Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 04:41 PM EDT

PDB ID	:	5UVF
Title	:	Crystal Structure of the Human vaccinia-related kinase bound to BI-D1870
Authors	:	Counago, R.M.; Bountra, C.; Arruda, P.; Edwards, A.M.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on	:	2017-02-20
Resolution	:	2.00 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:

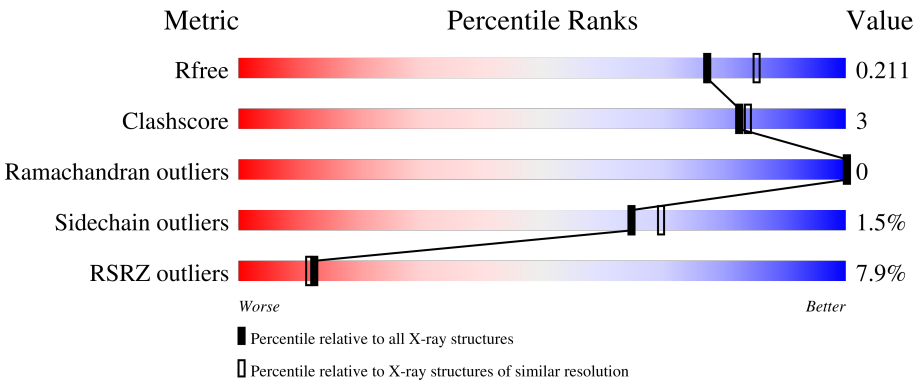
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	364	7% 83% • 13%
1	B	364	7% 83% • 13%
1	C	364	5% 78% • 17%
1	D	364	8% 76% 5% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10449 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
			Total	C	N	O	S			
1	A	317	2468	1581	416	459	12	0	0	0
1	B	316	2474	1584	419	459	12	0	0	0
1	C	301	2344	1501	401	430	12	0	0	0
1	D	296	2310	1481	400	417	12	0	0	0

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

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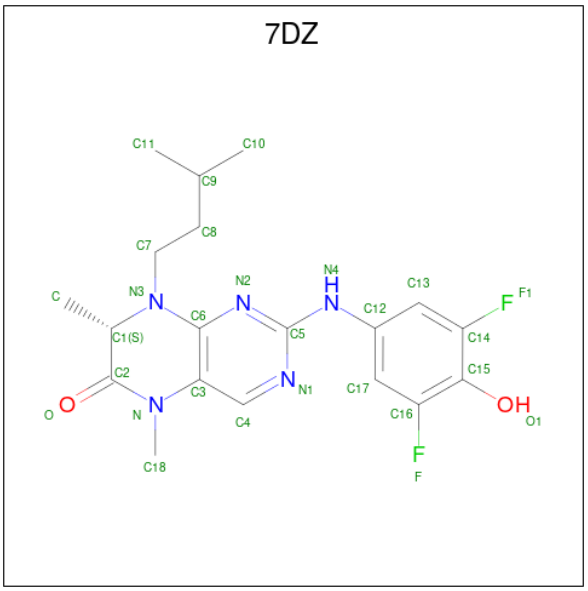
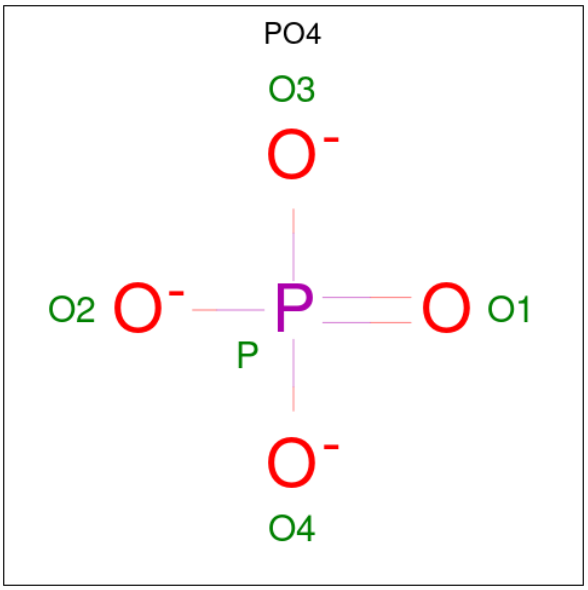
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	GLU	engineered mutation	UNP Q99986
B	293	ALA	LYS	engineered mutation	UNP Q99986
B	295	ALA	LYS	engineered mutation	UNP Q99986
B	359	ALA	LYS	engineered mutation	UNP Q99986
B	360	ALA	LYS	engineered mutation	UNP Q99986
C	1	SER	-	expression tag	UNP 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 (7S)-2-[(3,5-difluoro-4-hydroxyphenyl)amino]-5,7-dimethyl-8-(3-methylbutyl)-7,8-dihydropteridin-6(5H)-one (three-letter code: 7DZ) (formula: $C_{19}H_{23}F_2N_5O_2$).



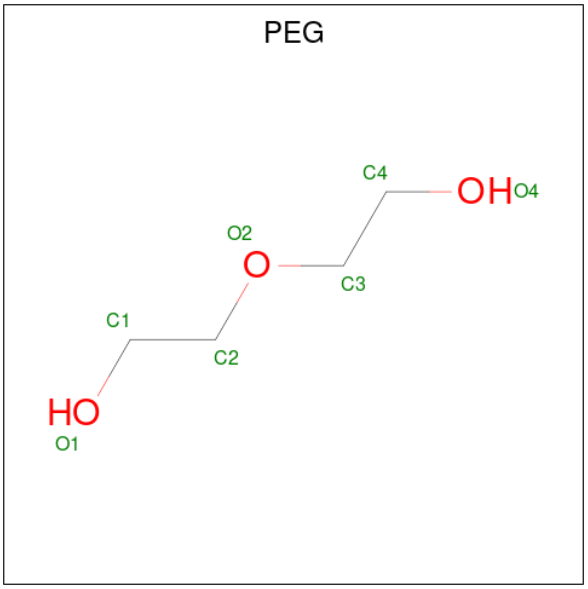
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	28	19	2	5	2	0	0
			Total	C	F	N	O		
2	B	1	28	19	2	5	2	0	0
			Total	C	F	N	O		
2	C	1	28	19	2	5	2	0	0
			Total	C	F	N	O		
2	D	1	28	19	2	5	2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: 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	B	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	D	1	5	4	1	0	0
			Total	O	P		
3	D	1	5	4	1	0	0
			Total	O	P		
3	D	1	5	4	1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	C	1	1	1	0	0

- Molecule 6 is water.

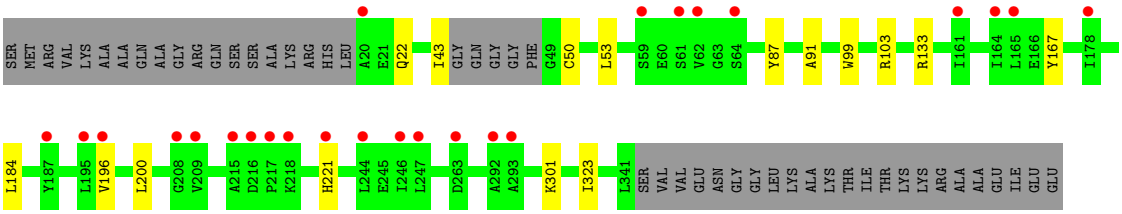
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	161	161	161	0	0
			Total	O		
6	B	193	193	193	0	0
			Total	O		
6	C	165	165	165	0	0
			Total	O		
6	D	164	164	164	0	0

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.

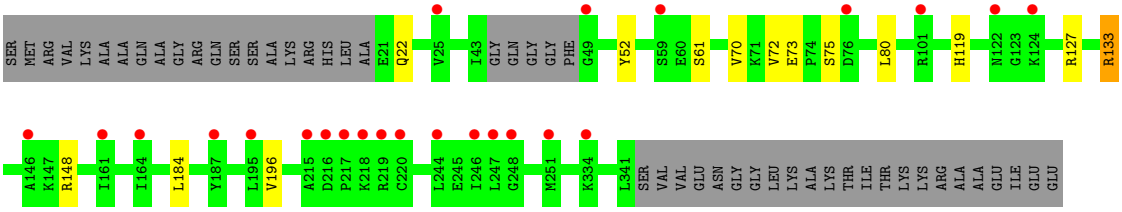
• Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:



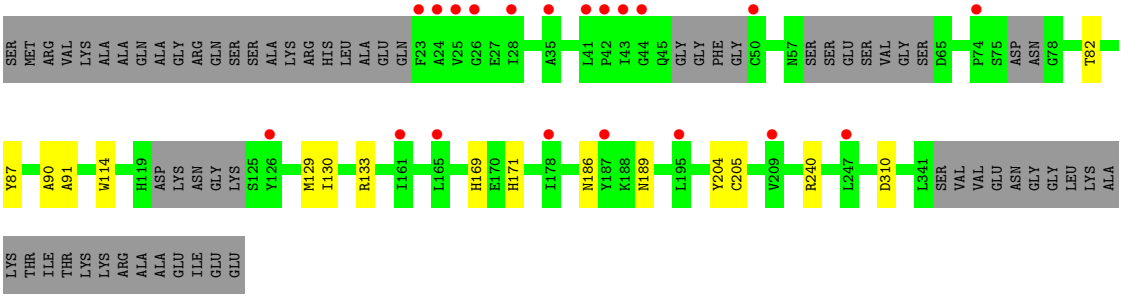
• Molecule 1: Serine/threonine-protein kinase VRK1

Chain B:



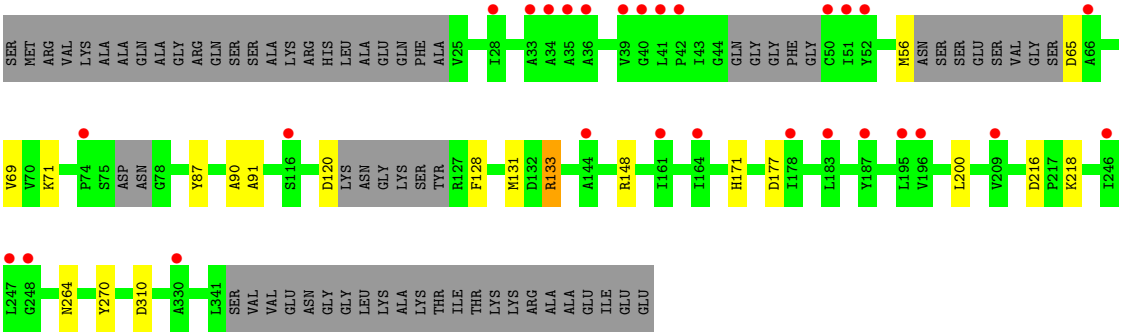
• Molecule 1: Serine/threonine-protein kinase VRK1

Chain C:



• Molecule 1: Serine/threonine-protein kinase VRK1

Chain D:


SER MET ARG VAL LYS ALA ALA GLN ALA GLY ARG GLN SER SER ALA LYS ARG HIS LEU ALA GLU GLN PHE ALA V25 I28 A33 A34 A35 A36 V39 G40 L41 P42 I43 G44 GLN GLY GLY PHE GLY C50 I51 Y52 M56 ASN SER SER GLU SER VAL GLY SER D65 A66
V69 V70 K71 P74 S75 ASP ASN G78 Y87 A90 A91 S116 D120 LYS ASN GLY LYS SER TYR R127 F128 M131 D132 R133 A144 R148 I161 I164 H171 D177 I178 L183 Y187 L195 V196 L200 V209 D216 P217 K218 I246
L247 G248 N264 Y270 D310 A330 L341 SER VAL VAL GLU ASN GLY GLY LEU LYS ALA ALA LYS THR ILE THR LYS LYS ARG ALA ALA GLU ILE GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.14Å 95.24Å 192.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.00 29.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.66-2.00) 96.8 (29.66-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.173 , 0.204 0.179 , 0.211	Depositor DCC
R_{free} test set	5538 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10449	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, CL, PEG, 7DZ

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	0.50	0/2527	0.63	0/3432
1	B	0.51	0/2532	0.61	0/3436
1	C	0.49	0/2399	0.60	0/3253
1	D	0.51	0/2364	0.60	0/3201
All	All	0.50	0/9822	0.61	0/13322

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	2468	0	2371	6	0
1	B	2474	0	2390	11	0
1	C	2344	0	2227	12	0
1	D	2310	0	2213	12	0
2	A	28	0	0	2	0
2	B	28	0	0	2	0
2	C	28	0	0	2	0
2	D	28	0	0	1	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	20	0	0	0	0
3	D	15	0	0	0	0
4	C	7	0	10	0	0
5	C	1	0	0	0	0
6	A	161	0	0	1	0
6	B	193	0	0	1	0
6	C	165	0	0	1	0
6	D	164	0	0	0	0
All	All	10449	0	9211	48	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 3.

All (48) 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:C:114:TRP:HB2	1:C:130:ILE:HG22	1.72	0.71
2:C:402:7DZ:O1	6:C:501:HOH:O	2.12	0.67
1:B:22:GLN:HG2	1:B:72:VAL:HG11	1.79	0.65
1:D:264:ASN:HB3	1:D:270:TYR:CD2	2.32	0.64
1:D:65:ASP:HA	1:D:133:ARG:HH21	1.64	0.63
1:C:87:TYR:HA	1:C:91:ALA:HB3	1.80	0.62
1:D:87:TYR:HA	1:D:91:ALA:HB3	1.82	0.61
1:B:73:GLU:HB2	1:B:80:LEU:HD22	1.83	0.59
1:D:90:ALA:HB1	1:D:171:HIS:HB3	1.87	0.56
1:B:22:GLN:NE2	1:B:119:HIS:ND1	2.50	0.56
2:B:402:7DZ:C	2:B:402:7DZ:C11	2.85	0.54
1:A:200:LEU:HD13	1:A:221:HIS:CG	2.43	0.53
1:C:114:TRP:HB2	1:C:130:ILE:CG2	2.39	0.52
1:B:148:ARG:HG2	1:B:148:ARG:HH11	1.75	0.51
2:B:402:7DZ:C13	2:B:402:7DZ:N2	2.73	0.51
1:C:90:ALA:HB1	1:C:171:HIS:HB3	1.92	0.50
2:A:401:7DZ:N2	2:A:401:7DZ:C13	2.75	0.50
1:C:87:TYR:HD2	1:C:129:MET:HE1	1.77	0.49
1:B:22:GLN:HE21	1:B:119:HIS:CE1	2.31	0.48
2:D:403:7DZ:N2	2:D:403:7DZ:C13	2.76	0.48
1:A:43:ILE:HG23	1:A:53:LEU:HG	1.95	0.48
1:B:52:TYR:HB2	1:B:70:VAL:CG1	2.44	0.48
2:C:402:7DZ:N2	2:C:402:7DZ:C13	2.77	0.48
1:D:90:ALA:CB	1:D:171:HIS:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:HG13	1:D:133:ARG:HG2	1.96	0.47
1:C:87:TYR:CD2	1:C:129:MET:HE1	2.49	0.47
1:D:216:ASP:OD1	1:D:218:LYS:HG2	2.14	0.47
1:D:65:ASP:HA	1:D:133:ARG:NH2	2.29	0.47
1:D:148:ARG:HH11	1:D:148:ARG:HG2	1.80	0.47
1:C:87:TYR:CD2	1:C:129:MET:CE	2.98	0.46
1:C:186:ASN:HB3	1:C:189:ASN:O	2.15	0.46
1:A:184:LEU:HD22	1:A:196:VAL:HG11	1.98	0.46
1:A:87:TYR:HD1	1:A:91:ALA:HB3	1.81	0.45
1:B:133:ARG:C	1:B:133:ARG:HD3	2.36	0.45
1:B:73:GLU:HB2	1:B:80:LEU:CD2	2.45	0.45
1:B:148:ARG:HG2	1:B:148:ARG:NH1	2.33	0.43
1:C:87:TYR:CD1	1:C:91:ALA:HB3	2.53	0.43
1:C:169:HIS:CG	1:C:240:ARG:HG2	2.54	0.42
1:C:204:TYR:CE2	1:C:205:CYS:HB2	2.54	0.42
2:A:401:7DZ:O1	6:A:501:HOH:O	2.22	0.42
1:D:177:ASP:HB2	1:D:200:LEU:HD11	2.01	0.42
1:A:99:TRP:CD2	1:A:167:TYR:HD2	2.38	0.41
1:B:184:LEU:HD22	1:B:196:VAL:HG11	2.02	0.41
1:A:301:LYS:HE3	1:A:323:ILE:HG12	2.02	0.41
1:C:90:ALA:CB	1:C:171:HIS:HB3	2.50	0.41
1:D:71:LYS:O	1:D:128:PHE:HA	2.21	0.40
1:D:131:MET:HE3	1:D:131:MET:HB3	1.90	0.40
1:B:127:ARG:HG3	6:B:613:HOH:O	2.21	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	313/364 (86%)	307 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/364 (86%)	308 (99%)	4 (1%)	0	100	100
1	C	291/364 (80%)	284 (98%)	7 (2%)	0	100	100
1	D	286/364 (79%)	281 (98%)	5 (2%)	0	100	100
All	All	1202/1456 (83%)	1180 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	251/304 (83%)	247 (98%)	4 (2%)	62	67
1	B	253/304 (83%)	250 (99%)	3 (1%)	71	76
1	C	232/304 (76%)	229 (99%)	3 (1%)	69	74
1	D	228/304 (75%)	224 (98%)	4 (2%)	59	63
All	All	964/1216 (79%)	950 (98%)	14 (2%)	65	69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	50	CYS
1	A	103	ARG
1	A	133	ARG
1	B	61	SER
1	B	75	SER
1	B	133	ARG
1	C	82	THR
1	C	133	ARG
1	C	310	ASP
1	D	56	MET
1	D	120	ASP
1	D	133	ARG

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Mol	Chain	Res	Type
1	D	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	22	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
3	PO4	D	402	-	4,4,4	1.27	0	6,6,6	0.38	0
2	7DZ	B	402	-	29,30,30	0.52	0	37,44,44	1.19	5 (13%)
3	PO4	C	403	-	4,4,4	1.18	0	6,6,6	0.55	0
3	PO4	A	402	-	4,4,4	1.22	0	6,6,6	0.52	0
3	PO4	C	401	-	4,4,4	1.33	0	6,6,6	0.54	0
3	PO4	C	405	-	4,4,4	1.10	0	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	D	401	-	4,4,4	1.29	0	6,6,6	0.49	0
2	7DZ	C	402	-	29,30,30	0.52	0	37,44,44	1.14	5 (13%)
3	PO4	C	404	-	4,4,4	1.17	0	6,6,6	0.35	0
4	PEG	C	406	-	6,6,6	0.46	0	5,5,5	0.39	0
3	PO4	B	401	-	4,4,4	1.57	0	6,6,6	0.57	0
2	7DZ	A	401	-	29,30,30	0.48	0	37,44,44	1.27	5 (13%)
3	PO4	A	403	-	4,4,4	1.17	0	6,6,6	0.43	0
3	PO4	D	404	-	4,4,4	1.17	0	6,6,6	0.48	0
2	7DZ	D	403	-	29,30,30	0.52	0	37,44,44	1.12	5 (13%)

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	7DZ	B	402	-	-	1/9/29/29	0/3/3/3
2	7DZ	C	402	-	-	0/9/29/29	0/3/3/3
4	PEG	C	406	-	-	1/4/4/4	-
2	7DZ	A	401	-	-	3/9/29/29	0/3/3/3
2	7DZ	D	403	-	-	2/9/29/29	0/3/3/3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	7DZ	C8-C7-N3	4.82	119.61	112.21
2	B	402	7DZ	C8-C7-N3	4.11	118.51	112.21
2	C	402	7DZ	C8-C7-N3	3.51	117.59	112.21
2	D	403	7DZ	C8-C7-N3	3.37	117.37	112.21
2	A	401	7DZ	F-C16-C15	2.83	119.23	117.13
2	D	403	7DZ	C17-C16-C15	-2.66	121.71	123.79
2	B	402	7DZ	C17-C16-C15	-2.60	121.76	123.79
2	C	402	7DZ	C13-C14-C15	-2.56	121.79	123.79
2	D	403	7DZ	C13-C14-C15	-2.50	121.83	123.79
2	C	402	7DZ	F-C16-C15	2.48	118.97	117.13
2	B	402	7DZ	C13-C14-C15	-2.43	121.89	123.79
2	A	401	7DZ	C17-C16-C15	-2.43	121.89	123.79
2	D	403	7DZ	F-C16-C15	2.42	118.92	117.13
2	C	402	7DZ	C17-C16-C15	-2.41	121.91	123.79
2	B	402	7DZ	F1-C14-C15	2.30	118.84	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	7DZ	C13-C14-C15	-2.24	122.04	123.79
2	C	402	7DZ	F1-C14-C15	2.20	118.76	117.13
2	A	401	7DZ	F1-C14-C15	2.16	118.74	117.13
2	B	402	7DZ	F-C16-C15	2.13	118.71	117.13
2	D	403	7DZ	F1-C14-C15	2.12	118.71	117.13

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	7DZ	C7-C8-C9-C11
2	D	403	7DZ	C7-C8-C9-C11
2	D	403	7DZ	C7-C8-C9-C10
2	A	401	7DZ	C7-C8-C9-C10
2	B	402	7DZ	C7-C8-C9-C11
4	C	406	PEG	C4-C3-O2-C2
2	A	401	7DZ	C8-C7-N3-C1

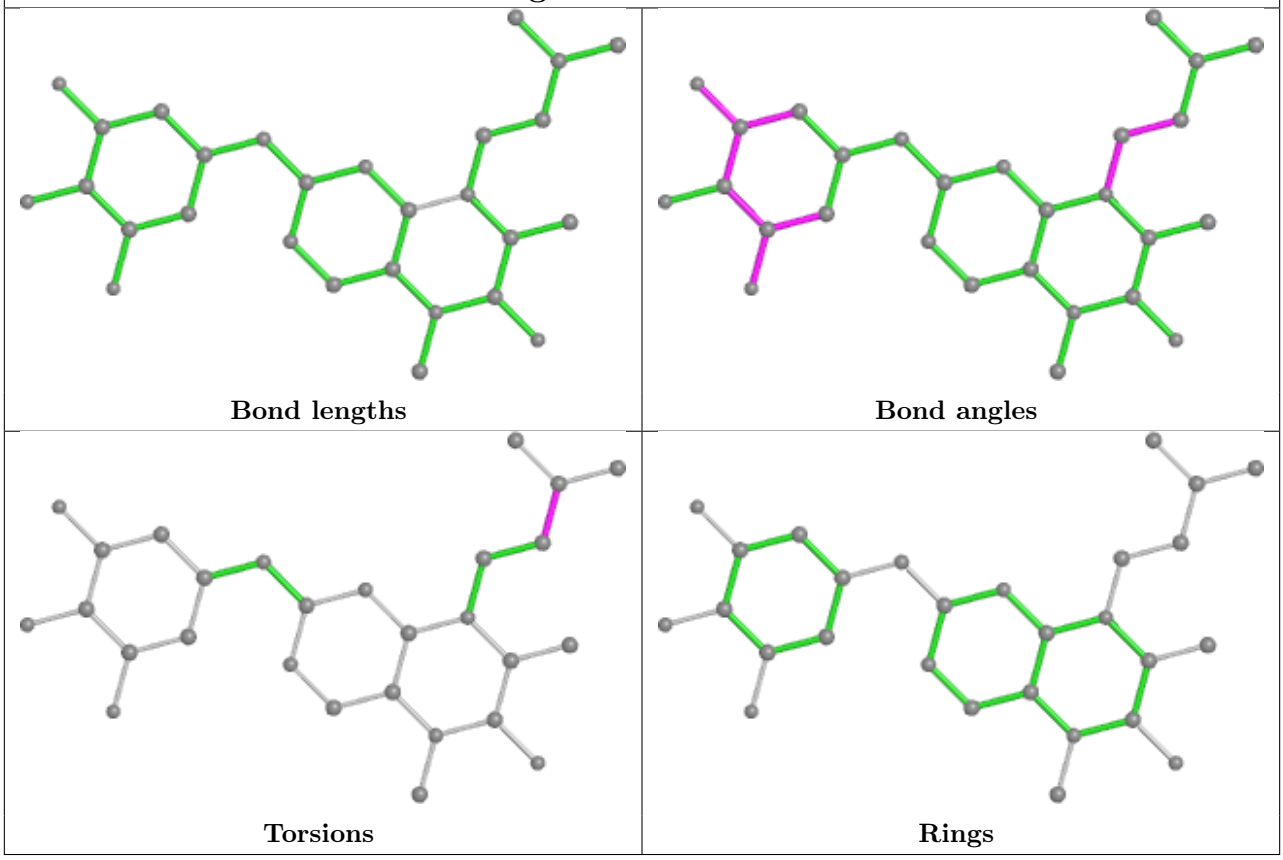
There are no ring outliers.

4 monomers are involved in 7 short contacts:

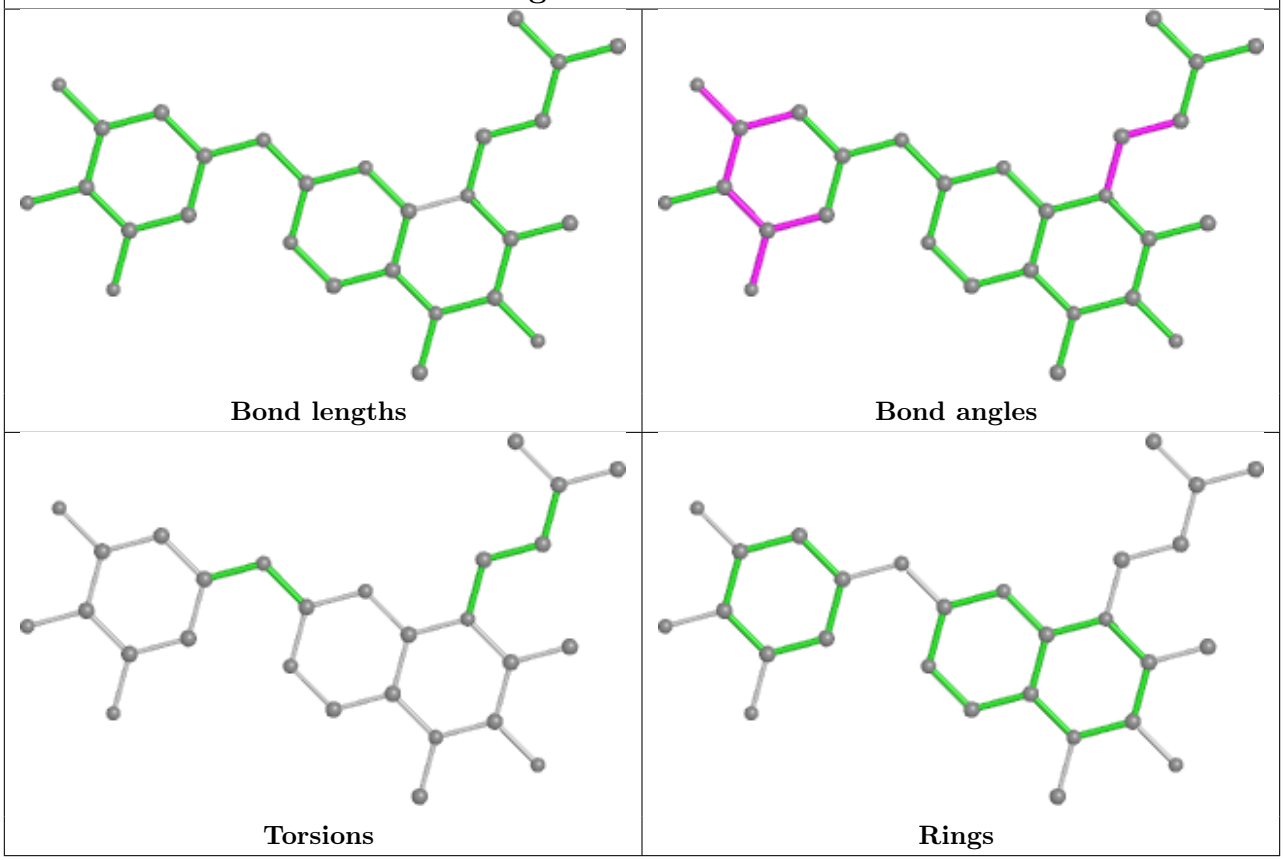
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	7DZ	2	0
2	C	402	7DZ	2	0
2	A	401	7DZ	2	0
2	D	403	7DZ	1	0

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.

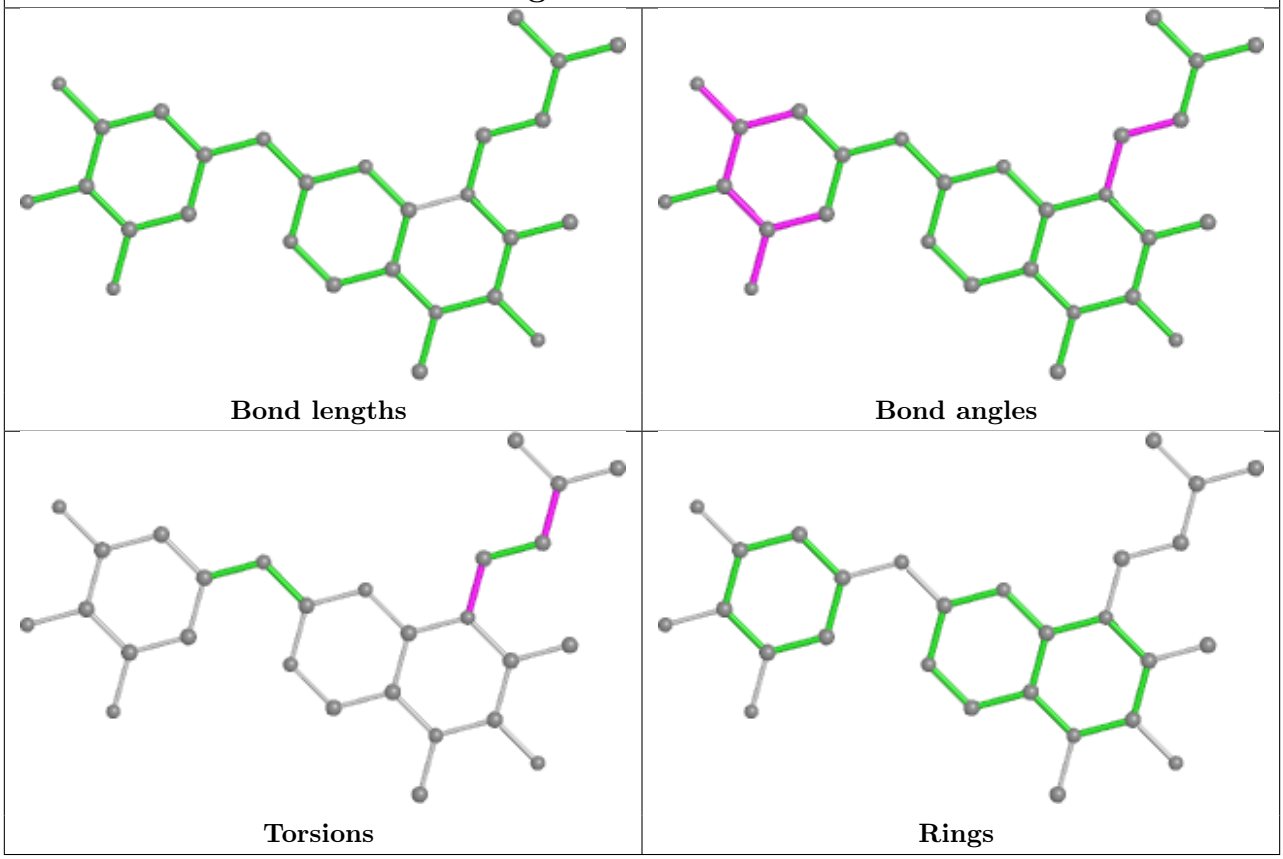
Ligand 7DZ B 402



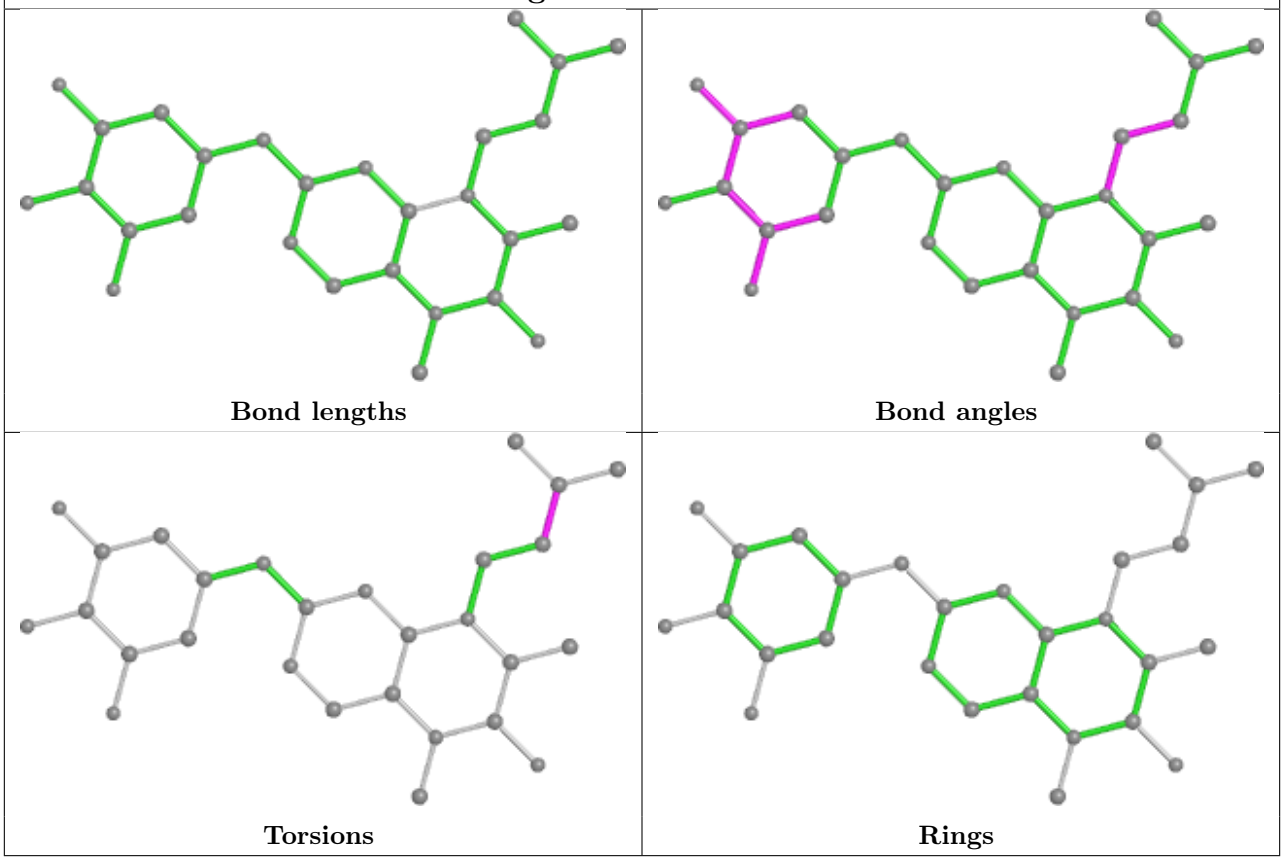
Ligand 7DZ C 402



Ligand 7DZ A 401



Ligand 7DZ D 403



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	317/364 (87%)	0.24	25 (7%)	12	11	35, 49, 79, 101	0
1	B	316/364 (86%)	0.14	24 (7%)	13	13	33, 49, 76, 90	0
1	C	301/364 (82%)	0.27	20 (6%)	18	17	30, 50, 88, 128	0
1	D	296/364 (81%)	0.32	28 (9%)	8	7	31, 48, 100, 130	0
All	All	1230/1456 (84%)	0.24	97 (7%)	12	11	30, 49, 87, 130	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	VAL	10.0
1	C	24	ALA	6.5
1	A	217	PRO	6.5
1	B	220	CYS	5.4
1	D	50	CYS	5.0
1	D	41	LEU	5.0
1	B	217	PRO	4.7
1	C	41	LEU	4.5
1	B	215	ALA	4.3
1	C	42	PRO	4.1
1	C	50	CYS	3.9
1	D	35	ALA	3.8
1	D	34	ALA	3.7
1	C	126	TYR	3.7
1	A	247	LEU	3.7
1	C	23	PHE	3.7
1	D	247	LEU	3.6
1	D	33	ALA	3.6
1	B	161	ILE	3.6
1	D	161	ILE	3.6
1	C	161	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	51	ILE	3.4
1	A	187	TYR	3.3
1	B	187	TYR	3.3
1	D	39	VAL	3.3
1	A	161	ILE	3.3
1	A	61	SER	3.3
1	A	215	ALA	3.2
1	D	40	GLY	3.2
1	B	219	ARG	3.2
1	D	52	TYR	3.2
1	C	44	GLY	3.0
1	A	293	ALA	3.0
1	B	247	LEU	3.0
1	D	195	LEU	3.0
1	D	246	ILE	3.0
1	D	36	ALA	2.9
1	D	66	ALA	2.9
1	C	43	ILE	2.8
1	A	178	ILE	2.8
1	C	28	ILE	2.8
1	A	263	ASP	2.8
1	D	74	PRO	2.8
1	C	247	LEU	2.8
1	D	178	ILE	2.7
1	B	218	LYS	2.7
1	A	64	SER	2.7
1	A	20	ALA	2.7
1	A	165	LEU	2.7
1	B	216	ASP	2.7
1	A	59	SER	2.6
1	D	209	VAL	2.6
1	A	196	VAL	2.6
1	D	187	TYR	2.6
1	A	246	ILE	2.6
1	D	28	ILE	2.6
1	A	208	GLY	2.6
1	B	122	ASN	2.5
1	B	248	GLY	2.4
1	A	195	LEU	2.4
1	C	165	LEU	2.4
1	A	221	HIS	2.4
1	D	330	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	101	ARG	2.3
1	B	59	SER	2.3
1	B	76	ASP	2.3
1	B	124	LYS	2.3
1	B	49	GLY	2.3
1	D	183	LEU	2.3
1	D	42	PRO	2.3
1	D	164	ILE	2.2
1	D	144	ALA	2.2
1	A	209	VAL	2.2
1	C	187	TYR	2.2
1	D	196	VAL	2.2
1	B	164	ILE	2.2
1	A	244	LEU	2.2
1	B	195	LEU	2.2
1	C	178	ILE	2.1
1	C	209	VAL	2.1
1	C	195	LEU	2.1
1	D	116	SER	2.1
1	A	292	ALA	2.1
1	D	248	GLY	2.1
1	B	251	MET	2.1
1	C	74	PRO	2.1
1	A	218	LYS	2.1
1	A	164	ILE	2.0
1	B	334	LYS	2.0
1	A	216	ASP	2.0
1	C	35	ALA	2.0
1	A	62	VAL	2.0
1	B	146	ALA	2.0
1	B	244	LEU	2.0
1	B	246	ILE	2.0
1	B	25	VAL	2.0
1	C	26	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

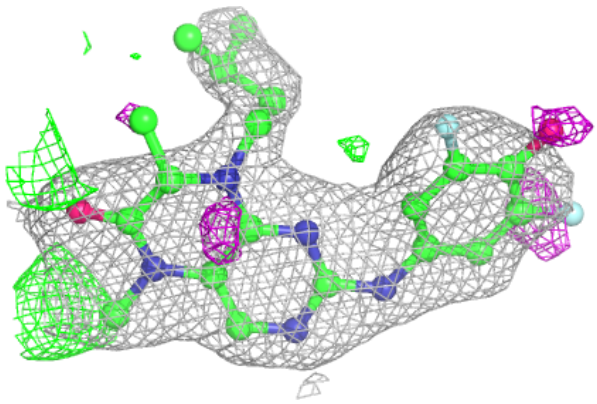
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

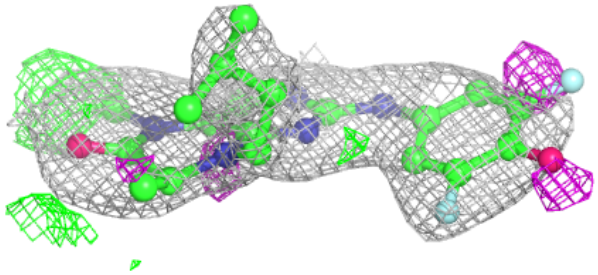
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7DZ	B	402	28/28	0.74	0.28	67,78,87,89	0
4	PEG	C	406	7/7	0.80	0.24	45,56,64,66	0
2	7DZ	A	401	28/28	0.88	0.17	55,66,72,73	0
5	CL	C	407	1/1	0.90	0.21	85,85,85,85	0
3	PO4	D	401	5/5	0.91	0.13	74,74,76,79	0
2	7DZ	C	402	28/28	0.92	0.14	46,65,75,77	0
2	7DZ	D	403	28/28	0.92	0.13	50,63,73,75	0
3	PO4	C	405	5/5	0.92	0.19	96,97,98,98	0
3	PO4	C	404	5/5	0.94	0.09	94,94,95,97	0
3	PO4	A	403	5/5	0.95	0.10	87,87,89,89	0
3	PO4	D	402	5/5	0.95	0.15	69,70,71,73	0
3	PO4	D	404	5/5	0.96	0.17	93,95,96,96	0
3	PO4	C	401	5/5	0.96	0.15	61,65,69,72	0
3	PO4	C	403	5/5	0.96	0.14	72,73,75,75	0
3	PO4	B	401	5/5	0.97	0.12	65,66,71,72	0
3	PO4	A	402	5/5	0.97	0.21	76,77,80,80	0

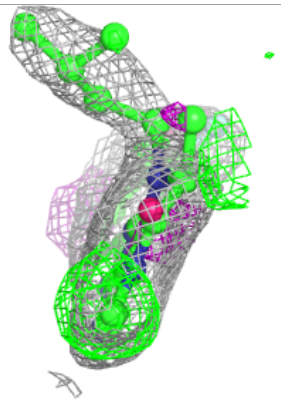
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7DZ B 402:

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

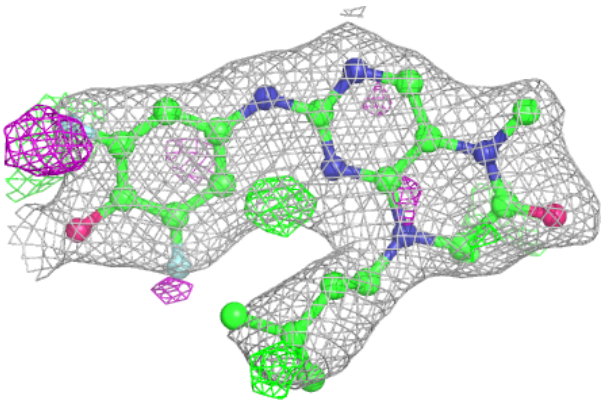


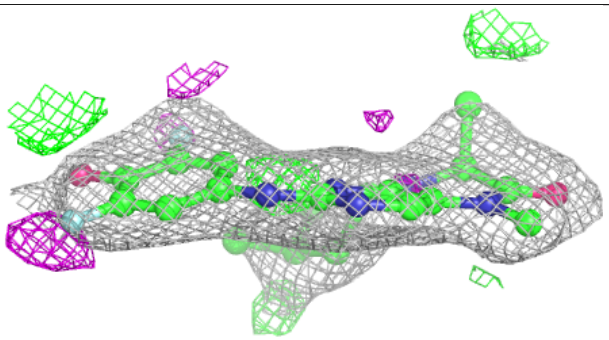


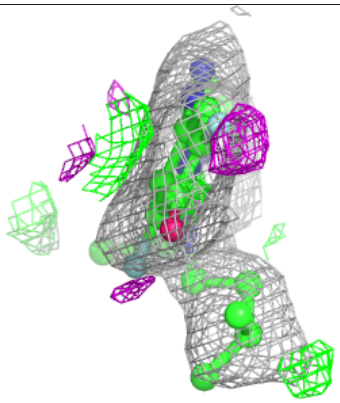


Electron density around 7DZ A 401:

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

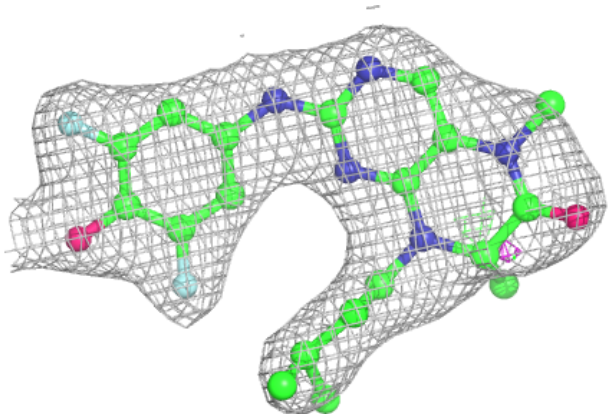


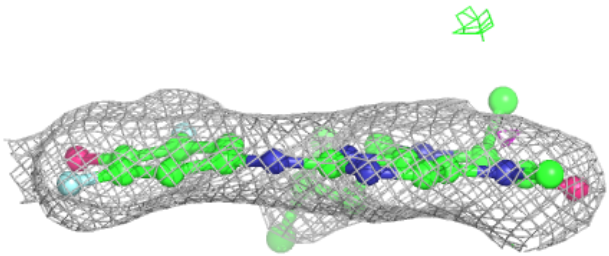


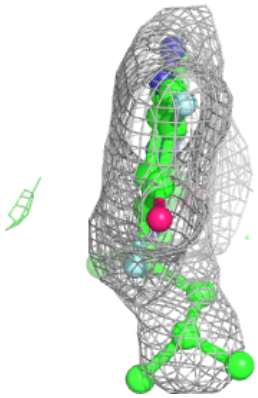


Electron density around 7DZ C 402:

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

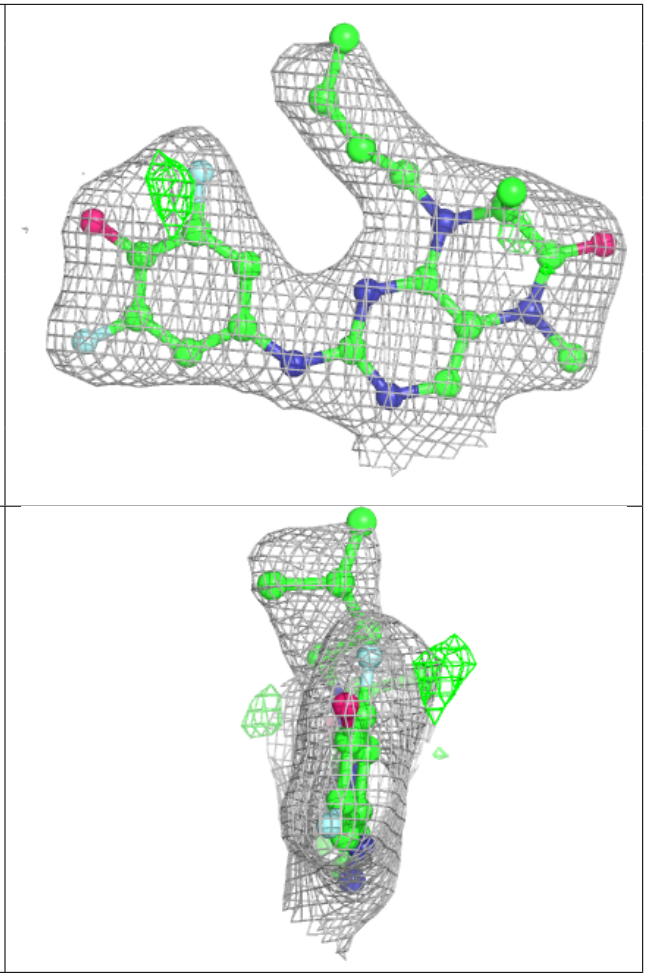






Electron density around 7DZ D 403:

$2mF_o$-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.