



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:44 am BST

PDB ID : 6BP0
Title : Crystal Structure of the Human vaccinia-related kinase 1 bound to (R)-2-phenylaminopteridinone inhibitor
Authors : Counago, R.M.; dos Reis, C.V.; de Souza, G.P.; Azevedo, A.; Guimaraes, C.; Mascarello, A.; Gama, F.; Ferreira, M.; Massirer, K.B.; Arruda, P.; Edwards, A.M.; Elkins, J.; Structural Genomics Consortium (SGC)
Deposited on : 2017-11-21
Resolution : 1.90 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

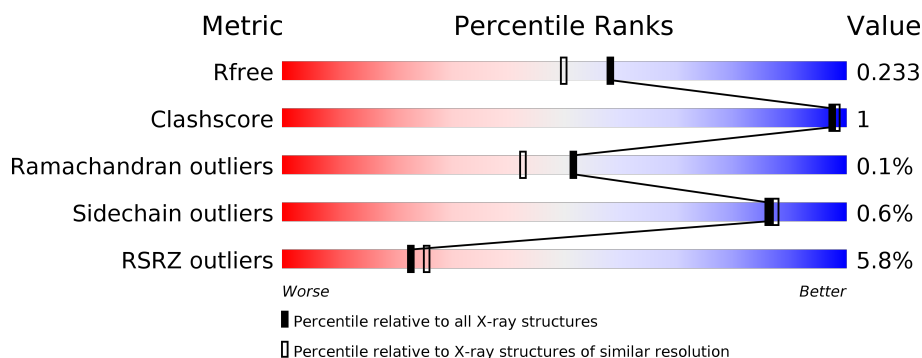
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	<div> <div>4%</div> <div>85%</div> <div>13%</div> </div>
1	B	364	<div> <div>7%</div> <div>82%</div> <div>16%</div> </div>
1	C	364	<div> <div>3%</div> <div>83%</div> <div>13%</div> </div>
1	D	364	<div> <div>6%</div> <div>83%</div> <div>15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	D	401	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10972 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 Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	2	0
			2513	1606	427	467	13			
1	B	304	Total	C	N	O	S	0	2	0
			2415	1548	414	441	12			
1	C	315	Total	C	N	O	S	0	3	0
			2495	1598	425	458	14			
1	D	311	Total	C	N	O	S	0	2	0
			2452	1573	419	448	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q99986
A	2	MET	-	expression tag	UNP Q99986
A	34	ALA	LYS	engineered mutation	UNP Q99986
A	35	ALA	LYS	engineered mutation	UNP Q99986
A	36	ALA	GLU	engineered mutation	UNP Q99986
A	212	ALA	GLU	engineered mutation	UNP Q99986
A	214	ALA	LYS	engineered mutation	UNP Q99986
A	215	ALA	GLU	engineered mutation	UNP Q99986
A	292	ALA	GLU	engineered mutation	UNP Q99986
A	293	ALA	LYS	engineered mutation	UNP Q99986
A	295	ALA	LYS	engineered mutation	UNP Q99986
A	359	ALA	LYS	engineered mutation	UNP Q99986
A	360	ALA	LYS	engineered mutation	UNP Q99986
B	1	SER	-	expression tag	UNP Q99986
B	2	MET	-	expression tag	UNP Q99986
B	34	ALA	LYS	engineered mutation	UNP Q99986
B	35	ALA	LYS	engineered mutation	UNP Q99986
B	36	ALA	GLU	engineered mutation	UNP Q99986
B	212	ALA	GLU	engineered mutation	UNP Q99986
B	214	ALA	LYS	engineered mutation	UNP Q99986
B	215	ALA	GLU	engineered mutation	UNP Q99986

Continued on next page...

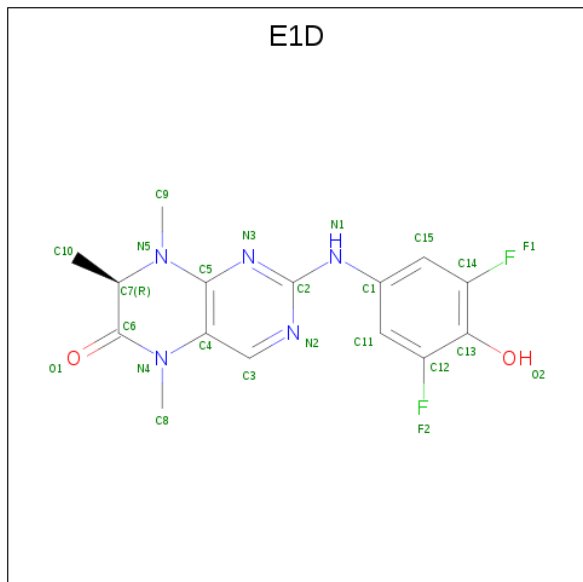
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	GLU	engineered mutation	UNP Q99986
B	293	ALA	LYS	engineered mutation	UNP Q99986
B	295	ALA	LYS	engineered mutation	UNP Q99986
B	359	ALA	LYS	engineered mutation	UNP Q99986
B	360	ALA	LYS	engineered mutation	UNP Q99986
C	1	SER	-	expression tag	UNP Q99986
C	2	MET	-	expression tag	UNP Q99986
C	34	ALA	LYS	engineered mutation	UNP Q99986
C	35	ALA	LYS	engineered mutation	UNP Q99986
C	36	ALA	GLU	engineered mutation	UNP Q99986
C	212	ALA	GLU	engineered mutation	UNP Q99986
C	214	ALA	LYS	engineered mutation	UNP Q99986
C	215	ALA	GLU	engineered mutation	UNP Q99986
C	292	ALA	GLU	engineered mutation	UNP Q99986
C	293	ALA	LYS	engineered mutation	UNP Q99986
C	295	ALA	LYS	engineered mutation	UNP Q99986
C	359	ALA	LYS	engineered mutation	UNP Q99986
C	360	ALA	LYS	engineered mutation	UNP Q99986
D	1	SER	-	expression tag	UNP Q99986
D	2	MET	-	expression tag	UNP Q99986
D	34	ALA	LYS	engineered mutation	UNP Q99986
D	35	ALA	LYS	engineered mutation	UNP Q99986
D	36	ALA	GLU	engineered mutation	UNP Q99986
D	212	ALA	GLU	engineered mutation	UNP Q99986
D	214	ALA	LYS	engineered mutation	UNP Q99986
D	215	ALA	GLU	engineered mutation	UNP Q99986
D	292	ALA	GLU	engineered mutation	UNP Q99986
D	293	ALA	LYS	engineered mutation	UNP Q99986
D	295	ALA	LYS	engineered mutation	UNP Q99986
D	359	ALA	LYS	engineered mutation	UNP Q99986
D	360	ALA	LYS	engineered mutation	UNP Q99986

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

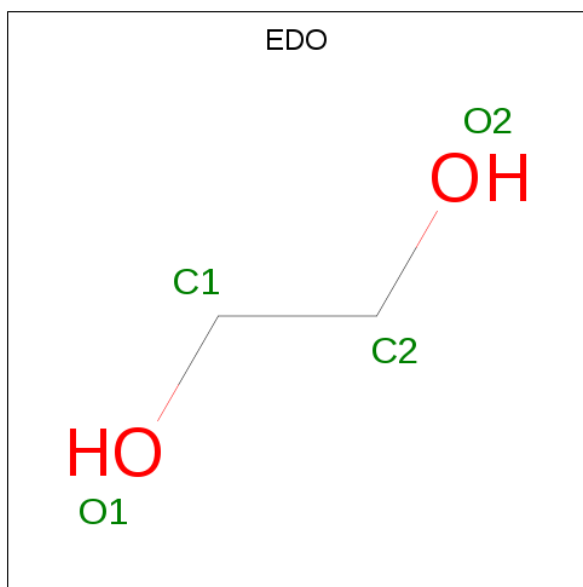
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Cl 3 3	0	0
2	A	2	Total Cl 2 2	0	0
2	D	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is (7R)-2-[(3,5-difluoro-4-hydroxyphenyl)amino]-5,7,8-trimethyl-7,8-dihydropteridin-6(5H)-one (three-letter code: E1D) (formula: $C_{15}H_{15}F_2N_5O_2$).



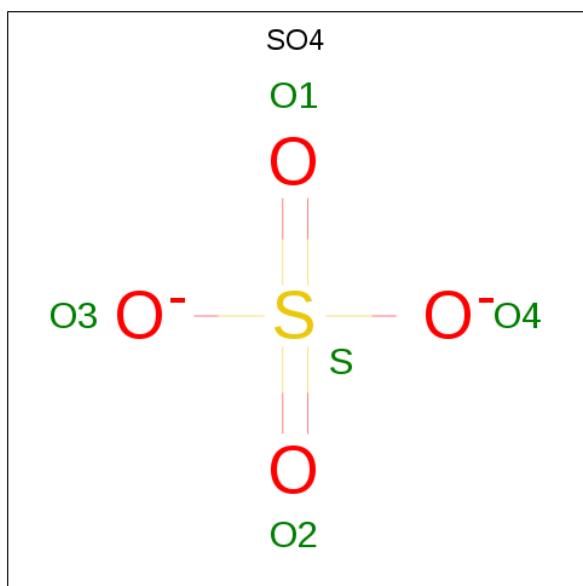
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			24	15	2	5	2		
3	D	1	Total	C	F	N	O	0	0
			24	15	2	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



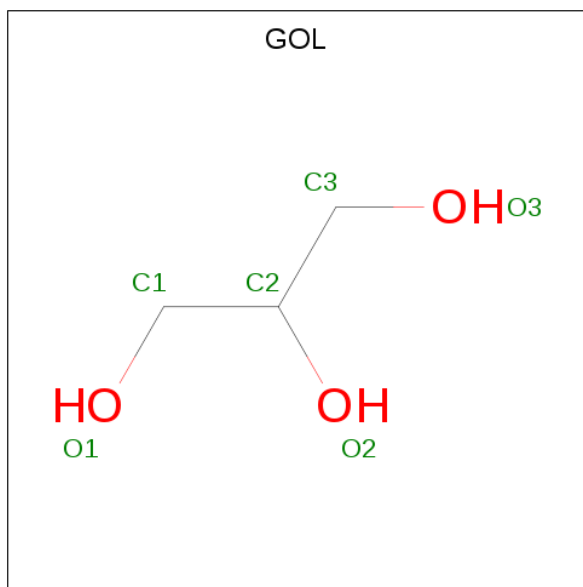
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



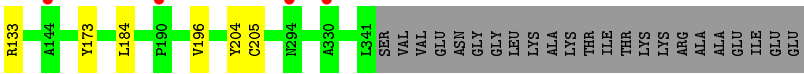
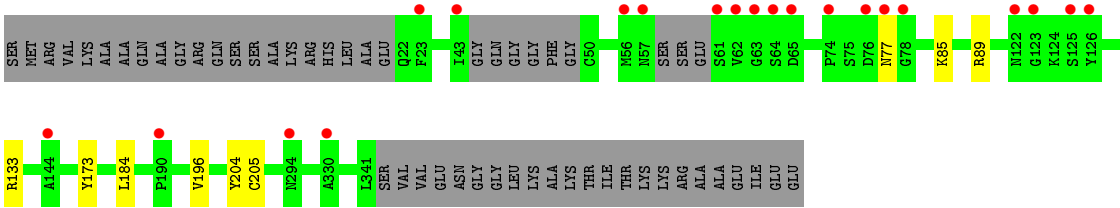
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	275	Total	O	0	0
			275	275		
7	B	197	Total	O	0	0
			197	197		
7	C	278	Total	O	0	0
			278	278		
7	D	257	Total	O	0	0
			257	257		

- Molecule 1: Serine/threonine-protein kinase VRK1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.22Å 95.12Å 193.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 1.90 19.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.81-1.90) 99.1 (19.81-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.187 , 0.226 0.196 , 0.233	Depositor DCC
R_{free} test set	6431 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, E1D, EDO, CL

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	0.55	0/2578	0.68	0/3494
1	B	0.55	0/2475	0.68	0/3354
1	C	0.54	0/2560	0.67	0/3470
1	D	0.58	0/2513	0.70	0/3409
All	All	0.56	0/10126	0.68	0/13727

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 [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	2513	0	2442	4	0
1	B	2415	0	2324	2	0
1	C	2495	0	2421	6	0
1	D	2452	0	2353	4	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	24	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	0	0	0
4	B	4	0	6	0	0
5	C	5	0	0	0	0
5	D	20	0	0	0	0
6	C	6	0	8	1	0
7	A	275	0	0	1	0
7	B	197	0	0	1	0
7	C	278	0	0	0	0
7	D	257	0	0	0	0
All	All	10972	0	9554	16	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 (16) 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:200:LEU:HD13	1:A:221:HIS:CG	2.38	0.58
1:D:89:ARG:NH1	1:D:173:TYR:OH	2.42	0.52
1:D:85:LYS:O	1:D:89:ARG:HG3	2.12	0.50
1:A:155:LEU:HD21	1:A:298:GLU:HG3	1.94	0.50
1:C:184:LEU:HD12	1:C:196:VAL:HG11	1.94	0.49
1:A:85:LYS:NZ	7:A:503:HOH:O	2.42	0.49
1:C:87:TYR:HB3	1:C:113:TYR:HB2	1.99	0.45
1:C:204:TYR:CE2	1:C:205:CYS:HB2	2.52	0.44
1:C:89:ARG:HH12	6:C:403:GOL:C3	2.31	0.43
1:B:319:ASN:HB3	7:B:669:HOH:O	2.18	0.43
1:D:184:LEU:HD22	1:D:196:VAL:HG11	2.00	0.43
1:D:204:TYR:CE2	1:D:205:CYS:HB2	2.55	0.42
1:C:200:LEU:HD13	1:C:221:HIS:CG	2.55	0.41
1:C:109:GLY:HA3	1:C:164:ILE:HD11	2.03	0.41
1:B:204:TYR:CE2	1:B:205[A]:CYS:HB2	2.56	0.40
1:A:204:TYR:CE2	1:A:205:CYS:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	315/364 (86%)	309 (98%)	6 (2%)	0	100	100
1	B	298/364 (82%)	289 (97%)	9 (3%)	0	100	100
1	C	314/364 (86%)	303 (96%)	11 (4%)	0	100	100
1	D	307/364 (84%)	300 (98%)	6 (2%)	1 (0%)	41	31
All	All	1234/1456 (85%)	1201 (97%)	32 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	77	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/304 (86%)	258 (99%)	2 (1%)	81	82
1	B	243/304 (80%)	241 (99%)	2 (1%)	81	82
1	C	256/304 (84%)	255 (100%)	1 (0%)	91	91
1	D	245/304 (81%)	244 (100%)	1 (0%)	91	91
All	All	1004/1216 (83%)	998 (99%)	6 (1%)	86	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	A	203	ARG
1	B	133	ARG
1	B	207	GLU
1	C	133	ARG
1	D	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	$\# Z > 2$
5	SO4	D	401	-	4,4,4	0.34	0	6,6,6	0.16	0
6	GOL	C	403	-	5,5,5	0.47	0	5,5,5	0.70	0
3	E1D	D	406	-	26,26,26	0.79	1 (3%)	34,39,39	1.19	4 (11%)
5	SO4	D	404	-	4,4,4	0.50	0	6,6,6	0.23	0
5	SO4	D	403	-	4,4,4	0.38	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	E1D	B	404	-	26,26,26	0.58	0	34,39,39	1.20	5 (14%)
4	EDO	B	405	-	3,3,3	0.45	0	2,2,2	0.28	0
5	SO4	D	402	-	4,4,4	0.28	0	6,6,6	0.37	0
5	SO4	C	401	-	4,4,4	0.18	0	6,6,6	0.40	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
3	E1D	B	404	-	-	0/4/24/24	0/3/3/3
6	GOL	C	403	-	-	2/4/4/4	-
3	E1D	D	406	-	-	0/4/24/24	0/3/3/3
4	EDO	B	405	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	406	E1D	C7-N5	2.95	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	406	E1D	C11-C12-C13	-2.68	121.69	123.79
3	B	404	E1D	F2-C12-C13	2.53	119.01	117.13
3	B	404	E1D	F1-C14-C13	2.46	118.96	117.13
3	D	406	E1D	F1-C14-C13	2.41	118.92	117.13
3	B	404	E1D	C15-C14-C13	-2.35	121.95	123.79
3	D	406	E1D	C9-N5-C7	2.30	119.37	116.19
3	D	406	E1D	C15-C14-C13	-2.24	122.03	123.79
3	B	404	E1D	C9-N5-C7	2.24	119.29	116.19
3	B	404	E1D	C11-C12-C13	-2.13	122.12	123.79

There are no chirality outliers.

All (3) torsion outliers are listed below:

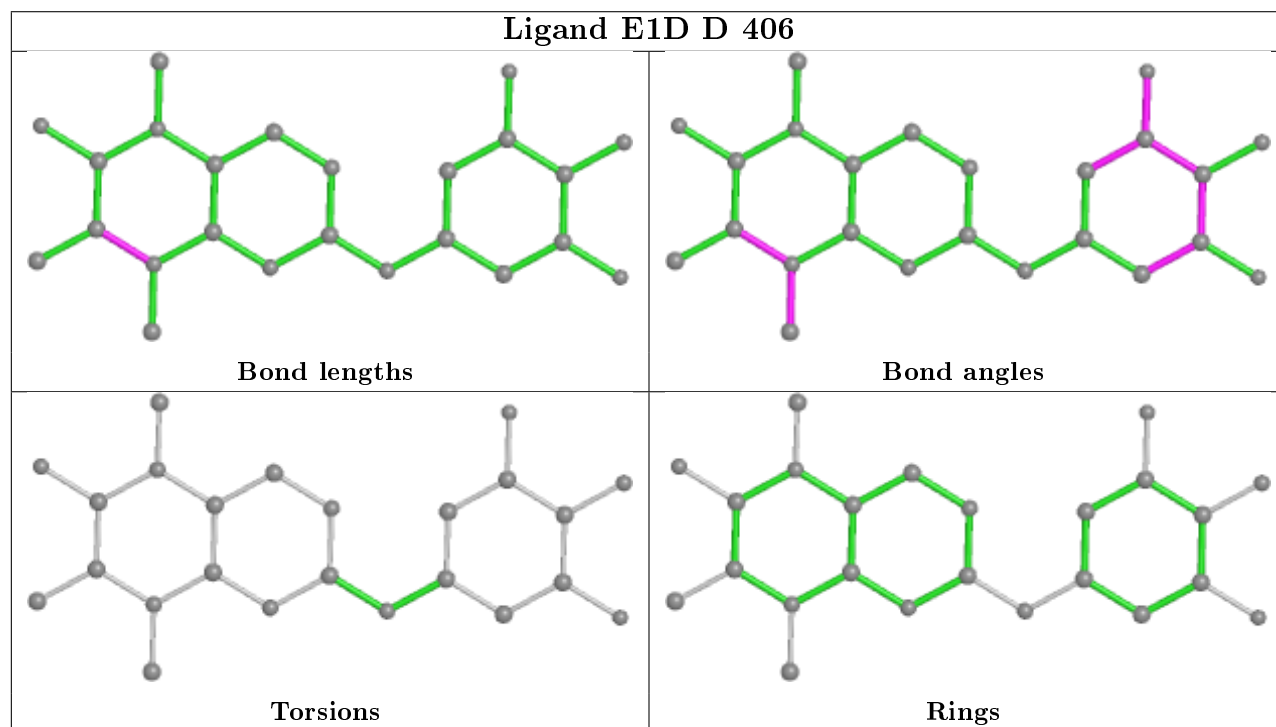
Mol	Chain	Res	Type	Atoms
6	C	403	GOL	C1-C2-C3-O3
6	C	403	GOL	O2-C2-C3-O3
4	B	405	EDO	O1-C1-C2-O2

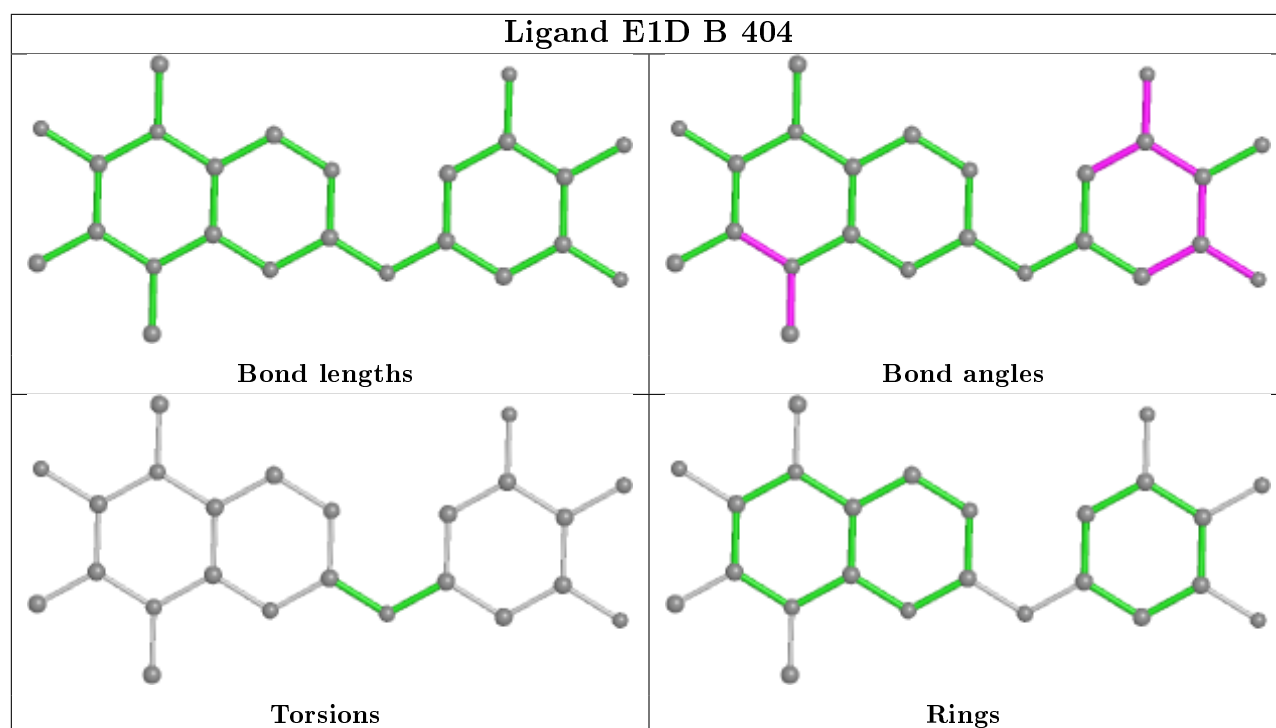
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	403	GOL	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/364 (87%)	0.13	15 (4%) 31 34	25, 35, 53, 77	0
1	B	304/364 (83%)	0.33	24 (7%) 12 14	24, 39, 73, 84	0
1	C	315/364 (86%)	0.13	12 (3%) 40 43	23, 36, 57, 75	0
1	D	311/364 (85%)	0.27	21 (6%) 17 19	21, 35, 68, 81	0
All	All	1247/1456 (85%)	0.21	72 (5%) 23 25	21, 36, 64, 84	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	CYS	6.3
1	B	126	TYR	5.2
1	D	77	ASN	4.7
1	A	220	CYS	4.6
1	B	36	ALA	4.6
1	B	34	ALA	4.5
1	C	217	PRO	4.5
1	B	33	ALA	4.5
1	A	217	PRO	4.4
1	A	291	PRO	4.3
1	B	25	VAL	4.1
1	D	76	ASP	4.1
1	D	78	GLY	3.9
1	C	122	ASN	3.9
1	D	62	VAL	3.8
1	D	63	GLY	3.8
1	D	330	ALA	3.7
1	B	77	ASN	3.6
1	A	123	GLY	3.6
1	D	123	GLY	3.6
1	B	42	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	43	ILE	3.4
1	A	292	ALA	3.4
1	A	20	ALA	3.4
1	C	187	TYR	3.4
1	A	293	ALA	3.3
1	B	24	ALA	3.3
1	D	61	SER	3.3
1	B	65	ASP	3.2
1	D	56	MET	3.2
1	B	74	PRO	3.2
1	C	123	GLY	3.1
1	A	49	GLY	3.1
1	C	59	SER	3.1
1	D	122	ASN	3.0
1	B	76	ASP	3.0
1	D	64	SER	2.9
1	C	126	TYR	2.9
1	B	120	ASP	2.9
1	B	57	ASN	2.8
1	D	294	ASN	2.8
1	D	43	ILE	2.7
1	A	187	TYR	2.7
1	A	332	GLY	2.7
1	B	64	SER	2.6
1	C	121	LYS	2.6
1	D	65	ASP	2.6
1	B	35	ALA	2.5
1	D	23	PHE	2.5
1	A	64	SER	2.4
1	B	187	TYR	2.4
1	C	65	ASP	2.4
1	D	125	SER	2.3
1	D	126	TYR	2.3
1	B	26	GLY	2.3
1	B	78	GLY	2.3
1	A	157	LEU	2.2
1	B	129	MET	2.2
1	B	58	SER	2.2
1	A	252	ILE	2.2
1	A	218	LYS	2.2
1	C	215	ALA	2.1
1	D	190	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	101	ARG	2.1
1	C	146	ALA	2.1
1	D	57	ASN	2.1
1	D	74	PRO	2.1
1	B	75	SER	2.0
1	B	66	ALA	2.0
1	B	67	PRO	2.0
1	D	144	ALA	2.0
1	C	64	SER	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, 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
5	SO4	D	401	5/5	0.50	0.78	190,197,201,202	0
6	GOL	C	403	6/6	0.71	0.27	59,62,66,67	0
2	CL	A	402	1/1	0.77	0.21	72,72,72,72	0
5	SO4	D	404	5/5	0.78	0.25	62,70,79,84	0
2	CL	D	405	1/1	0.80	0.08	80,80,80,80	0
2	CL	A	401	1/1	0.84	0.07	61,61,61,61	0
2	CL	B	401	1/1	0.84	0.07	71,71,71,71	0
2	CL	C	402	1/1	0.90	0.05	65,65,65,65	0
2	CL	B	403	1/1	0.92	0.04	62,62,62,62	0
4	EDO	B	405	4/4	0.92	0.22	35,39,40,40	0
3	E1D	B	404	24/24	0.93	0.10	38,49,59,62	0
5	SO4	D	402	5/5	0.93	0.19	54,58,61,67	0
3	E1D	D	406	24/24	0.95	0.09	31,37,47,49	0
5	SO4	C	401	5/5	0.97	0.10	46,46,54,59	0

Continued on next page...

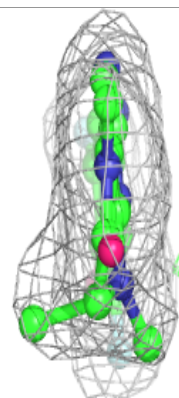
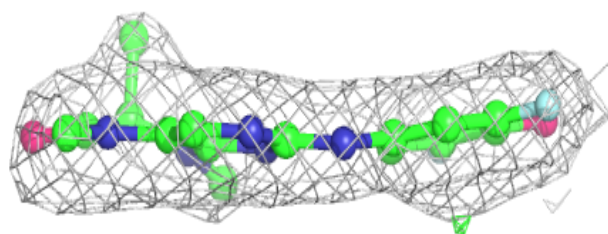
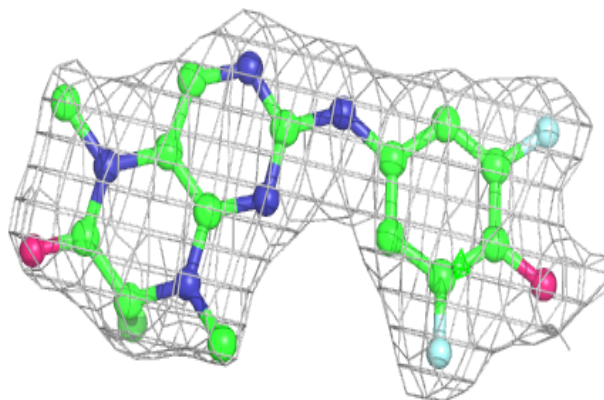
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	B	402	1/1	0.98	0.13	52,52,52,52	0
5	SO4	D	403	5/5	0.98	0.19	45,51,53,55	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.

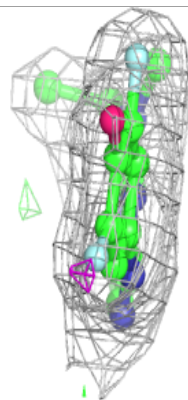
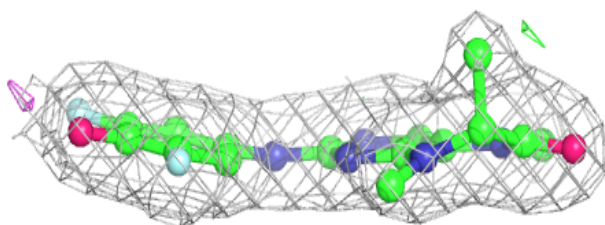
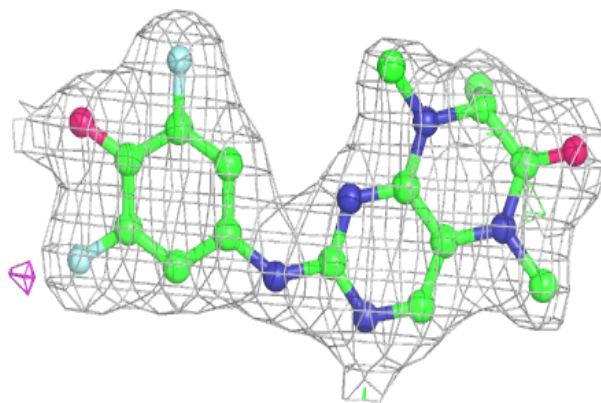
Electron density around E1D B 404:

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 E1D D 406:

$2mF_o-DF_c$ (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.