Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2023 – 12:04 PM EDT

PDB ID	:	8G6A
Title	:	Wildtype PTP1b in complex with DES6016
Authors	:	Greisman, J.B.; Willmore, L.; Yeh, C.Y.; Giordanetto, F.; Shahamadtar, S.; Nisonoff, H.; Maragakis, P.; Shaw, D.E.
Deposited on	:	2023-02-14
Resolution	:	1.62 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

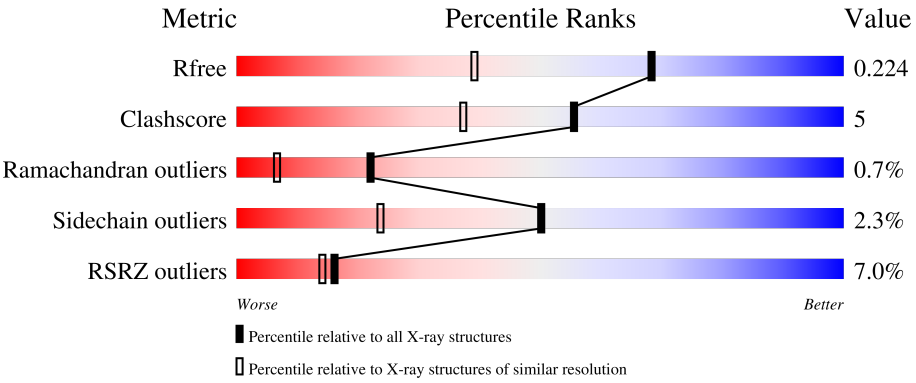
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	298	8% 78% 14% · 6%
1	B	298	6% 73% 20% · ·

2 Entry composition

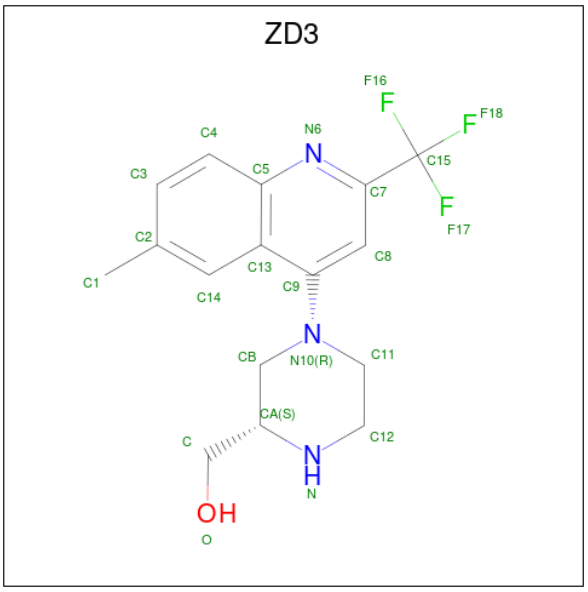
There are 7 unique types of molecules in this entry. The entry contains 5136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

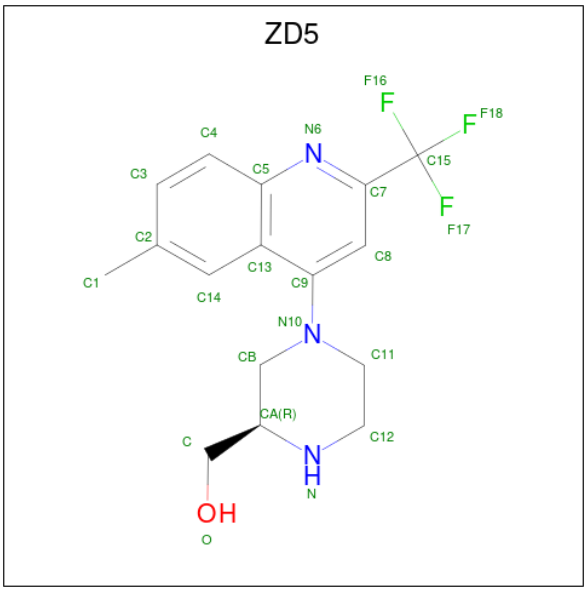
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	4	0
			2318	1473	398	430	17			
1	B	287	Total	C	N	O	S	0	13	0
			2392	1523	405	442	22			

- Molecule 2 is {(2S)-4-[6-methyl-2-(trifluoromethyl)quinolin-4-yl]piperazin-2-yl}methanol (three-letter code: ZD3) (formula: $C_{16}H_{18}F_3N_3O$) (labeled as "Ligand of Interest" by depositor).



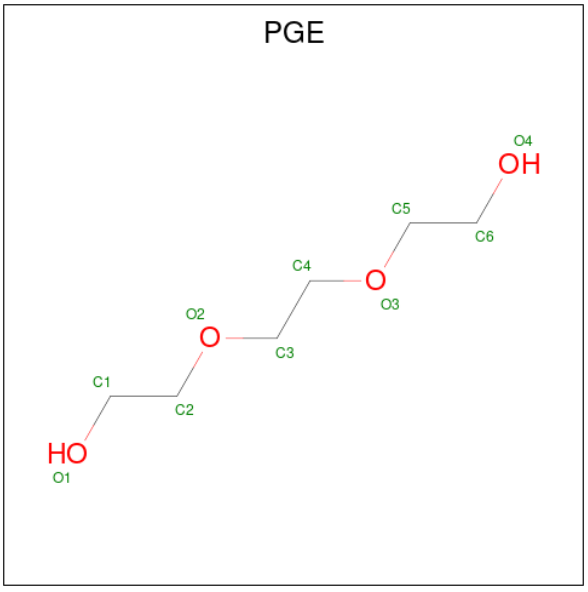
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	16	3	3	1		

- Molecule 3 is {(2R)-4-[6-methyl-2-(trifluoromethyl)quinolin-4-yl]piperazin-2-yl}methanol (three-letter code: ZD5) (formula: $C_{16}H_{18}F_3N_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			23	16	3	3	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

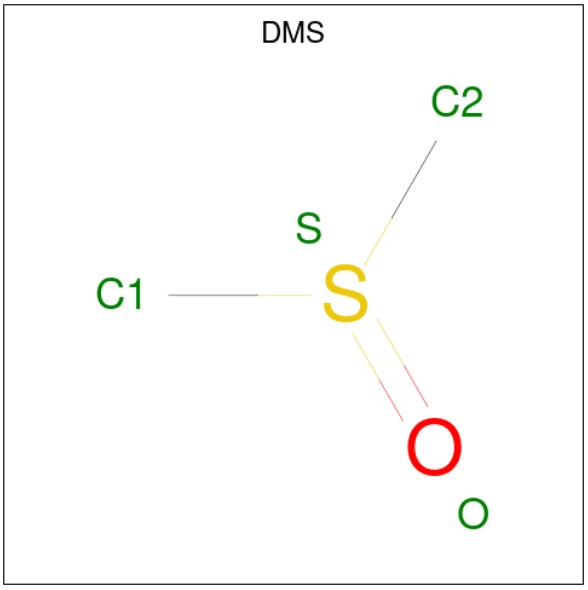


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 7 is water.

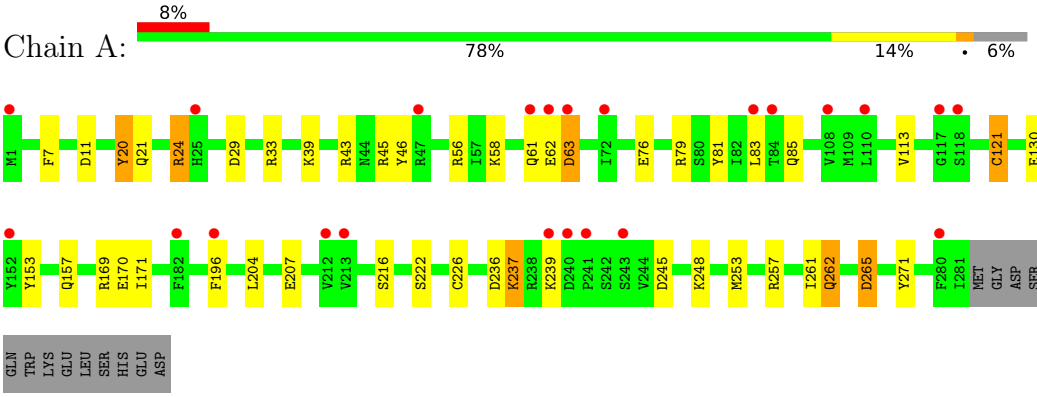
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	153	Total O 153 153	0	0
7	B	212	Total O 212 212	0	0

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.

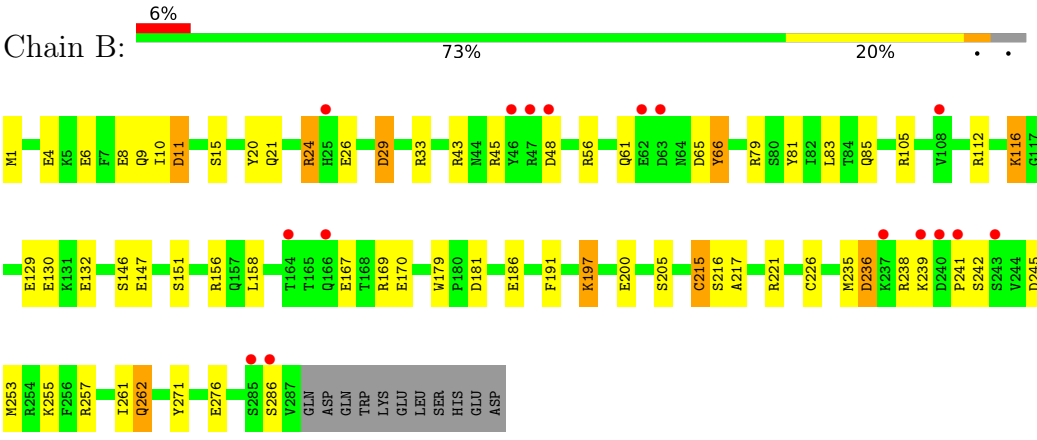
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 1

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.35Å 88.35Å 162.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.95 – 1.62 31.93 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.95-1.62) 99.9 (31.93-1.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.217 0.190 , 0.224	Depositor DCC
R_{free} test set	4175 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5136	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: MG, DMS, PGE, ZD5, ZD3

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	1.45	10/2383 (0.4%)	1.35	23/3211 (0.7%)
1	B	1.64	26/2484 (1.0%)	1.51	34/3345 (1.0%)
All	All	1.55	36/4867 (0.7%)	1.43	57/6556 (0.9%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	GLN	CG-CD	11.00	1.76	1.51
1	B	252	GLU	CD-OE2	9.58	1.36	1.25
1	B	186	GLU	CD-OE2	8.22	1.34	1.25
1	B	271	TYR	CE2-CZ	-7.95	1.28	1.38
1	B	170	GLU	CD-OE1	-7.76	1.17	1.25
1	B	20	TYR	CE1-CZ	-7.58	1.28	1.38
1	B	132	GLU	CD-OE2	-7.30	1.17	1.25
1	A	121	CYS	CB-SG	-6.93	1.70	1.82
1	B	146	SER	CB-OG	-6.81	1.33	1.42
1	A	147	GLU	CD-OE1	-6.80	1.18	1.25
1	B	130	GLU	CD-OE2	6.63	1.32	1.25
1	B	20	TYR	CG-CD2	-6.48	1.30	1.39
1	B	151	SER	CB-OG	-6.33	1.34	1.42
1	B	6	GLU	CD-OE2	6.25	1.32	1.25
1	A	46	TYR	CE1-CZ	6.15	1.46	1.38
1	A	153	TYR	CE1-CZ	6.11	1.46	1.38
1	B	170	GLU	CD-OE2	6.09	1.32	1.25
1	B	205	SER	CB-OG	-6.08	1.34	1.42
1	B	179	TRP	CZ3-CH2	-6.00	1.30	1.40
1	B	197	LYS	CA-CB	-5.98	1.40	1.53
1	A	20	TYR	CE1-CZ	-5.82	1.30	1.38
1	B	147	GLU	CD-OE1	-5.80	1.19	1.25
1	A	196	PHE	CB-CG	5.67	1.60	1.51
1	B	129	GLU	CD-OE2	-5.65	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLN	CD-NE2	5.59	1.46	1.32
1	B	191	PHE	CG-CD2	-5.51	1.30	1.38
1	B	26	GLU	CD-OE1	5.46	1.31	1.25
1	B	66	TYR	CE2-CZ	5.44	1.45	1.38
1	A	222	SER	CA-CB	5.44	1.61	1.52
1	A	262	GLN	CD-OE1	5.41	1.35	1.24
1	B	4	GLU	CD-OE1	5.29	1.31	1.25
1	B	8	GLU	CD-OE1	5.23	1.31	1.25
1	B	81	TYR	CE1-CZ	5.16	1.45	1.38
1	A	171	ILE	C-O	5.10	1.33	1.23
1	A	151	SER	CB-OG	-5.04	1.35	1.42
1	B	129	GLU	CG-CD	5.01	1.59	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	79	ARG	NE-CZ-NH2	11.70	126.15	120.30
1	B	11	ASP	CB-CG-OD1	11.58	128.72	118.30
1	B	257	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	B	235	MET	CG-SD-CE	-11.21	82.26	100.20
1	A	79	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	56	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	43	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	33	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	B	29	ASP	CB-CG-OD2	-9.07	110.13	118.30
1	A	236	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	B	158	LEU	CB-CG-CD2	-8.55	96.46	111.00
1	B	105	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	A	79	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	156	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	186	GLU	OE1-CD-OE2	-7.87	113.85	123.30
1	B	130	GLU	OE1-CD-OE2	-7.85	113.88	123.30
1	B	29	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	56	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	24	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	271	TYR	CB-CG-CD2	-7.49	116.50	121.00
1	B	56	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	276	GLU	OE1-CD-OE2	-7.44	114.37	123.30
1	B	245	ASP	CB-CG-OD1	7.38	124.95	118.30
1	A	271	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	B	262	GLN	CA-CB-CG	6.81	128.39	113.40
1	A	61	GLN	CB-CA-C	6.73	123.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	B	169	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	B	1	MET	CG-SD-CE	6.18	110.08	100.20
1	A	81	TYR	CB-CG-CD2	6.14	124.68	121.00
1	B	236	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	81	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	B	191	PHE	CB-CG-CD1	-5.99	116.61	120.80
1	A	130	GLU	OE1-CD-OE2	-5.99	116.12	123.30
1	A	33	ARG	CG-CD-NE	-5.96	99.27	111.80
1	A	253	MET	CG-SD-CE	-5.91	90.74	100.20
1	A	33	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	257	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	255	LYS	CD-CE-NZ	-5.77	98.43	111.70
1	B	271	TYR	CG-CD1-CE1	-5.74	116.71	121.30
1	A	153	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	B	65	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	A	7	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	B	147	GLU	N-CA-CB	-5.54	100.62	110.60
1	B	215[A]	CYS	CB-CA-C	5.52	121.44	110.40
1	B	215[B]	CYS	CB-CA-C	5.52	121.44	110.40
1	A	204	LEU	CB-CG-CD1	5.46	120.29	111.00
1	B	4	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	B	65	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	20	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	24	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	271	TYR	CD1-CE1-CZ	-5.24	115.09	119.80
1	A	245	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	58	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	A	265	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	B	186	GLU	CG-CD-OE2	5.09	128.49	118.30
1	A	169	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2318	0	2300	17	1
1	B	2392	0	2402	29	1
2	A	23	0	0	0	0
3	A	23	0	0	0	0
4	A	10	0	14	1	0
5	B	1	0	0	0	0
6	B	4	0	6	2	0
7	A	153	0	0	3	3
7	B	212	0	0	14	2
All	All	5136	0	4722	48	5

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 5.

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:B:262:GLN:CD	1:B:262:GLN:CG	1.76	1.53
1:B:43:ARG:HD3	7:B:404:HOH:O	1.43	1.16
1:B:215[B]:CYS:SG	7:B:544:HOH:O	2.03	1.07
1:B:9[A]:GLN:OE1	7:B:402:HOH:O	1.79	1.00
1:B:167:GLU:OE1	7:B:403:HOH:O	1.79	1.00
1:B:226[B]:CYS:SG	1:B:253[B]:MET:HE1	2.02	0.99
1:B:66:TYR:O	7:B:404:HOH:O	1.82	0.96
1:A:62:GLU:O	1:A:63:ASP:CB	2.16	0.94
1:B:21:GLN:HE22	1:B:24:ARG:HH11	1.20	0.90
1:A:62:GLU:O	1:A:63:ASP:HB2	1.72	0.89
1:B:226[B]:CYS:SG	1:B:253[B]:MET:CE	2.65	0.84
1:A:21:GLN:HE22	1:A:24:ARG:HH11	1.24	0.82
1:A:29:ASP:OD1	7:A:401:HOH:O	1.99	0.79
1:B:29:ASP:OD2	7:B:405:HOH:O	2.01	0.79
1:A:83:LEU:HD11	1:A:226[A]:CYS:SG	2.24	0.77
1:B:242:SER:OG	7:B:407:HOH:O	2.07	0.72
1:B:83:LEU:HD11	1:B:226[A]:CYS:SG	2.31	0.70
1:A:45:ARG:H	1:A:85:GLN:HE22	1.40	0.69
1:B:45:ARG:H	1:B:85:GLN:HE22	1.39	0.67
6:B:302:DMS:H13	7:B:508:HOH:O	1.96	0.63
1:B:242:SER:HB3	7:B:575:HOH:O	2.01	0.60
1:B:45:ARG:H	1:B:85:GLN:NE2	2.01	0.57
1:A:113:VAL:HG13	1:A:121:CYS:O	2.06	0.56
1:A:45:ARG:H	1:A:85:GLN:NE2	2.05	0.55
1:A:62:GLU:O	1:A:63:ASP:HB3	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:N	7:A:405:HOH:O	2.38	0.54
1:B:21:GLN:HE22	1:B:24:ARG:NH1	1.99	0.53
1:B:215[B]:CYS:SG	1:B:221:ARG:HD2	2.48	0.53
1:A:21:GLN:NE2	1:A:24:ARG:HH11	2.02	0.52
1:B:238:ARG:NH1	7:B:410:HOH:O	2.36	0.51
1:A:21:GLN:HE22	1:A:24:ARG:NH1	1.99	0.51
1:B:262:GLN:CD	1:B:262:GLN:CB	2.71	0.51
1:B:247:LYS:HB2	7:B:573:HOH:O	2.11	0.51
1:B:241:PRO:HG3	7:B:424:HOH:O	2.12	0.49
1:A:157:GLN:NE2	1:A:170:GLU:OE1	2.39	0.49
1:B:45:ARG:NH2	1:B:121[B]:CYS:HA	2.27	0.48
1:B:238:ARG:NH2	7:B:410:HOH:O	2.43	0.47
1:B:112:ARG:NH1	1:B:181:ASP:OD1	2.48	0.47
1:A:262:GLN:HB2	4:A:303:PGE:H2	1.98	0.46
1:B:197:LYS:NZ	1:B:200[B]:GLU:OE2	2.45	0.46
1:B:226[B]:CYS:SG	1:B:253[B]:MET:HE2	2.55	0.46
1:B:216[B]:SER:OG	1:B:217:ALA:N	2.44	0.44
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.53	0.44
1:B:10:ILE:HG23	1:B:15[B]:SER:HB2	2.00	0.42
1:B:48:ASP:OD1	1:B:48:ASP:N	2.51	0.42
1:A:216:SER:HB3	7:A:449:HOH:O	2.18	0.42
6:B:302:DMS:C1	7:B:508:HOH:O	2.64	0.41
1:A:76:GLU:O	1:A:237:LYS:HE3	2.20	0.41

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:423:HOH:O	7:A:541:HOH:O[5_554]	1.82	0.38
1:A:39:LYS:O	1:B:9[A]:GLN:NE2[4_545]	1.94	0.26
7:A:494:HOH:O	7:A:541:HOH:O[5_554]	2.00	0.20
7:A:516:HOH:O	7:B:573:HOH:O[4_545]	2.03	0.17
7:B:516:HOH:O	7:B:606:HOH:O[5_444]	2.14	0.06

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	283/298 (95%)	275 (97%)	6 (2%)	2 (1%)	22 7
1	B	298/298 (100%)	287 (96%)	9 (3%)	2 (1%)	22 7
All	All	581/596 (98%)	562 (97%)	15 (3%)	4 (1%)	22 7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	B	116	LYS
1	A	261	ILE
1	B	261	ILE

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	259/271 (96%)	253 (98%)	6 (2%)	50 24
1	B	273/271 (101%)	267 (98%)	6 (2%)	52 25
All	All	532/542 (98%)	520 (98%)	12 (2%)	50 24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	207	GLU
1	A	237	LYS
1	A	239	LYS
1	A	248	LYS
1	A	265	ASP
1	B	11	ASP
1	B	116	LYS

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Mol	Chain	Res	Type
1	B	118	SER
1	B	236	ASP
1	B	239	LYS
1	B	286	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	61	GLN
1	A	78	GLN
1	A	85	GLN
1	A	262	GLN
1	B	21	GLN
1	B	85	GLN
1	B	193	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ZD3	A	301	-	25,25,25	1.05	1 (4%)	31,37,37	2.27	6 (19%)
3	ZD5	A	302	-	25,25,25	0.99	1 (4%)	31,37,37	2.27	8 (25%)
4	PGE	A	303	-	9,9,9	0.50	0	8,8,8	0.81	0
6	DMS	B	302	-	3,3,3	0.51	0	3,3,3	1.40	1 (33%)

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	ZD3	A	301	-	-	2/12/34/34	0/3/3/3
3	ZD5	A	302	-	-	3/12/34/34	0/3/3/3
4	PGE	A	303	-	-	3/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ZD3	C7-N6	3.53	1.35	1.31
3	A	302	ZD5	C7-N6	2.82	1.34	1.31

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ZD3	C15-C7-N6	6.39	120.50	114.79
3	A	302	ZD5	C8-C7-N6	-6.35	121.54	125.50
3	A	302	ZD5	C15-C7-N6	6.10	120.24	114.79
2	A	301	ZD3	C8-C9-N10	-5.51	111.58	120.64
2	A	301	ZD3	C-CA-N	5.32	114.77	109.17
2	A	301	ZD3	C13-C9-N10	5.13	129.26	119.04
3	A	302	ZD5	C13-C9-N10	3.86	126.73	119.04
3	A	302	ZD5	F17-C15-C7	3.73	118.84	112.47
3	A	302	ZD5	F18-C15-C7	-3.60	106.32	112.47
3	A	302	ZD5	C8-C9-N10	-3.55	114.80	120.64
2	A	301	ZD3	C8-C7-N6	-3.55	123.28	125.50
2	A	301	ZD3	C8-C7-C15	-3.08	116.21	120.10
3	A	302	ZD5	C11-N10-C9	2.83	124.69	116.46
3	A	302	ZD5	CB-CA-C	-2.28	107.18	111.76
6	B	302	DMS	O-S-C1	2.26	118.06	106.54

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ZD3	O-C-CA-CB
2	A	301	ZD3	O-C-CA-N
3	A	302	ZD5	C13-C9-N10-CB
4	A	303	PGE	O3-C5-C6-O4
3	A	302	ZD5	C8-C9-N10-CB
3	A	302	ZD5	O-C-CA-CB
4	A	303	PGE	C1-C2-O2-C3
4	A	303	PGE	O2-C3-C4-O3

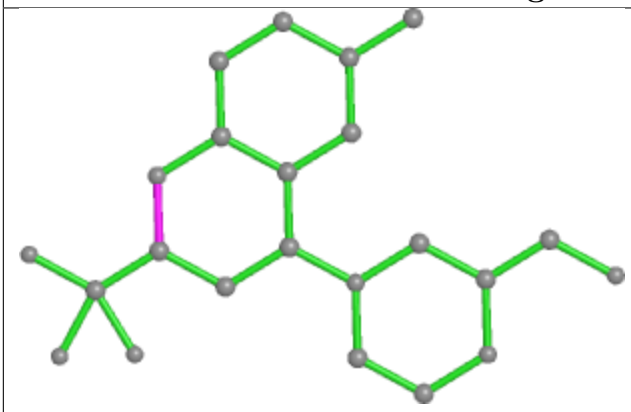
There are no ring outliers.

2 monomers are involved in 3 short contacts:

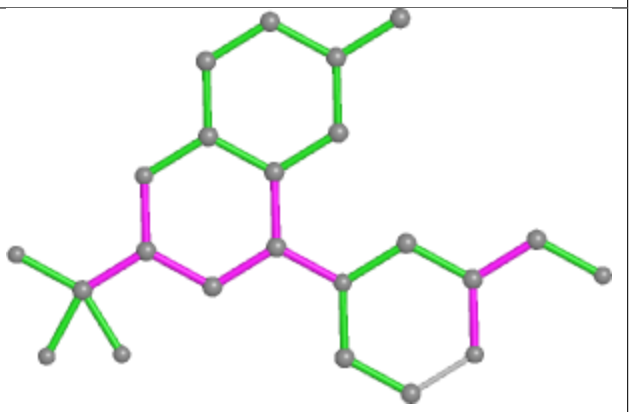
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	PGE	1	0
6	B	302	DMS	2	0

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.

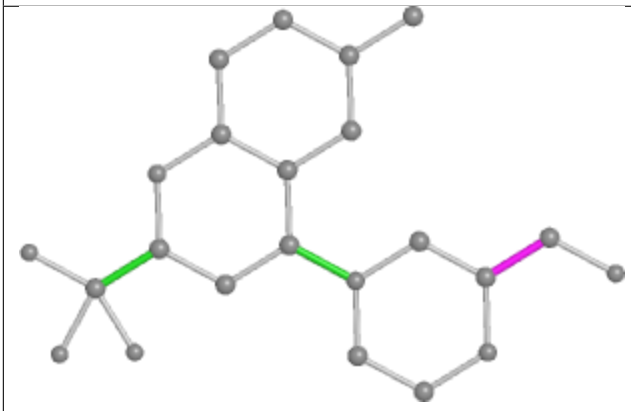
Ligand ZD3 A 301



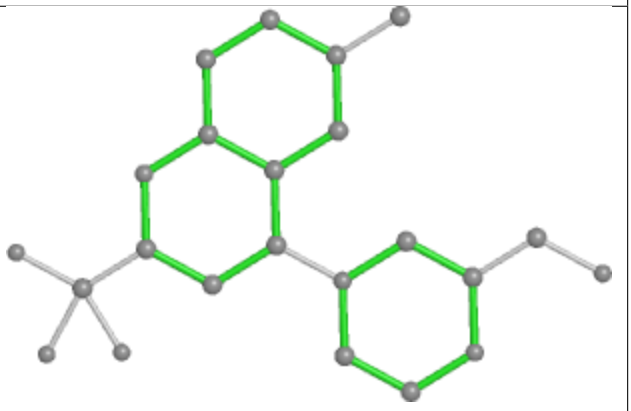
Bond lengths



Bond angles

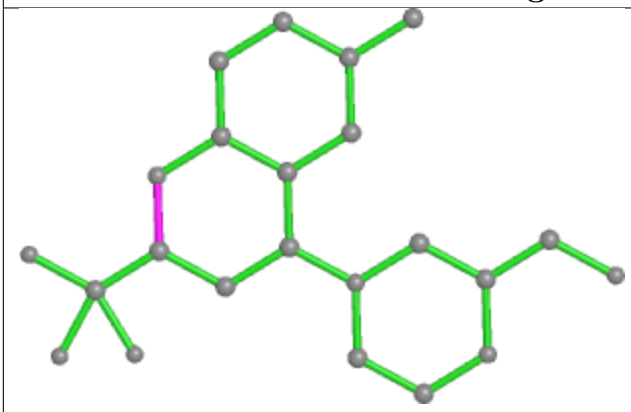


Torsions

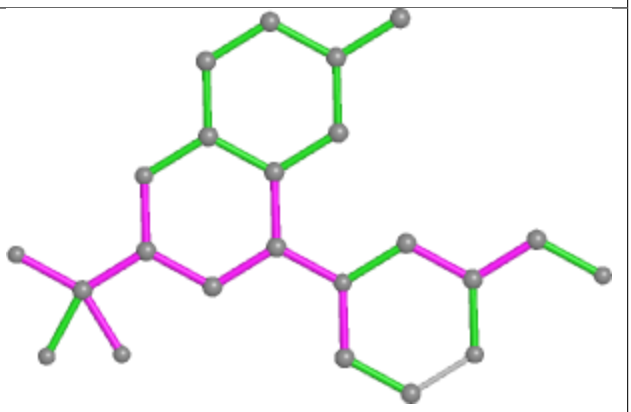


Rings

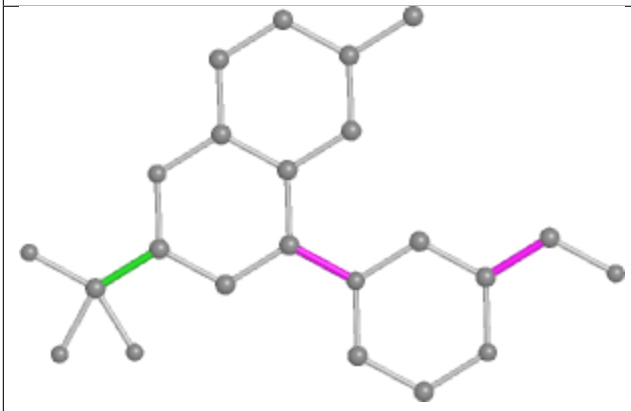
Ligand ZD5 A 302



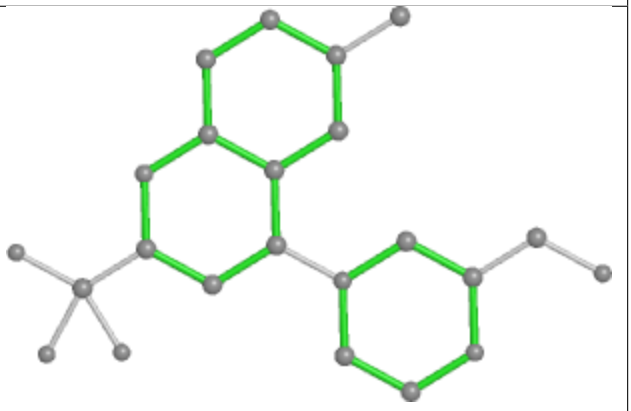
Bond lengths



Bond angles



Torsions



Rings

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	281/298 (94%)	0.25	23 (8%)	11	9	20, 32, 56, 90	0
1	B	287/298 (96%)	0.10	17 (5%)	22	19	16, 25, 52, 77	0
All	All	568/596 (95%)	0.18	40 (7%)	16	14	16, 29, 55, 90	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	LYS	8.9
1	A	62	GLU	4.4
1	B	239	LYS	4.2
1	A	117	GLY	4.2
1	A	63	ASP	4.0
1	A	83	LEU	3.8
1	A	240	ASP	3.8
1	A	213	VAL	3.6
1	B	237	LYS	3.5
1	A	196	PHE	3.4
1	B	285	SER	3.4
1	B	62	GLU	3.3
1	A	182	PHE	2.9
1	A	241	PRO	2.9
1	B	166	GLN	2.9
1	B	119	LEU	2.8
1	A	61	GLN	2.8
1	A	243	SER	2.7
1	A	152	TYR	2.7
1	A	118	SER	2.7
1	B	243	SER	2.7
1	B	47	ARG	2.6
1	A	1	MET	2.6
1	B	286	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	VAL	2.5
1	A	108	VAL	2.5
1	B	240	ASP	2.4
1	B	46	TYR	2.4
1	A	25[A]	HIS	2.4
1	B	63	ASP	2.4
1	A	72	ILE	2.3
1	B	241	PRO	2.3
1	A	110	LEU	2.3
1	A	280	PHE	2.3
1	B	25[A]	HIS	2.2
1	B	108	VAL	2.2
1	B	164	THR	2.1
1	A	84	THR	2.1
1	A	47	ARG	2.0
1	B	48	ASP	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, 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.

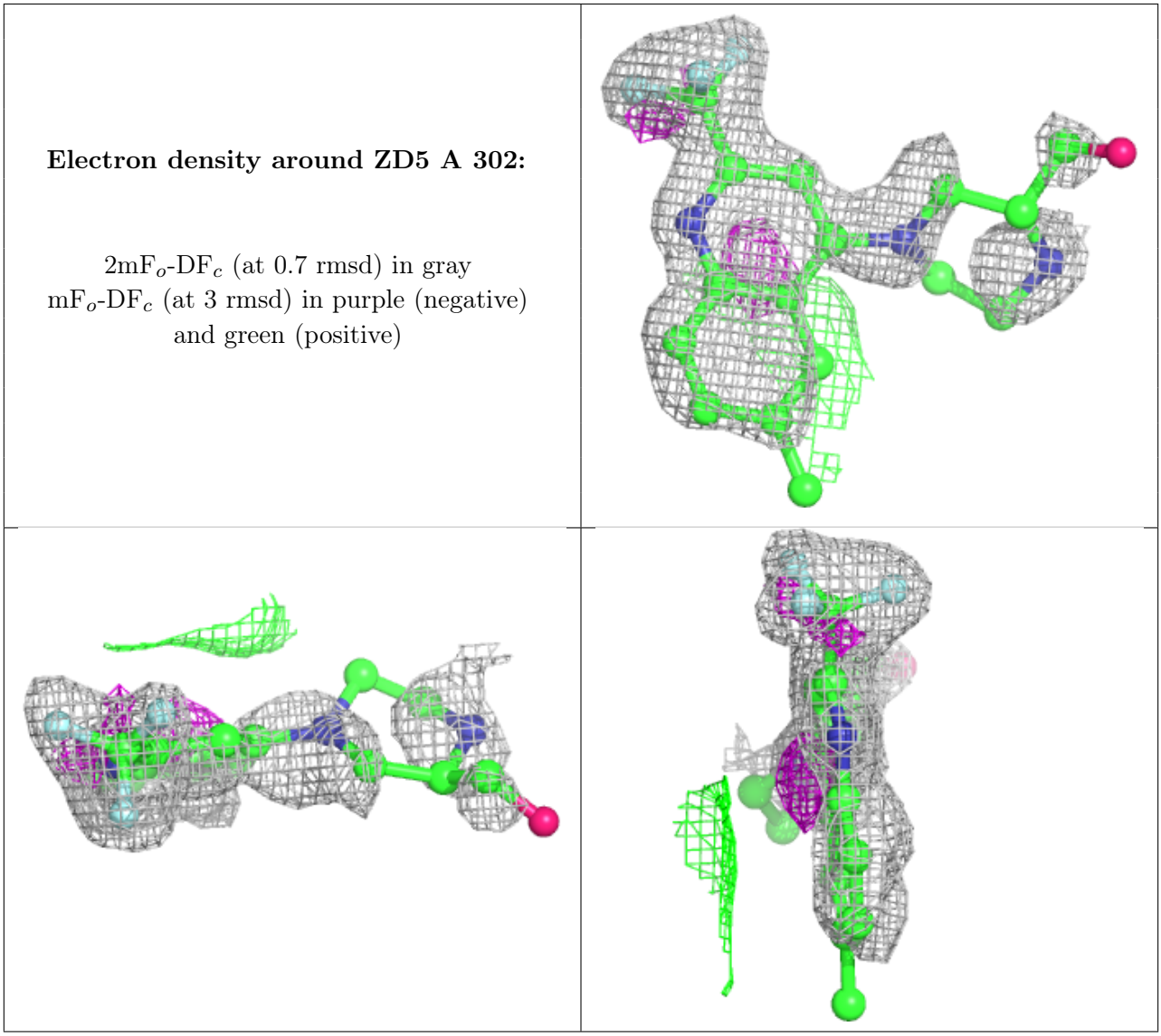
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGE	A	303	10/10	0.60	0.17	48,54,63,63	0
3	ZD5	A	302	23/23	0.77	0.35	46,86,100,104	0
2	ZD3	A	301	23/23	0.79	0.22	47,61,69,71	0
5	MG	B	301	1/1	0.91	0.13	52,52,52,52	0
6	DMS	B	302	4/4	0.97	0.38	40,45,49,52	0

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.

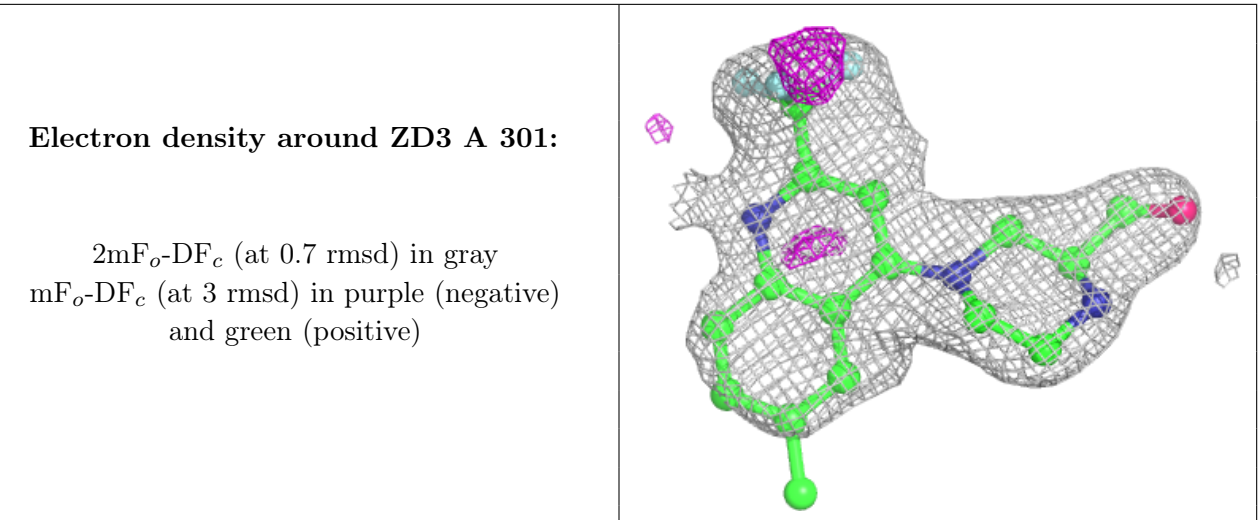
Electron density around ZD5 A 302:

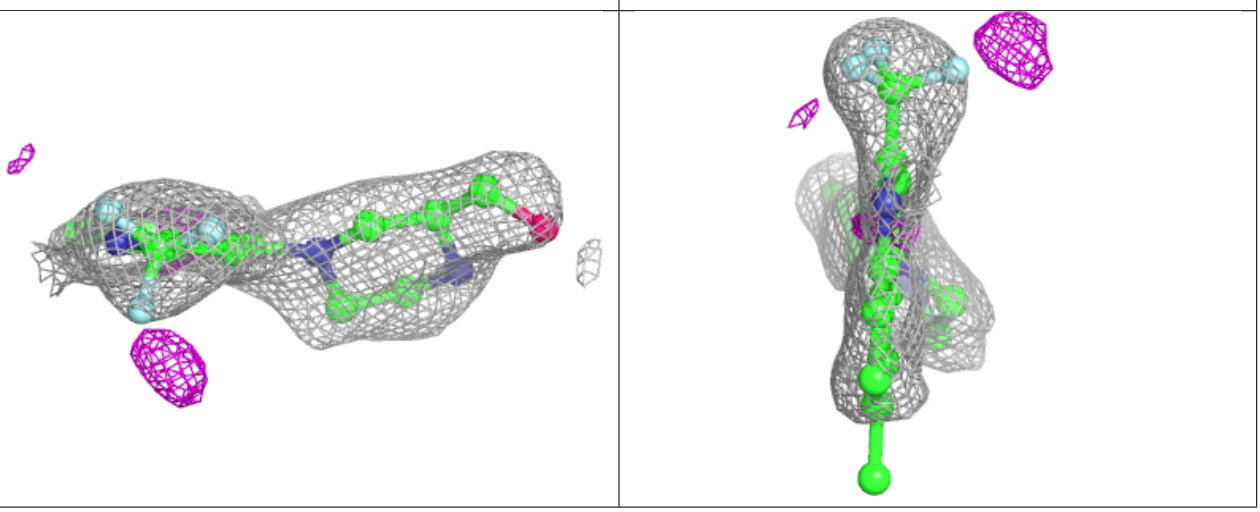
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZD3 A 301:

$2mF_o$-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.