Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 10:36 AM UTC

PDB ID	:	5EHR / pdb_00005ehr
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 (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:

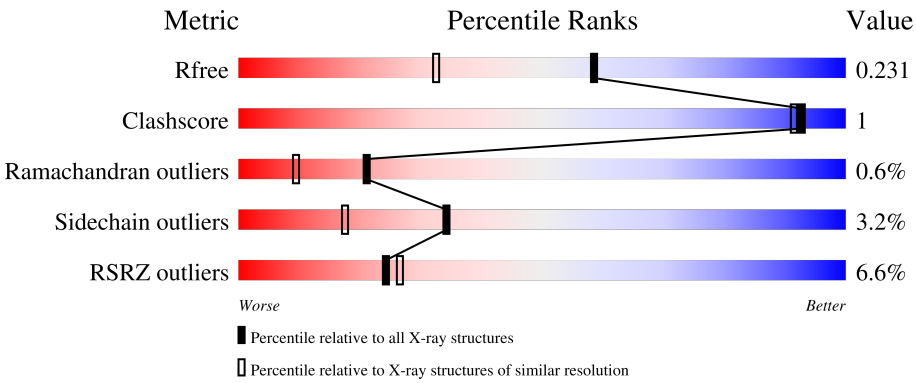
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	526	5% 87% 5% • 8%
1	B	526	7% 80% 9% 11%

2 Entry composition (i)

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.

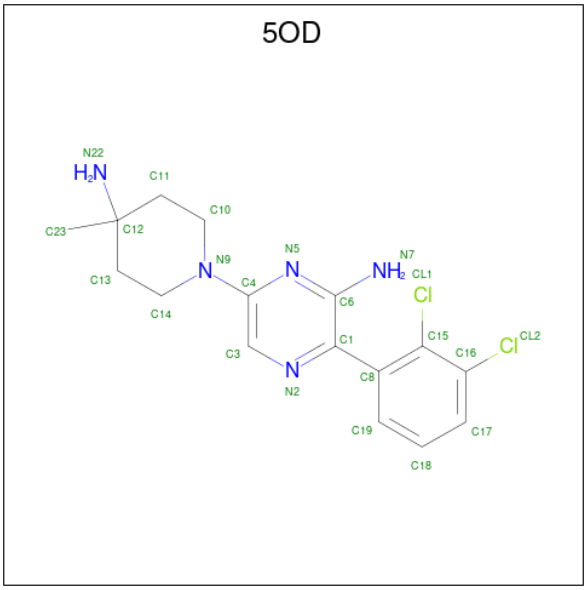
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

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

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 (CCD ID: 5OD) (formula: $C_{16}H_{19}Cl_2N_5$).



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

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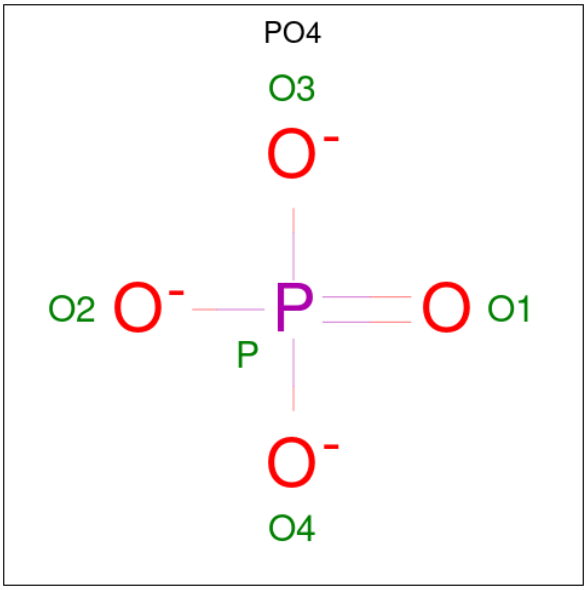
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	N		
2	B	1	23	16	2	5	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is water.

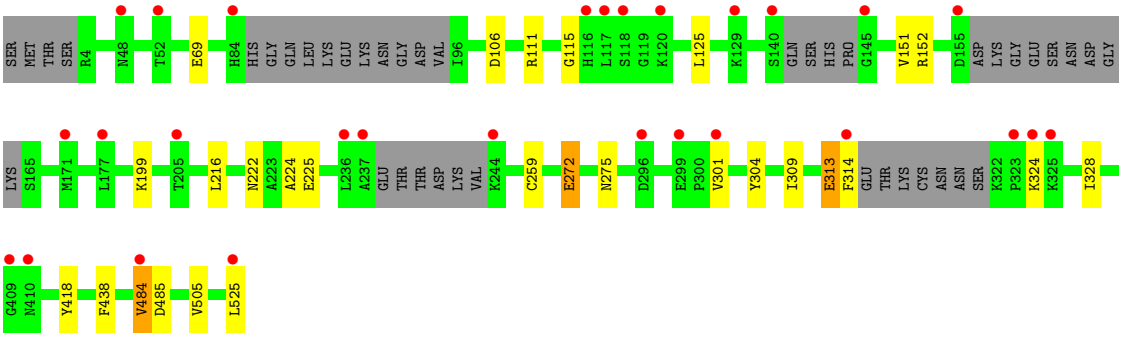
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	343	343	343	0	0
			Total	O		
4	B	327	327	327	0	0

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.

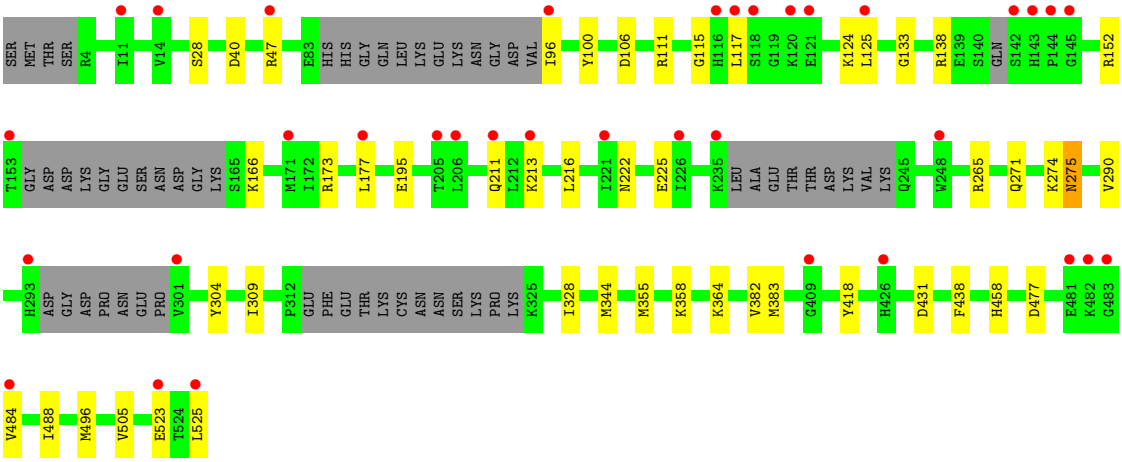
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 11

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 24.89 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.89-1.70) 97.8 (24.89-1.70)	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 , 38.2	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 (i)

5.1 Standard geometry (i)

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	0.84	0/4034	1.08	4/5438 (0.1%)
1	B	0.82	1/3907 (0.0%)	1.10	6/5266 (0.1%)
All	All	0.83	1/7941 (0.0%)	1.09	10/10704 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	496	MET	SD-CE	5.09	1.92	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	40	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	106	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	106	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	314	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	275	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	304	TYR	N-CA-C	5.35	118.21	109.59
1	B	275	ASN	CA-CB-CG	5.30	117.90	112.60
1	B	431	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	304	TYR	N-CA-C	5.20	117.95	109.59
1	B	358	LYS	N-CA-C	-5.03	104.04	110.53

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	3944	0	3896	10	0
1	B	3824	0	3781	13	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	23	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 (23) 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:H	1:A:272:GLU:HG2	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:28:SER:HA	1:B:100:TYR:O	2.18	0.44
1:B:271:GLN:HA	1:B:274:LYS:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:VAL:HG23	1:B:383:MET:HE2	2.01	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:O	1:A:301:VAL:HG13	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%)	16 5
1	B	458/526 (87%)	447 (98%)	9 (2%)	2 (0%)	30 16
All	All	934/1052 (89%)	907 (97%)	21 (2%)	6 (1%)	21 9

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%)	421 (97%)	13 (3%)	36	19
1	B	421/468 (90%)	405 (96%)	16 (4%)	29	13
All	All	855/936 (91%)	826 (97%)	29 (3%)	34	16

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

Mol	Chain	Res	Type
1	A	69	GLU
1	A	111[A]	ARG
1	A	111[B]	ARG
1	A	151	VAL
1	A	152	ARG
1	A	199	LYS
1	A	259[A]	CYS
1	A	259[B]	CYS
1	A	272	GLU
1	A	313	GLU
1	A	484	VAL
1	A	485	ASP
1	A	525	LEU
1	B	47	ARG
1	B	96	ILE
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	477	ASP
1	B	484	VAL
1	B	488	ILE
1	B	523	GLU
1	B	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	196	HIS
1	A	211	GLN
1	A	281	ASN
1	A	394	HIS
1	A	426	HIS
1	B	79	GLN
1	B	200	ASN
1	B	211	GLN
1	B	256	GLN
1	B	257	GLN
1	B	281	ASN
1	B	335	GLN
1	B	446	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 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	$\#\|Z\| > 2$
3	PO4	A	604	-	4,4,4	2.56	2 (50%)	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5OD	B	601	-	25,25,25	1.37	5 (20%)	30,37,37	1.60	9 (30%)
3	PO4	B	602	-	4,4,4	2.52	2 (50%)	6,6,6	0.52	0
3	PO4	A	602	-	4,4,4	2.17	1 (25%)	6,6,6	0.31	0
3	PO4	B	603	-	4,4,4	2.07	2 (50%)	6,6,6	0.55	0
3	PO4	B	604	-	4,4,4	2.60	2 (50%)	6,6,6	0.52	0
2	5OD	A	601	-	25,25,25	1.36	4 (16%)	30,37,37	1.50	6 (20%)
3	PO4	A	603	-	4,4,4	2.57	2 (50%)	6,6,6	0.58	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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	604	PO4	P-O1	4.32	1.60	1.50
3	A	603	PO4	P-O1	4.31	1.60	1.50
3	A	604	PO4	P-O1	4.28	1.60	1.50
3	B	602	PO4	P-O1	4.01	1.59	1.50
2	A	601	5OD	C11-C12	3.09	1.58	1.54
2	B	601	5OD	C1-C6	-2.92	1.41	1.45
2	B	601	5OD	C11-C12	2.76	1.58	1.54
2	B	601	5OD	C23-C12	2.72	1.56	1.53
3	A	602	PO4	P-O1	2.64	1.56	1.50
2	A	601	5OD	C1-C6	-2.54	1.42	1.45
2	B	601	5OD	C13-C12	2.50	1.57	1.54
2	A	601	5OD	C23-C12	2.44	1.55	1.53
3	B	603	PO4	P-O1	2.32	1.56	1.50
2	B	601	5OD	C4-N5	2.18	1.37	1.34
3	B	604	PO4	P-O4	2.09	1.60	1.54
2	A	601	5OD	C13-C12	2.05	1.57	1.54
3	A	604	PO4	P-O2	2.04	1.60	1.54
3	A	603	PO4	P-O4	2.02	1.60	1.54
3	B	603	PO4	P-O4	2.02	1.60	1.54
3	B	602	PO4	P-O2	2.00	1.60	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	5OD	N5-C4-N9	3.58	121.08	116.56
2	A	601	5OD	N5-C4-N9	3.34	120.78	116.56
2	B	601	5OD	C1-C6-N5	-3.15	118.03	120.08
2	A	601	5OD	C1-C6-N7	3.04	123.66	121.11
2	A	601	5OD	C6-C1-N2	-2.87	119.64	121.10
2	A	601	5OD	C10-N9-C14	2.72	117.69	111.57
2	B	601	5OD	C1-C6-N7	2.69	123.37	121.11
2	B	601	5OD	C8-C1-C6	2.45	125.47	122.36
2	B	601	5OD	C15-C16-CL2	-2.44	118.27	120.51
2	A	601	5OD	C8-C1-C6	2.42	125.44	122.36
2	B	601	5OD	C11-C10-N9	-2.41	106.16	110.53
2	A	601	5OD	C3-C4-N5	-2.27	118.36	121.22
2	B	601	5OD	C3-C4-N5	-2.26	118.36	121.22
2	B	601	5OD	C10-N9-C14	2.13	116.35	111.57
2	B	601	5OD	C6-C1-N2	-2.11	120.03	121.10

There are no chirality outliers.

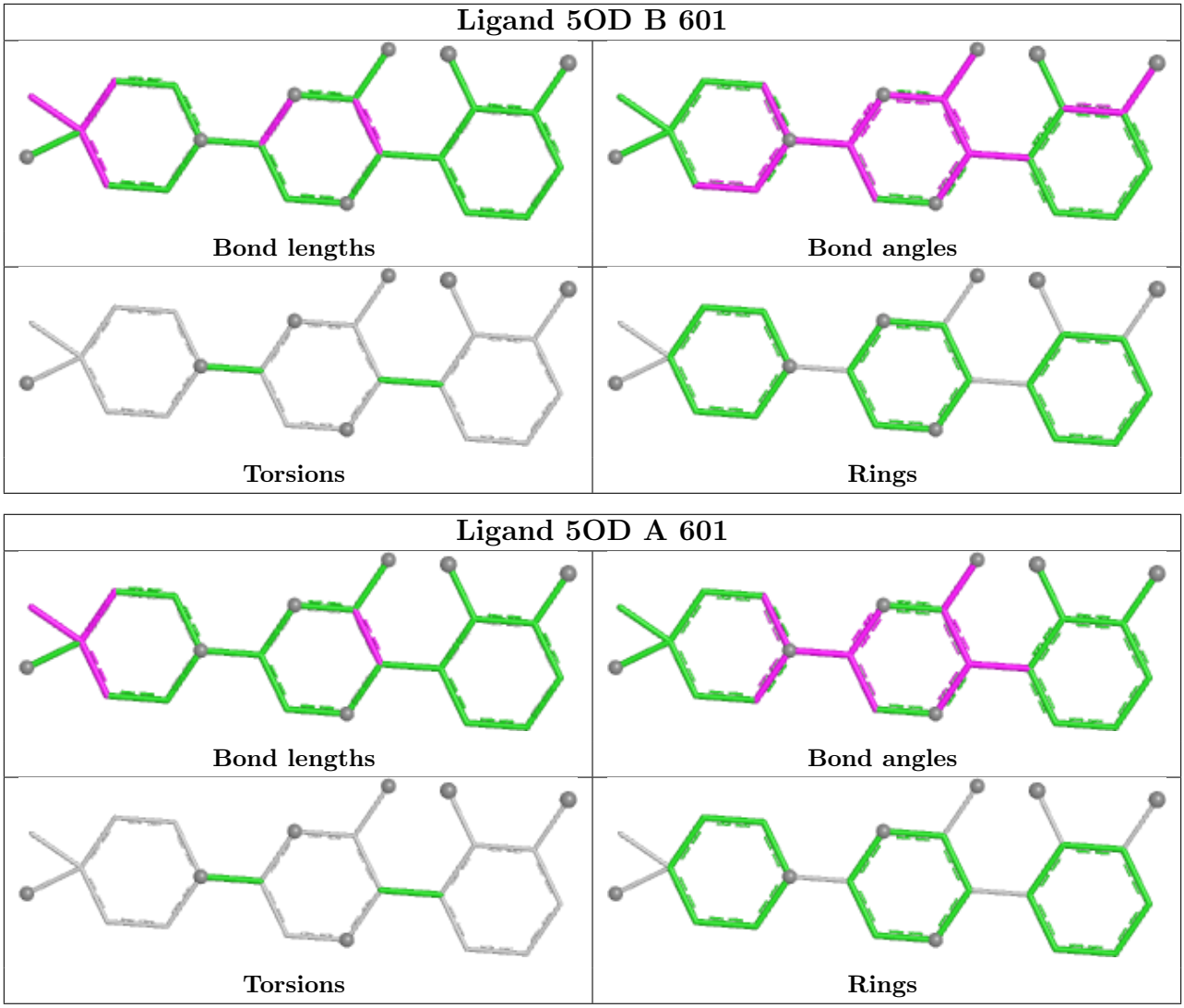
There are no torsion outliers.

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.



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	485/526 (92%)	0.37	28 (5%)	29	32	11, 27, 53, 77	3 (0%)
1	B	470/526 (89%)	0.41	35 (7%)	20	22	15, 27, 53, 73	2 (0%)
All	All	955/1052 (90%)	0.39	63 (6%)	24	26	11, 27, 53, 77	5 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	THR	5.4
1	B	117	LEU	4.7
1	A	237	ALA	4.5
1	A	117	LEU	4.3
1	A	314	PHE	4.2
1	B	301	VAL	4.2
1	B	484	VAL	4.2
1	A	325	LYS	3.8
1	B	206	LEU	3.7
1	A	525	LEU	3.5
1	B	525	LEU	3.5
1	A	84	HIS	3.5
1	A	323	PRO	3.5
1	B	142	SER	3.2
1	B	120	LYS	3.2
1	B	409	GLY	3.0
1	A	171	MET	3.0
1	B	96	ILE	3.0
1	A	116	HIS	2.8
1	A	120	LYS	2.8
1	A	145	GLY	2.8
1	B	248	TRP	2.7
1	B	213	LYS	2.7
1	B	11	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	2.6
1	B	121	GLU	2.6
1	A	52	THR	2.5
1	B	116	HIS	2.5
1	A	118	SER	2.5
1	A	155	ASP	2.5
1	B	235	LYS	2.5
1	B	47	ARG	2.4
1	B	426	HIS	2.4
1	B	177	LEU	2.4
1	A	244	LYS	2.4
1	A	301	VAL	2.4
1	B	144	PRO	2.3
1	A	409	GLY	2.3
1	B	481	GLU	2.3
1	A	324	LYS	2.3
1	B	482	LYS	2.3
1	A	484	VAL	2.3
1	B	205	THR	2.2
1	B	226	ILE	2.2
1	A	236	LEU	2.2
1	B	483	GLY	2.2
1	B	293	HIS	2.2
1	B	221	ILE	2.2
1	B	523	GLU	2.2
1	A	129	LYS	2.2
1	B	153	THR	2.2
1	A	296	ASP	2.1
1	B	14	VAL	2.1
1	A	299	GLU	2.1
1	B	145	GLY	2.1
1	B	143	HIS	2.1
1	A	410	ASN	2.1
1	B	118	SER	2.0
1	A	177	LEU	2.0
1	B	125	LEU	2.0
1	A	48	ASN	2.0
1	B	171	MET	2.0
1	B	211	GLN	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 oligosaccharides in this entry.

6.4 Ligands (i)

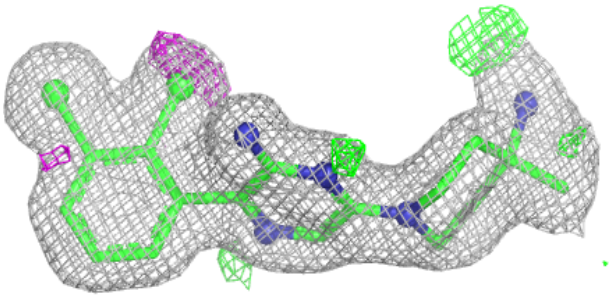
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

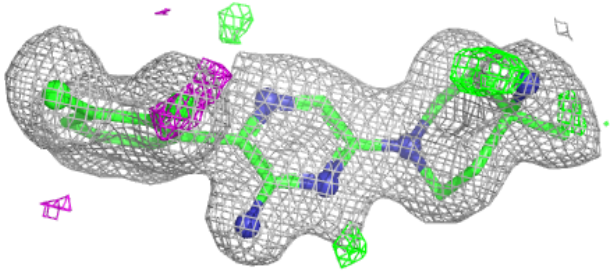
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	B	604	5/5	0.73	0.14	54,55,57,60	0
3	PO4	B	603	5/5	0.75	0.14	70,71,71,72	0
3	PO4	A	602	5/5	0.76	0.15	61,61,63,64	0
3	PO4	A	604	5/5	0.77	0.15	61,65,67,67	0
3	PO4	A	603	5/5	0.85	0.11	45,49,51,51	0
2	5OD	B	601	23/23	0.96	0.07	20,23,32,32	0
2	5OD	A	601	23/23	0.96	0.08	19,23,29,33	0
3	PO4	B	602	5/5	0.97	0.07	34,34,35,43	0

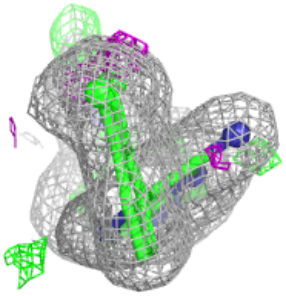
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5OD 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)

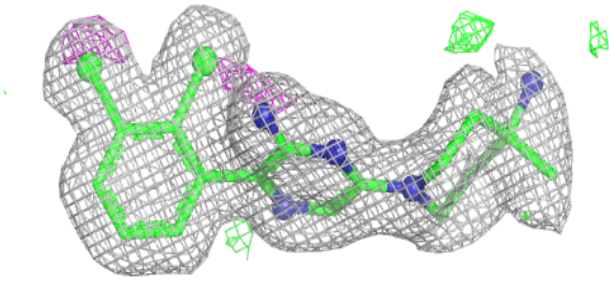


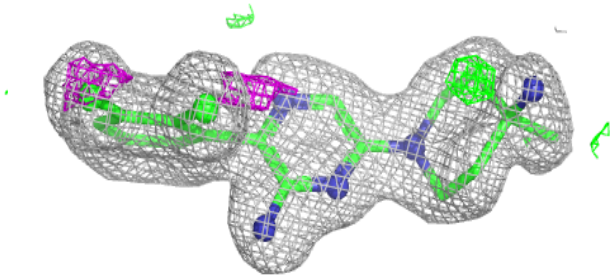


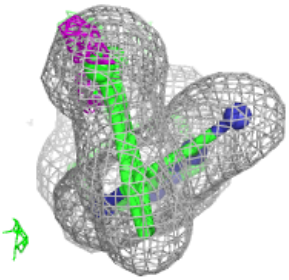


Electron density around 5OD A 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.