Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 10:46 PM EDT

PDB ID	:	5HLN
Title	:	X-RAY CRYSTAL STRUCTURE OF GSK3B IN COMPLEX WITH CHIR99021
Authors	:	White, A.; Lakshminarasimhan, D.; Nadupalli, A.; Suto, R.K.
Deposited on	:	2016-01-15
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

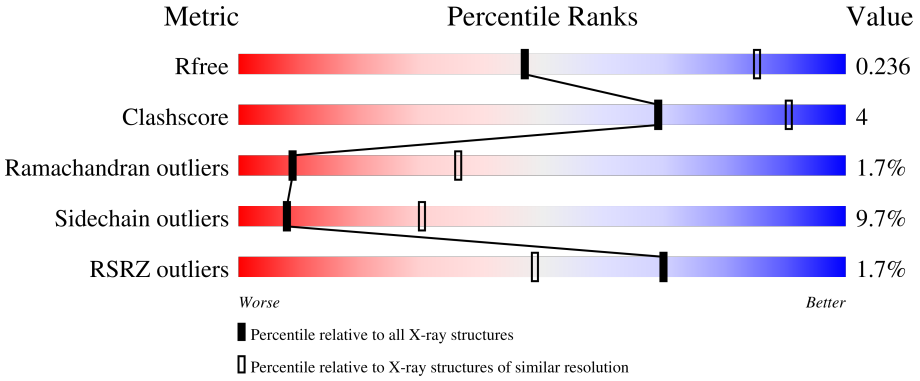
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	424	67% 13% • 18%
1	B	424	?% 65% 15% • 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5652 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.

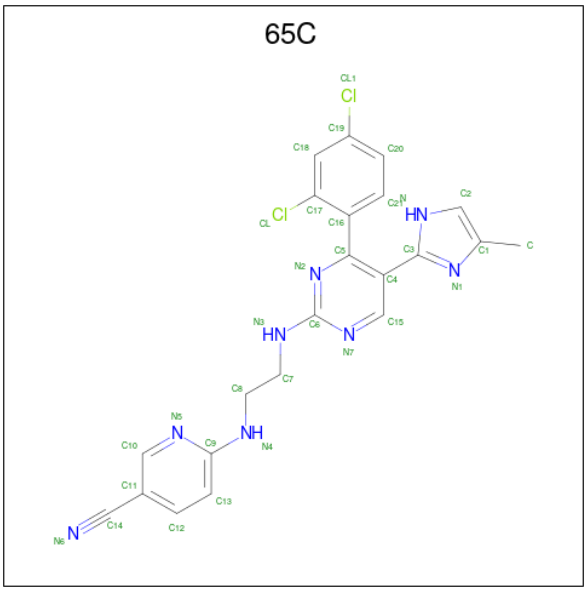
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	347	2781	1787	476	506	1	11	0	0	0
1	B	347	2781	1789	477	504		11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P49841
A	-2	SER	-	expression tag	UNP P49841
A	-1	PRO	-	expression tag	UNP P49841
A	0	GLY	-	expression tag	UNP P49841
B	-3	GLY	-	expression tag	UNP P49841
B	-2	SER	-	expression tag	UNP P49841
B	-1	PRO	-	expression tag	UNP P49841
B	0	GLY	-	expression tag	UNP P49841

- Molecule 2 is CHIR99021 (three-letter code: 65C) (formula: $C_{22}H_{18}Cl_2N_8$).

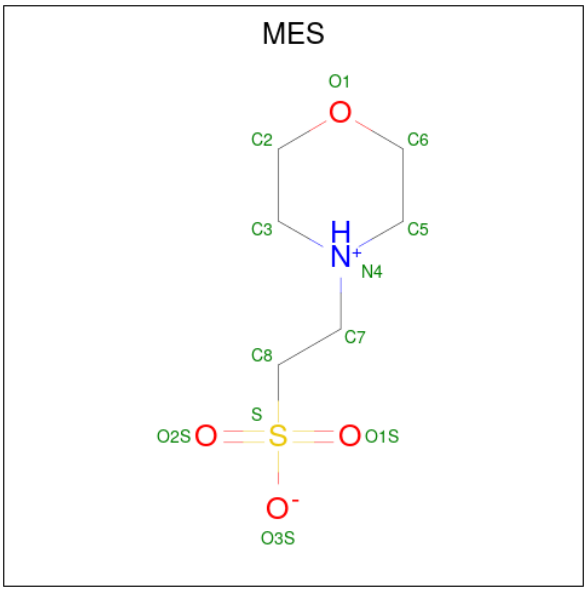


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	N		
2	A	1	32	22	2	8	0	0
			Total	C	Cl	N		
2	B	1	32	22	2	8	0	0

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

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



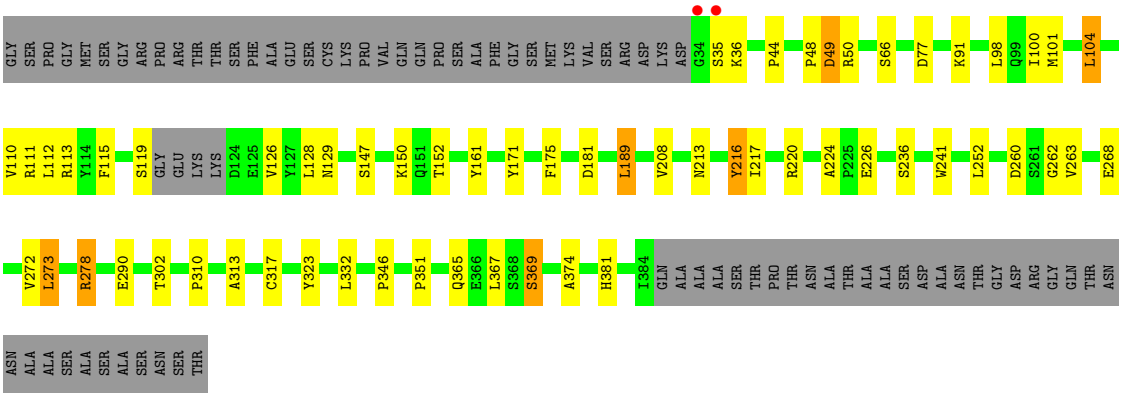
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0

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.

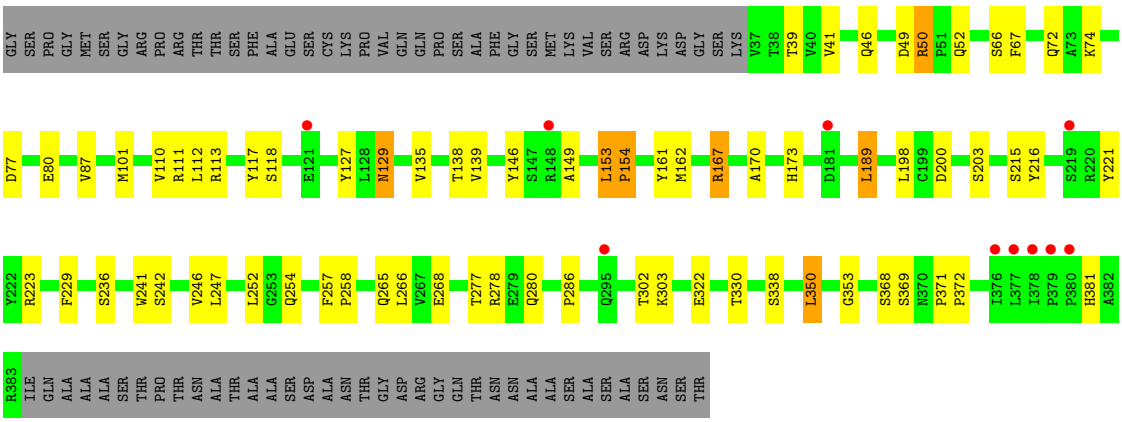
• Molecule 1: Glycogen synthase kinase-3 beta

Chain A: 67% 13% • 18%



• Molecule 1: Glycogen synthase kinase-3 beta

Chain B: 2% 65% 15% • 18%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	163.52Å 163.52Å 84.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.28 – 3.10 39.28 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.28-3.10) 99.3 (39.28-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.170 , 0.236 0.173 , 0.236	Depositor DCC
R_{free} test set	1210 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	99.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5652	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 65C, MG, PTR

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	0.64	0/2833	0.88	3/3853 (0.1%)
1	B	0.58	0/2838	0.81	0/3860
All	All	0.61	0/5671	0.85	3/7713 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	113	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	111	ARG	NE-CZ-NH2	5.33	122.96	120.30

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	2781	0	2798	17	0
1	B	2781	0	2802	29	0
2	A	32	0	0	0	0
2	B	32	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	13	0	0
4	B	12	0	13	0	0
All	All	5652	0	5626	42	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 4.

All (42) 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:216:PTR:O1P	1:B:216:PTR:OH	2.16	0.63
1:A:101:MET:HB3	1:A:112:LEU:HD22	1.80	0.62
1:A:216:PTR:O3P	1:B:216:PTR:OH	2.18	0.60
1:B:129:ASN:HD22	1:B:129:ASN:N	1.99	0.60
1:A:216:PTR:P	1:B:216:PTR:OH	2.60	0.59
1:B:50:ARG:NH1	1:B:52:GLN:OE1	2.38	0.56
1:A:100:ILE:O	1:A:104:LEU:HD22	2.06	0.55
1:A:48:PRO:O	1:A:50:ARG:N	2.40	0.55
1:B:74:LYS:HA	1:B:80:GLU:O	2.06	0.55
1:B:146:TYR:CE2	1:B:154:PRO:HD2	2.43	0.53
1:B:173:HIS:CD2	1:B:236:SER:HB3	2.46	0.50
1:B:161:TYR:CZ	1:B:189:LEU:HD12	2.47	0.49
1:B:153:LEU:HD23	1:B:154:PRO:HD2	1.94	0.49
1:B:129:ASN:N	1:B:129:ASN:ND2	2.61	0.48
1:B:242:SER:O	1:B:246:VAL:HG23	2.13	0.48
1:B:167:ARG:O	1:B:170:ALA:HB3	2.15	0.47
1:A:161:TYR:CZ	1:A:189:LEU:HD13	2.50	0.47
1:A:224:ALA:HA	1:A:241:TRP:CD1	2.50	0.47
1:B:257:PHE:O	1:B:265:GLN:NE2	2.47	0.46
1:A:346:PRO:HB3	1:A:381:HIS:CD2	2.50	0.46
1:B:277:THR:OG1	1:B:280:GLN:HG3	2.15	0.46
1:B:371:PRO:N	1:B:372:PRO:HD2	2.31	0.46
1:B:67:PHE:O	1:B:87:VAL:HG12	2.17	0.45
1:A:310:PRO:O	1:A:313:ALA:HB3	2.16	0.44
1:B:101:MET:HB3	1:B:112:LEU:HD22	1.98	0.44
1:B:135:VAL:O	2:B:501:65C:N4	2.50	0.44
1:A:332:LEU:HD21	1:A:367:LEU:HA	1.99	0.44
1:B:117:TYR:HA	1:B:127:TYR:O	2.17	0.44
1:B:241:TRP:CD1	1:B:241:TRP:C	2.91	0.44
1:A:273:LEU:HD12	1:A:323:TYR:CD2	2.53	0.43
1:B:221:TYR:CE1	1:B:258:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PHE:CZ	1:B:266:LEU:HD21	2.54	0.43
1:B:162:MET:HG3	1:B:247:LEU:HD13	2.00	0.43
1:A:104:LEU:HB2	1:A:171:TYR:HE2	1.84	0.43
1:B:46:GLN:HE21	1:B:46:GLN:HA	1.84	0.42
1:A:175:PHE:CE1	1:A:365:GLN:NE2	2.88	0.42
1:B:350:LEU:O	1:B:353:GLY:N	2.53	0.41
1:A:98:LEU:HB2	1:A:128:LEU:HD21	2.02	0.41
1:A:115:PHE:HA	1:A:129:ASN:O	2.21	0.41
1:B:111:ARG:NH1	1:B:113:ARG:HD3	2.36	0.41
1:A:262:GLY:HA2	1:B:216:PTR:CE2	2.51	0.40
1:B:139:VAL:HG22	1:B:189:LEU:HD13	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	342/424 (81%)	306 (90%)	30 (9%)	6 (2%)	8 34
1	B	344/424 (81%)	304 (88%)	34 (10%)	6 (2%)	9 36
All	All	686/848 (81%)	610 (89%)	64 (9%)	12 (2%)	9 36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	B	49	ASP
1	B	381	HIS
1	A	236	SER
1	A	374	ALA
1	B	149	ALA
1	A	278	ARG

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Mol	Chain	Res	Type
1	A	369	SER
1	B	200	ASP
1	A	181	ASP
1	B	286	PRO
1	B	154	PRO

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	308/365 (84%)	277 (90%)	31 (10%)	7	28
1	B	308/365 (84%)	279 (91%)	29 (9%)	8	32
All	All	616/730 (84%)	556 (90%)	60 (10%)	8	30

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	36	LYS
1	A	44	PRO
1	A	49	ASP
1	A	66	SER
1	A	77	ASP
1	A	91	LYS
1	A	104	LEU
1	A	110	VAL
1	A	119	SER
1	A	126	VAL
1	A	147	SER
1	A	150	LYS
1	A	152	THR
1	A	189	LEU
1	A	208	VAL
1	A	213	ASN
1	A	217	ILE

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Mol	Chain	Res	Type
1	A	226	GLU
1	A	252	LEU
1	A	260	ASP
1	A	263	VAL
1	A	268	GLU
1	A	272	VAL
1	A	273	LEU
1	A	278	ARG
1	A	290	GLU
1	A	302	THR
1	A	317	CYS
1	A	351	PRO
1	A	369	SER
1	B	39	THR
1	B	41	VAL
1	B	50	ARG
1	B	66	SER
1	B	72	GLN
1	B	77	ASP
1	B	110	VAL
1	B	118	SER
1	B	129	ASN
1	B	138	THR
1	B	153	LEU
1	B	167	ARG
1	B	189	LEU
1	B	198	LEU
1	B	203	SER
1	B	215	SER
1	B	223	ARG
1	B	252	LEU
1	B	254	GLN
1	B	268	GLU
1	B	278	ARG
1	B	302	THR
1	B	303	LYS
1	B	322	GLU
1	B	330	THR
1	B	338	SER
1	B	350	LEU
1	B	368	SER
1	B	369	SER

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	129	ASN
1	A	365	GLN
1	B	46	GLN
1	B	129	ASN
1	B	206	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	PTR	A	216	1	15,16,17	0.92	1 (6%)	19,22,24	1.53	3 (15%)
1	PTR	B	216	1	11,12,17	0.61	0	12,15,24	0.42	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
1	PTR	A	216	1	-	4/10/11/13	0/1/1/1
1	PTR	B	216	1	-	3/5/6/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	PTR	P-OH	2.22	1.62	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	PTR	O2P-P-OH	-3.19	95.26	105.24
1	A	216	PTR	O3P-P-O2P	3.01	119.15	107.64
1	A	216	PTR	P-OH-CZ	2.42	131.52	123.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	216	PTR	O-C-CA-CB
1	B	216	PTR	O-C-CA-CB
1	B	216	PTR	CA-CB-CG-CD1
1	A	216	PTR	CZ-OH-P-O1P
1	B	216	PTR	CA-CB-CG-CD2
1	A	216	PTR	CA-CB-CG-CD2
1	A	216	PTR	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	216	PTR	3	0
1	B	216	PTR	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 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	MES	A	503	-	12,12,12	2.09	2 (16%)	14,16,16	2.58	3 (21%)
2	65C	A	501	-	33,35,35	1.57	4 (12%)	43,48,48	2.82	17 (39%)
4	MES	B	503	-	12,12,12	2.20	1 (8%)	14,16,16	2.22	5 (35%)
2	65C	B	501	-	33,35,35	1.40	3 (9%)	43,48,48	2.73	12 (27%)

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	MES	A	503	-	-	4/6/14/14	0/1/1/1
2	65C	A	501	-	-	2/17/17/17	0/4/4/4
4	MES	B	503	-	-	6/6/14/14	0/1/1/1
2	65C	B	501	-	-	2/17/17/17	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	MES	C8-S	-7.04	1.67	1.77
2	A	501	65C	C11-C14	-6.63	1.29	1.44
4	A	503	MES	C8-S	-6.23	1.68	1.77
2	B	501	65C	C11-C14	-5.92	1.31	1.44
2	A	501	65C	C4-C5	-3.04	1.38	1.41
2	B	501	65C	C17-CL	2.86	1.80	1.73
4	A	503	MES	O1S-S	2.79	1.53	1.45
2	A	501	65C	C3-N	2.60	1.39	1.35
2	A	501	65C	C17-CL	2.47	1.79	1.73
2	B	501	65C	C19-CL1	2.44	1.79	1.74

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	65C	C4-C3-N1	-8.39	112.98	123.67
4	A	503	MES	O1S-S-C8	8.13	116.71	106.92
2	B	501	65C	C4-C3-N	8.02	133.91	123.67
2	B	501	65C	N7-C6-N2	-7.65	119.30	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	65C	C4-C3-N1	-7.00	114.75	123.67
2	A	501	65C	N7-C6-N2	-6.96	119.96	126.55
2	A	501	65C	C4-C3-N	5.63	130.85	123.67
2	A	501	65C	C10-N5-C9	5.48	123.38	117.82
2	B	501	65C	C-C1-N1	5.37	132.43	119.98
2	A	501	65C	C-C1-C2	-4.89	116.20	129.07
2	B	501	65C	C-C1-C2	-4.79	116.48	129.07
4	B	503	MES	O2S-S-C8	4.66	112.53	106.92
4	B	503	MES	O3S-S-C8	4.24	112.62	105.77
2	A	501	65C	C-C1-N1	4.23	129.79	119.98
2	A	501	65C	C15-C4-C5	4.20	119.30	115.69
2	B	501	65C	C15-N7-C6	4.11	122.08	115.88
2	A	501	65C	C8-C7-N3	-3.94	103.24	111.46
4	B	503	MES	O1S-S-C8	-3.86	102.27	106.92
2	B	501	65C	C10-N5-C9	3.64	121.51	117.82
2	A	501	65C	C15-N7-C6	3.27	120.81	115.88
4	A	503	MES	O2S-S-C8	-3.17	103.10	106.92
2	A	501	65C	C18-C17-C16	-2.98	119.79	121.91
2	B	501	65C	C18-C17-C16	-2.96	119.80	121.91
2	A	501	65C	C4-C15-N7	-2.94	119.86	124.49
2	B	501	65C	C4-C15-N7	-2.92	119.89	124.49
2	A	501	65C	C13-C9-N5	-2.86	118.11	122.57
2	A	501	65C	C12-C11-C14	2.69	124.47	119.99
2	B	501	65C	C21-C16-C17	2.53	120.43	117.63
2	B	501	65C	C13-C9-N5	-2.39	118.84	122.57
2	A	501	65C	N3-C6-N2	2.34	121.24	117.19
4	B	503	MES	O2S-S-O1S	-2.28	106.05	113.95
2	A	501	65C	C13-C9-N4	2.28	125.95	121.04
2	A	501	65C	C4-C5-N2	-2.24	118.18	121.61
4	B	503	MES	C7-N4-C5	2.20	116.87	111.23
2	B	501	65C	N3-C6-N2	2.19	120.98	117.19
4	A	503	MES	O3S-S-C8	2.17	109.28	105.77
2	A	501	65C	C17-C18-C19	2.12	121.09	118.71

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	MES	N4-C7-C8-S
4	A	503	MES	C7-C8-S-O1S
4	B	503	MES	C8-C7-N4-C3
4	B	503	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
4	B	503	MES	N4-C7-C8-S
4	B	503	MES	C7-C8-S-O1S
4	B	503	MES	C7-C8-S-O2S
4	B	503	MES	C7-C8-S-O3S
4	A	503	MES	C7-C8-S-O3S
2	B	501	65C	N-C3-C4-C15
2	A	501	65C	N-C3-C4-C15
2	B	501	65C	N1-C3-C4-C15
4	A	503	MES	C7-C8-S-O2S
2	A	501	65C	N1-C3-C4-C15

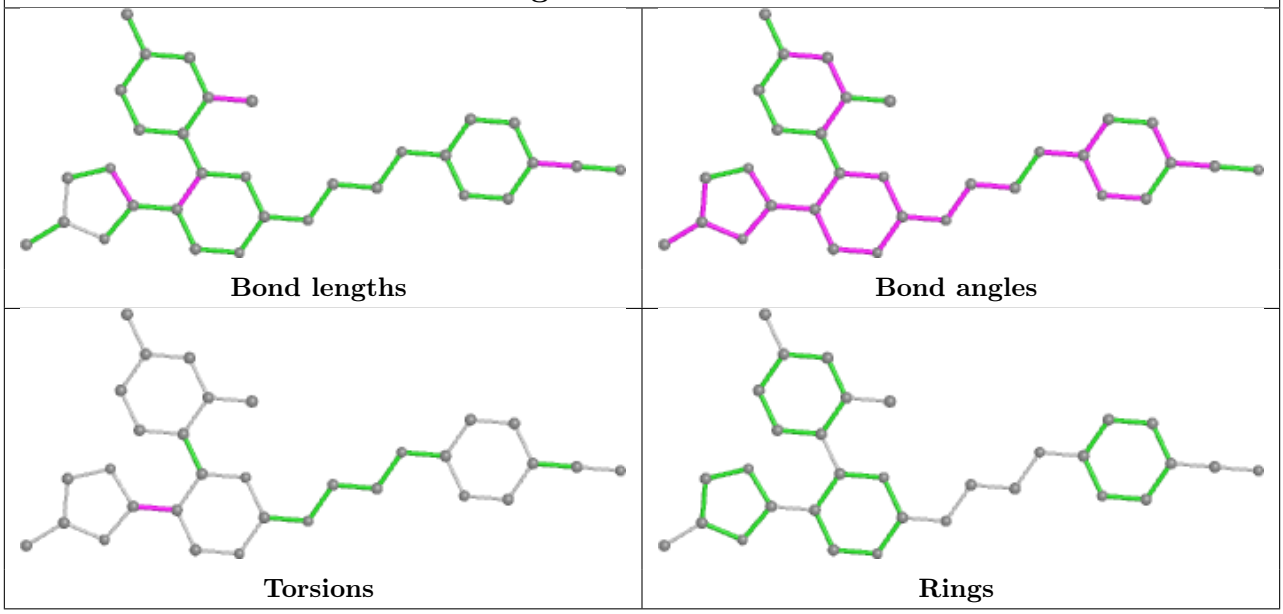
There are no ring outliers.

1 monomer is involved in 1 short contact:

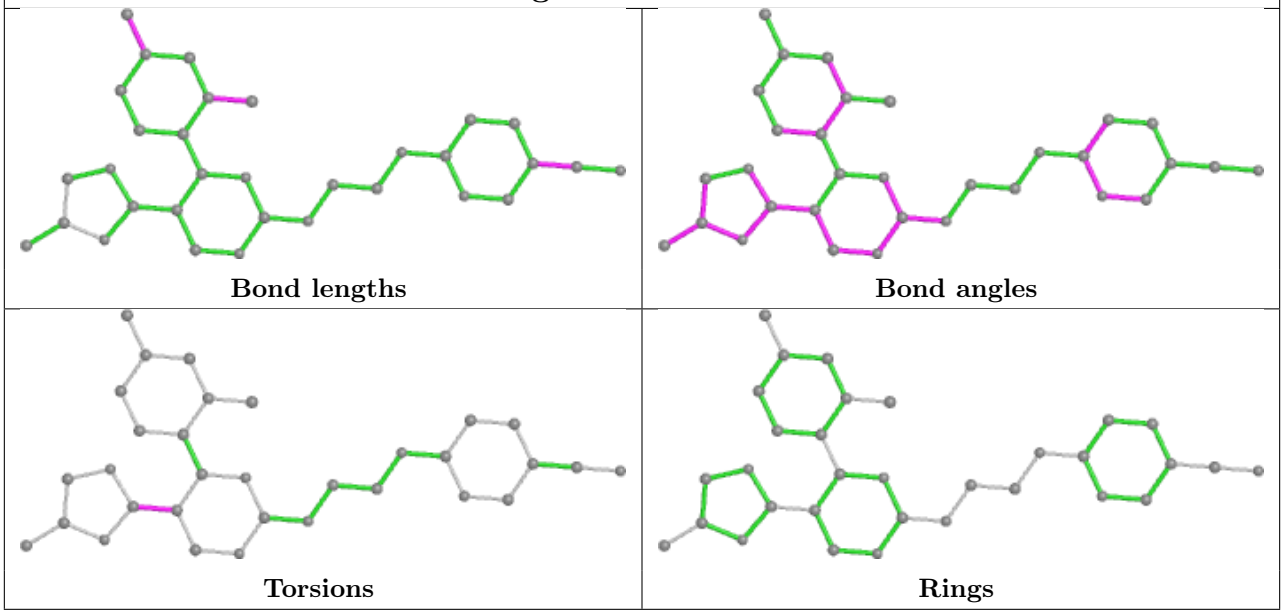
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	65C	1	0

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 65C A 501



Ligand 65C B 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	346/424 (81%)	-0.24	2 (0%)	89	78	65, 87, 124, 158	0
1	B	346/424 (81%)	0.12	10 (2%)	51	28	82, 111, 145, 171	0
All	All	692/848 (81%)	-0.06	12 (1%)	70	49	65, 99, 140, 171	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	SER	4.0
1	B	378	ILE	3.8
1	B	219	SER	3.7
1	B	379	PRO	3.4
1	B	181	ASP	3.0
1	B	121	GLU	2.6
1	B	376	ILE	2.4
1	B	148	ARG	2.3
1	B	295	GLN	2.2
1	B	377	LEU	2.1
1	B	380	PRO	2.0
1	A	34	GLY	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	PTR	A	216	16/17	0.97	0.23	82,92,108,109	0
1	PTR	B	216	12/17	0.97	0.24	87,104,112,112	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

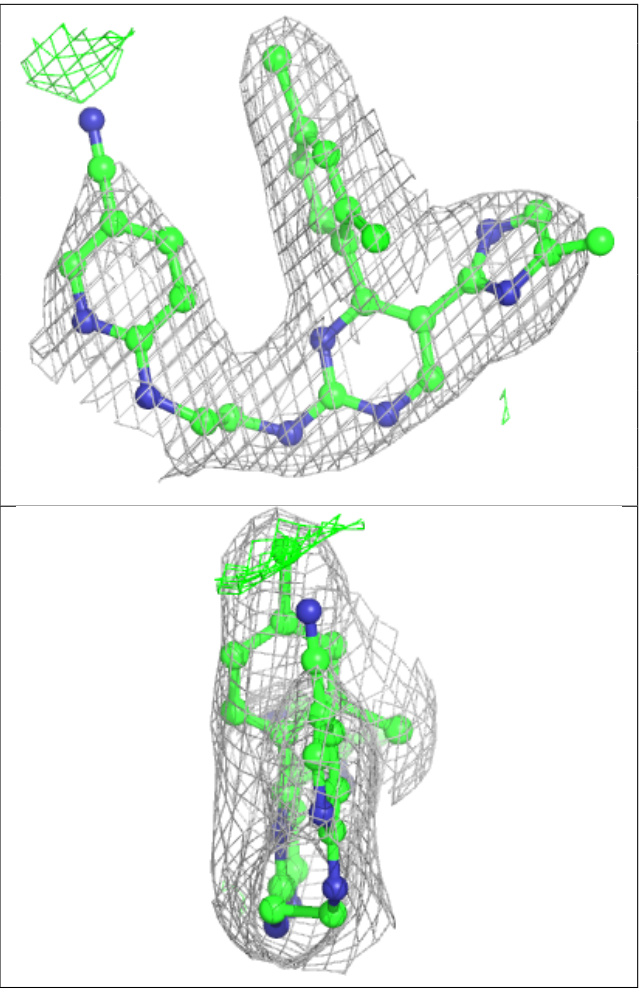
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	502	1/1	0.77	0.19	97,97,97,97	0
3	MG	A	502	1/1	0.87	0.26	107,107,107,107	0
4	MES	A	503	12/12	0.92	0.33	104,116,129,143	0
2	65C	B	501	32/32	0.95	0.20	95,104,111,118	0
4	MES	B	503	12/12	0.95	0.22	95,108,118,119	0
2	65C	A	501	32/32	0.96	0.18	60,72,85,93	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.

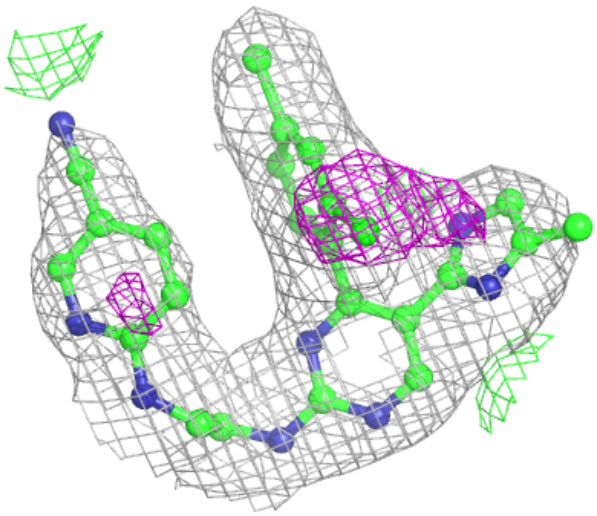
Electron density around 65C B 501:

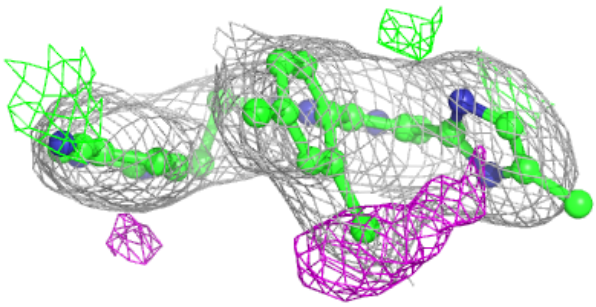
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

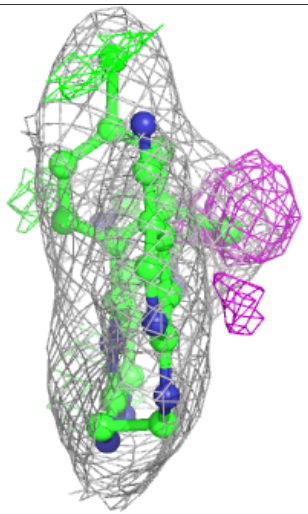


Electron density around 65C A 501:

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.