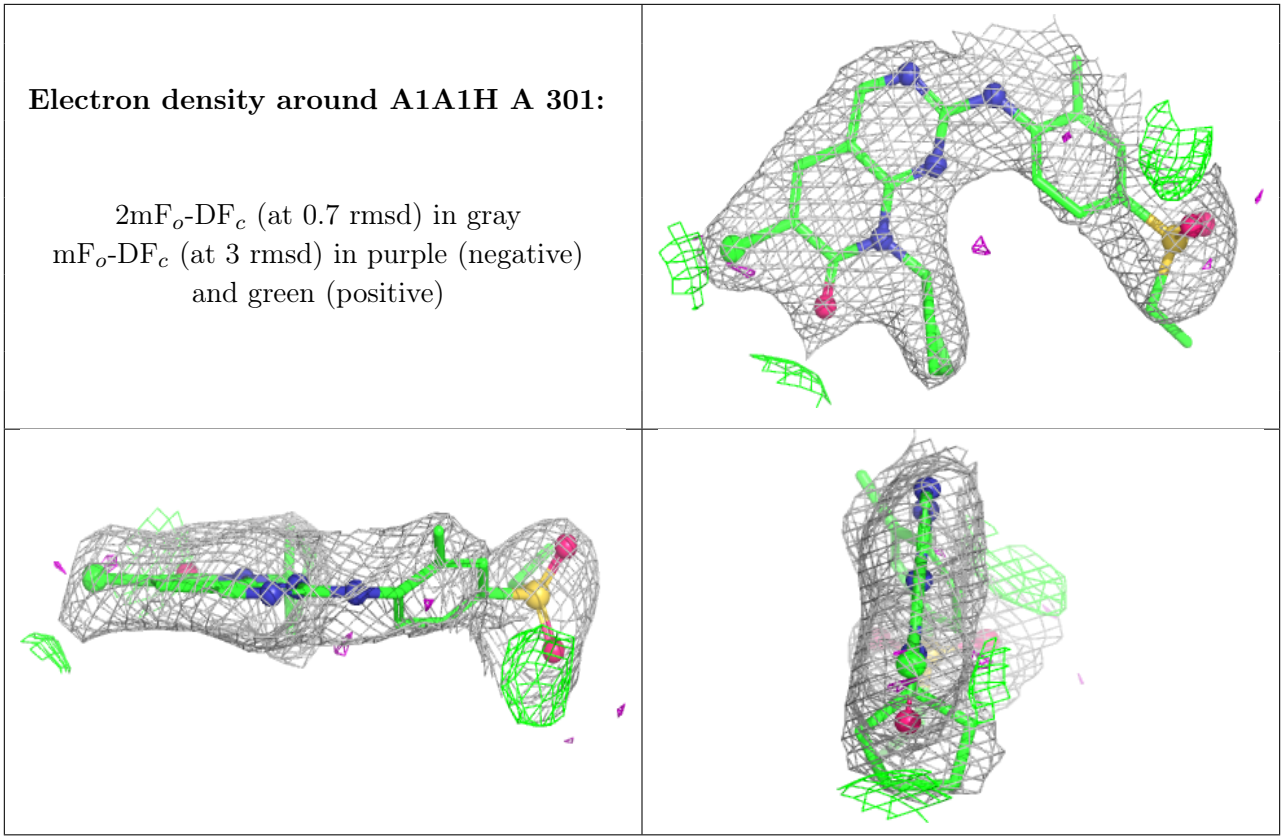
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	403	6/6	0.77	0.16	58,66,69,73	0
5	GOL	B	404	6/6	0.82	0.13	63,66,78,81	0
5	GOL	B	402	6/6	0.84	0.15	56,63,75,75	0
6	EDO	B	407	4/4	0.84	0.15	58,60,63,64	0
6	EDO	B	406	4/4	0.85	0.15	59,65,66,69	0
6	EDO	B	405	4/4	0.85	0.15	53,58,60,70	0
4	PEG	B	401	7/7	0.88	0.13	56,61,69,70	0
3	A1A1H	A	301	30/30	0.91	0.11	60,74,95,103	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 A1A1H A 301:

$2mF_o$-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.