Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:57 pm BST

PDB ID	:	5EHR
Title	:	Non-receptor Protein Tyrosine Phosphatase SHP2 in Complex with Allosteric Inhibitor SHP099
Authors	:	Stams, T.; Fodor, M.
Deposited on	:	2015-10-28
Resolution	:	1.70 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:

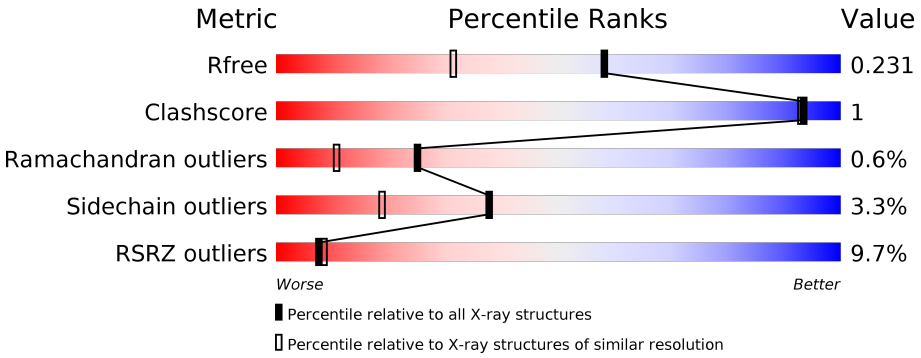
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	526	10%, 88%, 8%
1	B	526	8%, 81%, 8%, 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8514 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.

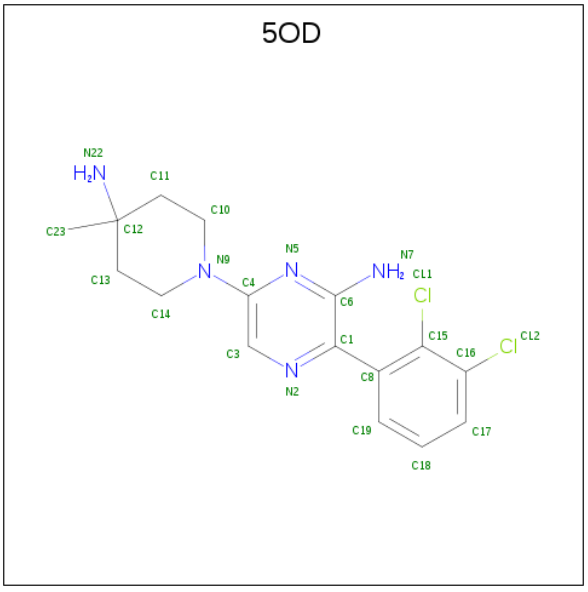
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	3	0
			3944	2489	699	737	19			
1	B	470	Total	C	N	O	S	0	2	0
			3824	2414	680	711	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q06124
B	0	SER	-	expression tag	UNP Q06124

- Molecule 2 is 6-(4-azanyl-4-methyl-piperidin-1-yl)-3-[2,3-bis(chloranyl)phenyl]pyrazin-2-amine (three-letter code: 5OD) (formula: $C_{16}H_{19}Cl_2N_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			23	16	2	5		

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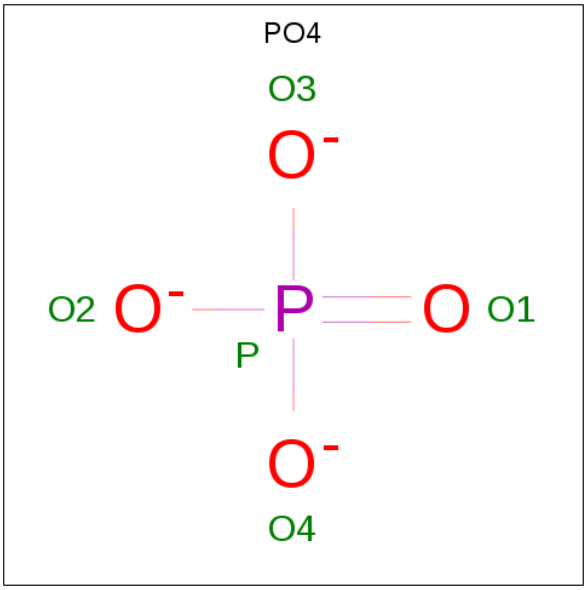
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C Cl N 23 16 2 5	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

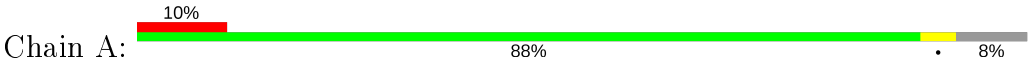
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	343	Total O 343 343	0	0
4	B	327	Total O 327 327	0	0

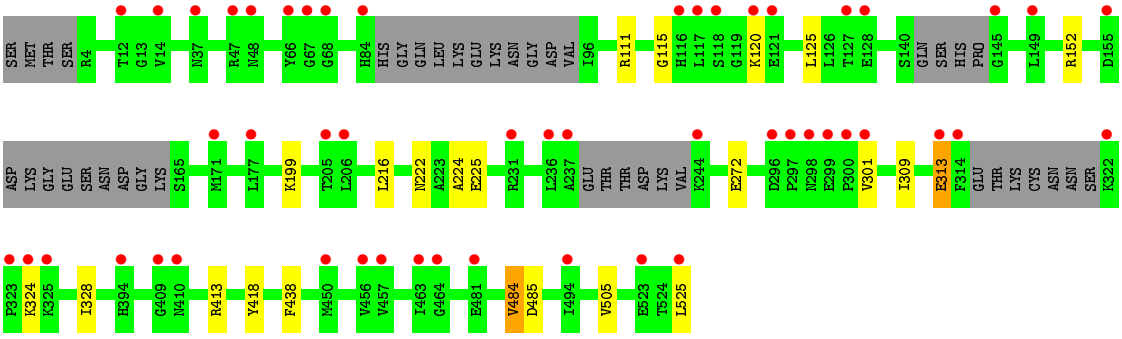
3 Residue-property plots (i)

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: Tyrosine-protein phosphatase non-receptor type 11

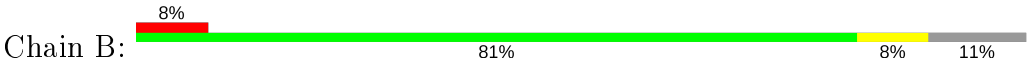
Chain A:

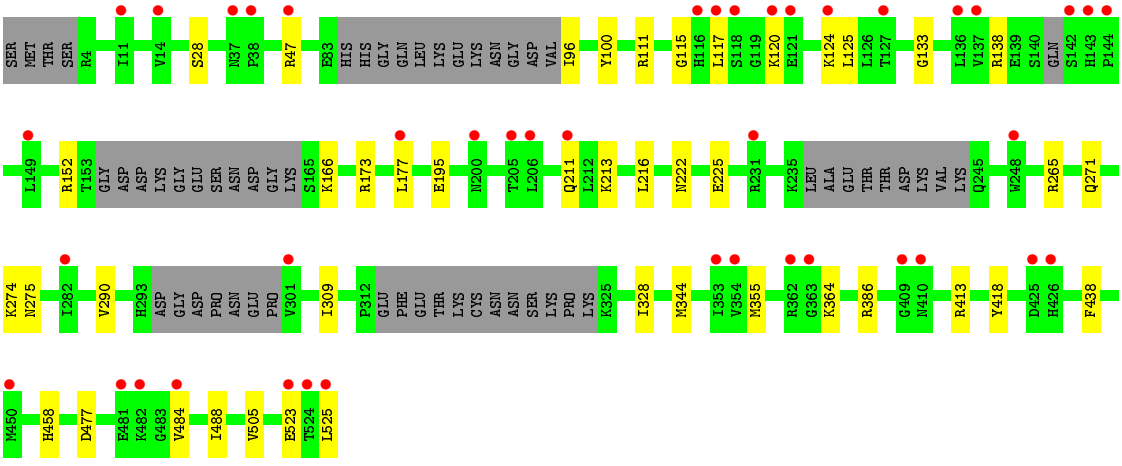




- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.19Å 213.79Å 55.89Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	24.89 – 1.70 24.44 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.89-1.70) 97.8 (24.44-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.70Å)	Xtriage
Refinement program	BUSTER BUSTER 2.11.5	Depositor
R, R_{free}	0.195 , 0.221 0.200 , 0.231	Depositor DCC
R_{free} test set	5755 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8514	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: PO4, 5OD

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	0.52	0/4034	0.63	0/5438
1	B	0.50	0/3907	0.63	0/5266
All	All	0.51	0/7941	0.63	0/10704

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	3944	0	3896	10	0
1	B	3824	0	3781	12	0
2	A	23	0	0	0	0
2	B	23	0	0	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	343	0	0	0	0
4	B	327	0	0	1	0
All	All	8514	0	7677	22	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 1.

All (22) 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:272:GLU:HB2	1:A:301:VAL:HG11	1.13	1.12
1:A:272:GLU:CB	1:A:301:VAL:HG11	1.95	0.94
1:A:272:GLU:HB2	1:A:301:VAL:CG1	2.06	0.80
1:B:111[A]:ARG:HD3	2:B:601:5OD:CL1	2.44	0.54
1:B:222:ASN:O	1:B:225:GLU:HG2	2.11	0.51
1:A:222:ASN:O	1:A:225:GLU:HG2	2.12	0.48
1:B:125:LEU:HB3	1:B:216:LEU:HD21	1.96	0.47
1:A:309:ILE:HD13	1:A:328:ILE:HG12	1.97	0.46
1:A:272:GLU:HG2	1:A:272:GLU:H	1.58	0.45
1:A:125:LEU:HB3	1:A:216:LEU:HD21	1.98	0.45
1:A:224:ALA:HB2	1:A:484:VAL:HG13	1.98	0.45
1:A:418:TYR:HB3	1:A:438:PHE:CE1	2.53	0.44
1:B:271:GLN:HA	1:B:274:LYS:HE3	2.00	0.44
1:B:28:SER:HA	1:B:100:TYR:O	2.18	0.44
1:B:195:GLU:HG2	4:B:824:HOH:O	2.19	0.42
1:B:309:ILE:HD13	1:B:328:ILE:HG12	2.01	0.42
1:B:290:VAL:HG11	1:B:344:MET:HG3	2.01	0.42
1:B:355:MET:HG3	1:B:458:HIS:CE1	2.55	0.42
1:B:133:GLY:HA3	1:B:213:LYS:HB2	2.03	0.41
1:B:418:TYR:HB3	1:B:438:PHE:CE1	2.55	0.41
1:B:117:LEU:O	1:B:138:ARG:HD2	2.21	0.41
1:A:301:VAL:HG13	1:A:301:VAL:O	2.20	0.41

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	476/526 (90%)	460 (97%)	12 (2%)	4 (1%)	19 6
1	B	458/526 (87%)	447 (98%)	9 (2%)	2 (0%)	34 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	934/1052 (89%)	907 (97%)	21 (2%)	6 (1%)	25 11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	A	313	GLU
1	A	324	LYS
1	A	505	VAL
1	B	505	VAL
1	B	115	GLY

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	434/468 (93%)	424 (98%)	10 (2%)	50 33
1	B	421/468 (90%)	402 (96%)	19 (4%)	27 10
All	All	855/936 (91%)	826 (97%)	29 (3%)	38 18

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111[A]	ARG
1	A	111[B]	ARG
1	A	120	LYS
1	A	152	ARG
1	A	199	LYS
1	A	313	GLU
1	A	413	ARG
1	A	484	VAL
1	A	485	ASP
1	A	525	LEU
1	B	47	ARG
1	B	96	ILE

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Mol	Chain	Res	Type
1	B	120	LYS
1	B	124	LYS
1	B	152	ARG
1	B	166	LYS
1	B	173	ARG
1	B	177	LEU
1	B	211	GLN
1	B	265	ARG
1	B	275	ASN
1	B	364	LYS
1	B	386	ARG
1	B	413	ARG
1	B	477	ASP
1	B	484	VAL
1	B	488	ILE
1	B	523	GLU
1	B	525	LEU

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

Mol	Chain	Res	Type
1	A	211	GLN
1	A	281	ASN
1	B	37	ASN
1	B	211	GLN
1	B	256	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)

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)

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	$\#\|Z\| > 2$
3	PO4	B	604	-	4,4,4	2.51	2 (50%)	6,6,6	0.50	0
3	PO4	B	603	-	4,4,4	2.00	1 (25%)	6,6,6	0.52	0
3	PO4	A	603	-	4,4,4	2.49	1 (25%)	6,6,6	0.55	0
3	PO4	A	602	-	4,4,4	2.10	1 (25%)	6,6,6	0.28	0
2	5OD	B	601	-	23,25,25	1.20	3 (13%)	28,37,37	1.63	8 (28%)
2	5OD	A	601	-	23,25,25	1.18	2 (8%)	28,37,37	1.48	5 (17%)
3	PO4	B	602	-	4,4,4	2.43	1 (25%)	6,6,6	0.49	0
3	PO4	A	604	-	4,4,4	2.48	1 (25%)	6,6,6	0.57	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
2	5OD	B	601	-	-	0/8/20/20	0/3/3/3
2	5OD	A	601	-	-	0/8/20/20	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	604	PO4	P-O1	4.17	1.60	1.50
3	A	603	PO4	P-O1	4.15	1.60	1.50
3	A	604	PO4	P-O1	4.12	1.60	1.50
3	B	602	PO4	P-O1	3.86	1.59	1.50
2	B	601	5OD	C1-C6	-2.96	1.41	1.45
2	B	601	5OD	C23-C12	2.68	1.56	1.53
2	A	601	5OD	C1-C6	-2.57	1.42	1.45
3	A	602	PO4	P-O1	2.52	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	5OD	C23-C12	2.40	1.55	1.53
3	B	603	PO4	P-O1	2.21	1.56	1.50
2	B	601	5OD	C4-N5	2.05	1.37	1.34
3	B	604	PO4	P-O4	2.03	1.60	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	5OD	N5-C4-N9	4.04	121.08	116.55
2	A	601	5OD	N5-C4-N9	3.77	120.78	116.55
2	B	601	5OD	C1-C6-N5	-3.16	118.03	120.09
2	A	601	5OD	C1-C6-N7	3.07	123.66	121.11
2	A	601	5OD	C10-N9-C14	2.80	117.69	111.52
2	B	601	5OD	C1-C6-N7	2.71	123.37	121.11
2	B	601	5OD	C8-C1-C6	2.53	125.47	122.34
2	A	601	5OD	C8-C1-C6	2.50	125.44	122.34
2	B	601	5OD	C11-C10-N9	-2.36	106.16	110.34
2	B	601	5OD	C15-C16-CL2	-2.31	118.27	120.52
2	B	601	5OD	C10-N9-C14	2.19	116.35	111.52
2	A	601	5OD	C3-C4-N5	-2.19	118.36	121.32
2	B	601	5OD	C3-C4-N5	-2.18	118.36	121.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

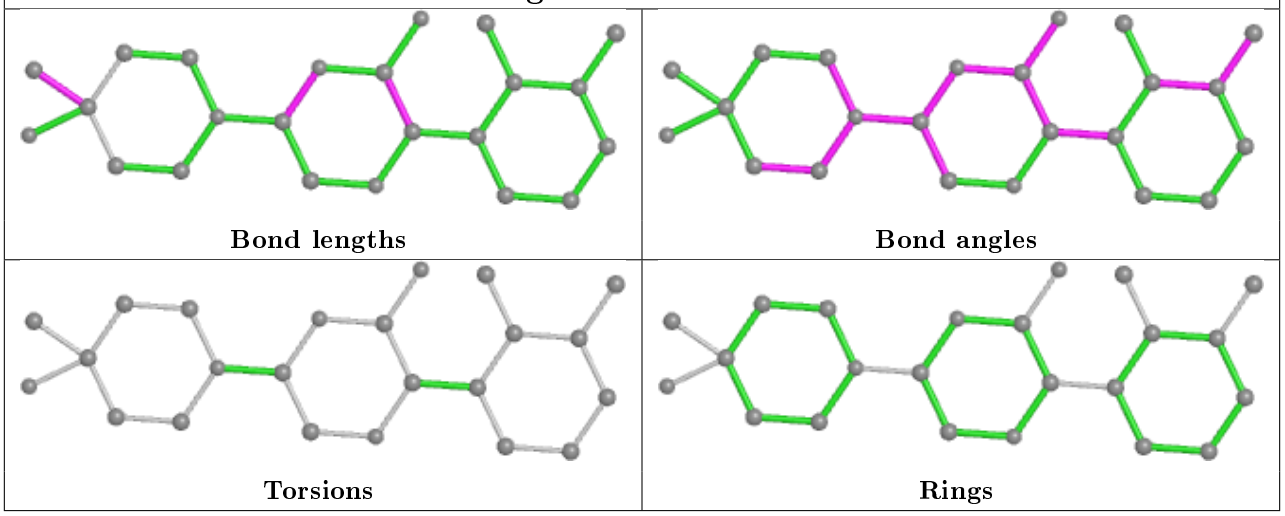
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	5OD	1	0

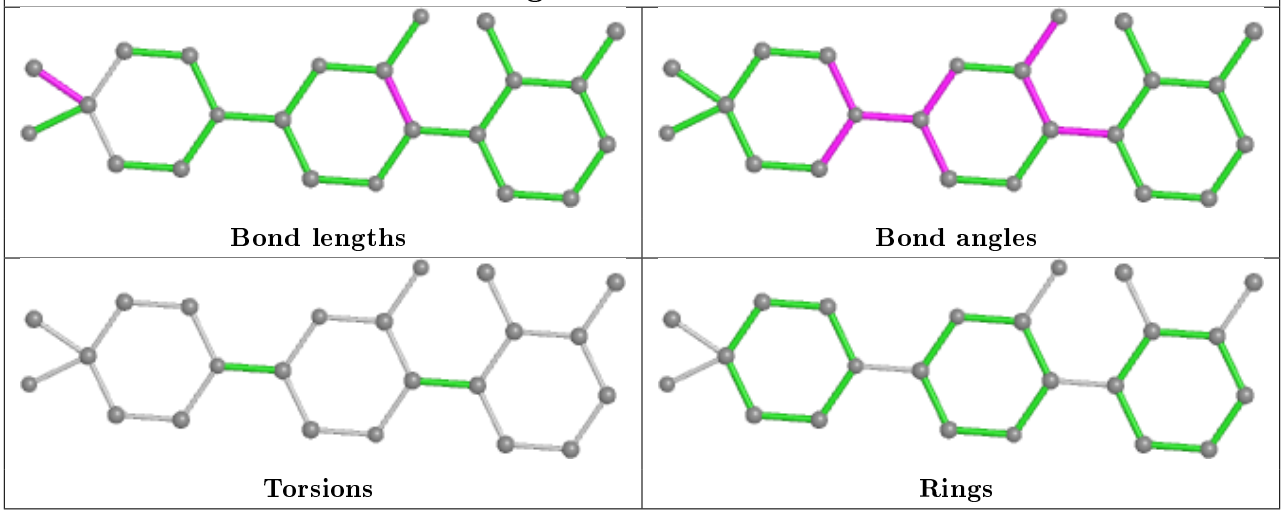
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 5OD B 601



Ligand 5OD A 601



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, 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	485/526 (92%)	0.62	51 (10%) 6 7	14, 27, 53, 77	0
1	B	470/526 (89%)	0.61	42 (8%) 9 11	15, 28, 53, 73	0
All	All	955/1052 (90%)	0.61	93 (9%) 7 8	14, 27, 53, 77	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	THR	9.6
1	A	116	HIS	6.6
1	B	116	HIS	6.3
1	B	301	VAL	5.8
1	A	236	LEU	5.8
1	B	120	LYS	5.7
1	B	144	PRO	5.4
1	B	205	THR	5.1
1	B	426	HIS	4.9
1	B	525	LEU	4.8
1	A	323	PRO	4.7
1	A	314	PHE	4.5
1	B	127	THR	4.4
1	B	121	GLU	4.3
1	B	409	GLY	4.3
1	B	143	HIS	4.3
1	B	206	LEU	4.2
1	A	300	PRO	4.1
1	B	177	LEU	4.1
1	A	48	ASN	4.0
1	B	142	SER	3.9
1	A	394	HIS	3.8
1	A	237	ALA	3.8
1	A	525	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	14	VAL	3.7
1	A	313	GLU	3.7
1	A	298	ASN	3.7
1	A	120	LYS	3.7
1	A	155	ASP	3.7
1	A	409	GLY	3.6
1	A	296	ASP	3.6
1	B	450	MET	3.3
1	A	171	MET	3.2
1	B	425	ASP	3.2
1	A	177	LEU	3.2
1	A	301	VAL	3.2
1	A	145	GLY	3.1
1	A	66	TYR	3.1
1	B	481	GLU	3.1
1	A	118	SER	3.1
1	B	363	GLY	3.0
1	A	117	LEU	3.0
1	A	206	LEU	3.0
1	A	523	GLU	2.9
1	B	124	LYS	2.8
1	B	362	ARG	2.8
1	A	68	GLY	2.8
1	B	136	LEU	2.7
1	A	297	PRO	2.7
1	B	37	ASN	2.7
1	A	325	LYS	2.6
1	A	481	GLU	2.6
1	B	117	LEU	2.6
1	A	464	GLY	2.6
1	A	244	LYS	2.6
1	A	128	GLU	2.6
1	A	456	VAL	2.6
1	A	47	ARG	2.5
1	A	299	GLU	2.5
1	B	523	GLU	2.5
1	A	450	MET	2.5
1	B	200	ASN	2.5
1	B	211	GLN	2.5
1	A	127	THR	2.5
1	B	118	SER	2.4
1	B	231	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	11	ILE	2.3
1	A	410	ASN	2.3
1	B	282	ILE	2.3
1	B	248	TRP	2.3
1	B	47	ARG	2.3
1	B	524	THR	2.3
1	A	84	HIS	2.3
1	B	353	ILE	2.2
1	A	324	LYS	2.2
1	A	457	VAL	2.2
1	B	482	LYS	2.2
1	A	463	ILE	2.2
1	A	37	ASN	2.2
1	A	322	LYS	2.2
1	A	121	GLU	2.1
1	A	231	ARG	2.1
1	B	137	VAL	2.1
1	B	484	VAL	2.1
1	A	12	THR	2.1
1	A	149	LEU	2.1
1	B	149	LEU	2.1
1	B	38	PRO	2.1
1	A	67	GLY	2.1
1	A	494	ILE	2.1
1	A	14	VAL	2.1
1	B	354	VAL	2.0
1	B	410	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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,

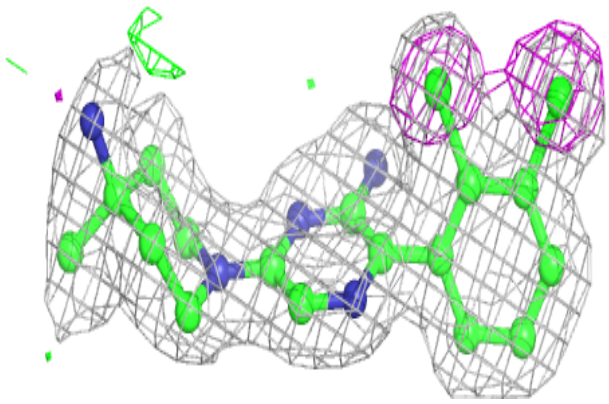
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

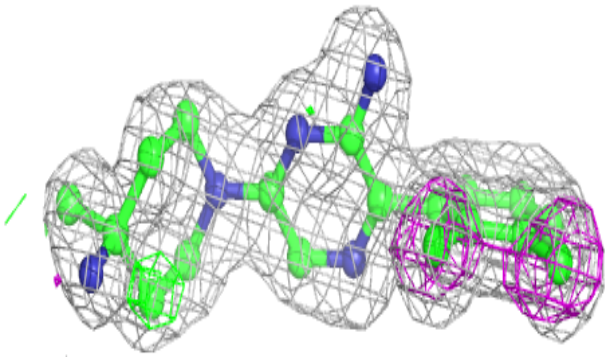
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	B	604	5/5	0.82	0.25	54,55,57,60	0
3	PO4	A	602	5/5	0.83	0.20	61,61,63,64	0
3	PO4	A	603	5/5	0.86	0.16	45,49,51,51	0
3	PO4	A	604	5/5	0.86	0.17	61,65,67,67	0
3	PO4	B	603	5/5	0.92	0.14	70,71,71,72	0
2	5OD	A	601	23/23	0.95	0.10	19,23,29,33	0
2	5OD	B	601	23/23	0.95	0.10	20,23,32,32	0
3	PO4	B	602	5/5	0.98	0.10	34,34,35,43	0

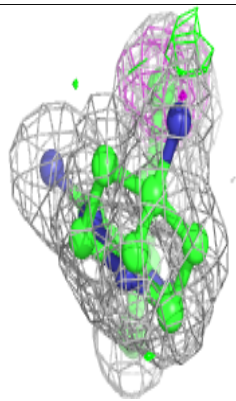
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5OD A 601:

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

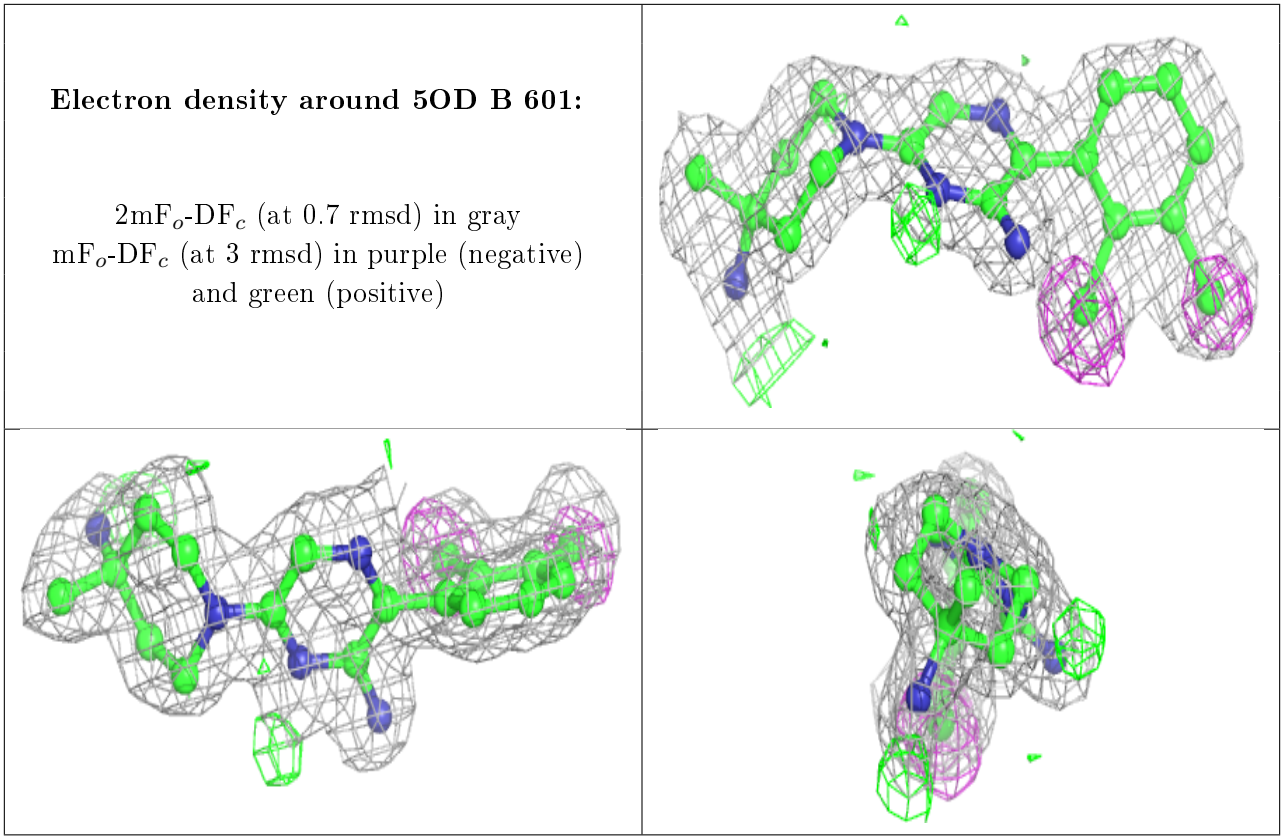






Electron density around 5OD B 601:

$2mF_o$-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

There are no such residues in this entry.