



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:01 AM UTC

PDB ID : 8G6A / pdb_00008g6a
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 : 4-5-2 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

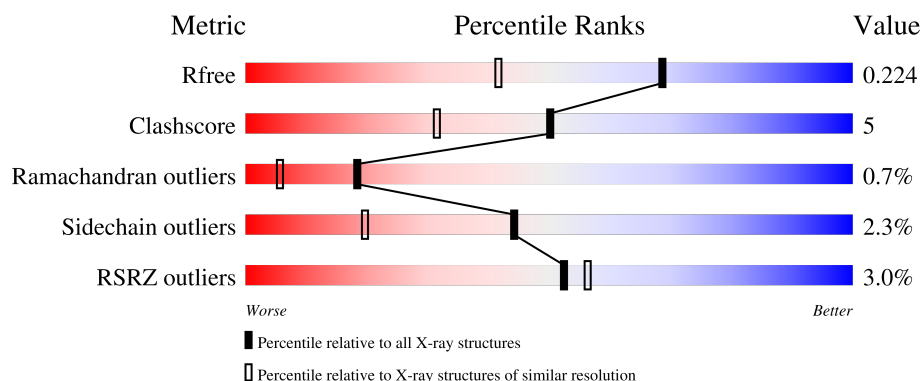
1 Overall quality at a glance

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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (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 $\leq 5\%$. 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	298	
1	B	298	

2 Entry composition [i](#)

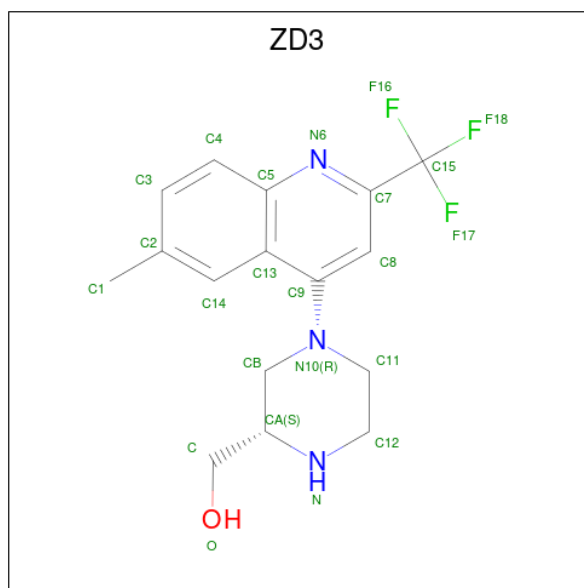
There are 7 unique types of molecules in this entry. The entry contains 5136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

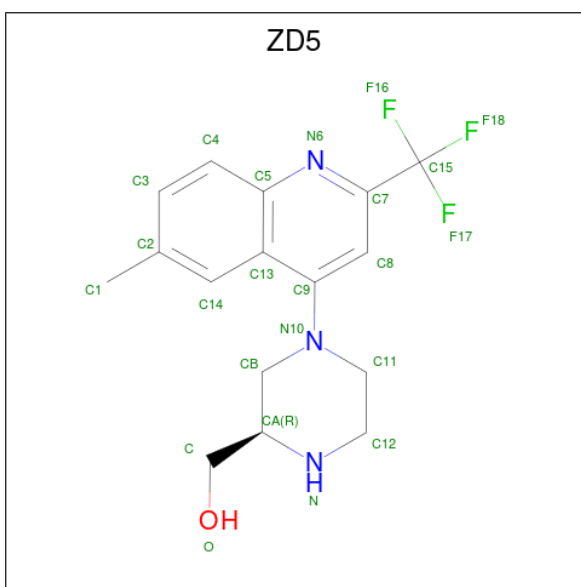
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	4	0
			2318	1473	398	430	17			
1	B	287	Total	C	N	O	S	0	13	0
			2392	1523	405	442	22			

- Molecule 2 is {(2S)-4-[6-methyl-2-(trifluoromethyl)quinolin-4-yl]piperazin-2-yl}methanol (CCD ID: ZD3) (formula: C₁₆H₁₈F₃N₃O) (labeled as "Ligand of Interest" by depositor).



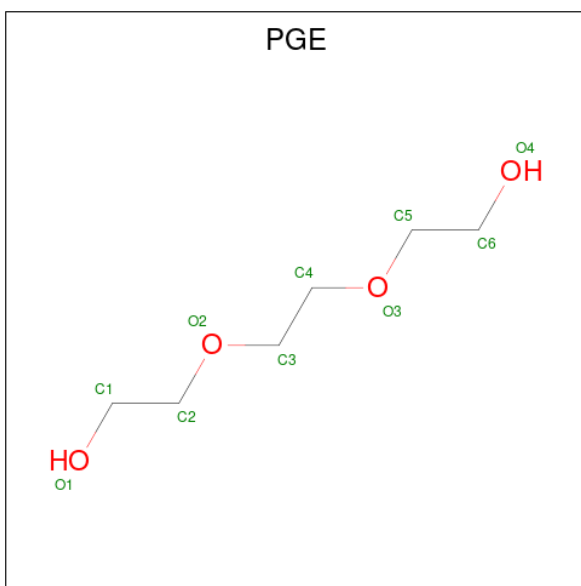
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	16	3	3	1		

- Molecule 3 is {(2R)-4-[6-methyl-2-(trifluoromethyl)quinolin-4-yl]piperazin-2-yl}methanol (CCD ID: ZD5) (formula: C₁₆H₁₈F₃N₃O).



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 (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

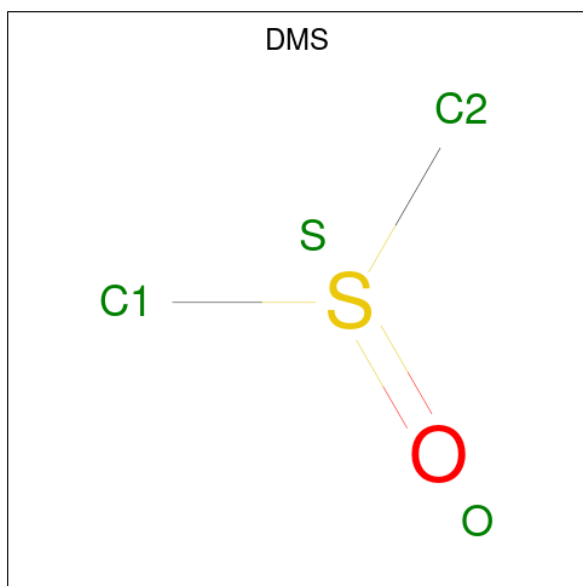


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

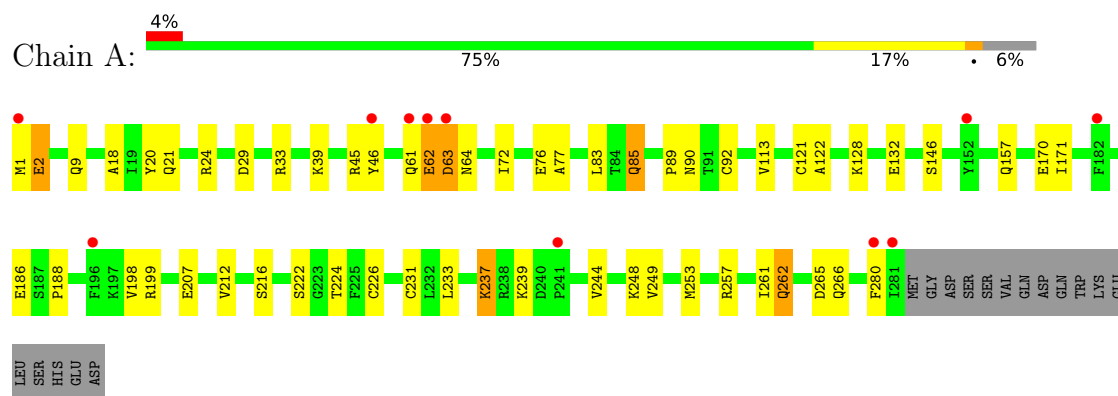
- Molecule 7 is water.

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

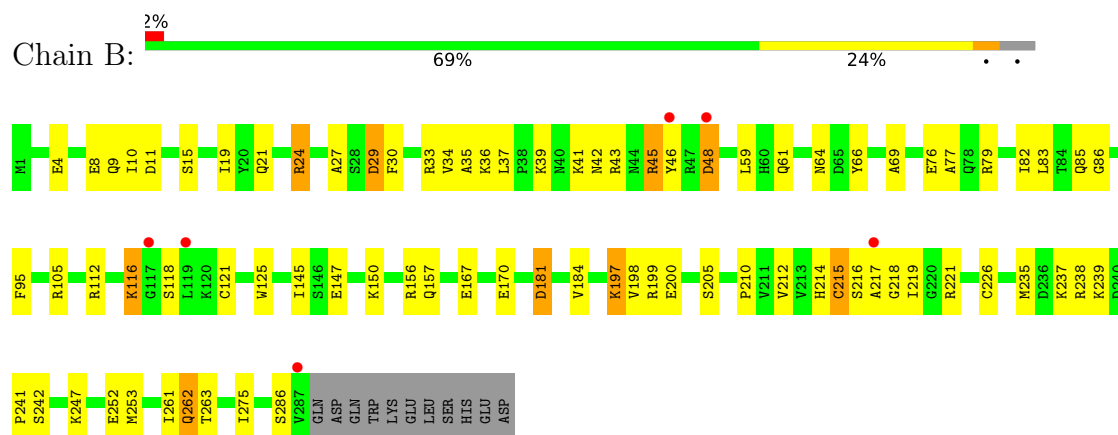
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

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 31.95 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.95-1.62) 99.9 (31.95-1.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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: ZD3, MG, PGE, ZD5, DMS

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	1.77	29/2383 (1.2%)	1.43	11/3211 (0.3%)
1	B	1.94	46/2484 (1.9%)	1.55	18/3345 (0.5%)
All	All	1.86	75/4867 (1.5%)	1.49	29/6556 (0.4%)

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	GLN	CG-CD	9.72	1.76	1.52
1	A	171	ILE	C-O	8.35	1.33	1.24
1	B	197	LYS	CA-CB	-8.01	1.40	1.53
1	B	19	ILE	CA-C	-7.93	1.43	1.52
1	A	257	ARG	CA-C	-7.78	1.42	1.52
1	A	18	ALA	N-CA	7.54	1.55	1.46
1	A	231	CYS	N-CA	7.50	1.55	1.46
1	B	212	VAL	N-CA	-7.24	1.37	1.46
1	A	2	GLU	C-O	6.99	1.32	1.23
1	B	95	PHE	N-CA	6.86	1.54	1.46
1	A	146	SER	C-O	6.76	1.31	1.23
1	A	46	TYR	N-CA	6.64	1.54	1.46
1	A	262	GLN	CD-OE1	6.47	1.35	1.23
1	B	61	GLN	CD-NE2	6.46	1.46	1.33
1	B	214	HIS	N-CA	-6.37	1.37	1.45
1	A	122	ALA	CA-C	6.34	1.61	1.53
1	A	253	MET	C-O	6.31	1.31	1.24
1	B	125	TRP	N-CA	6.29	1.50	1.45
1	A	199	ARG	N-CA	-6.29	1.39	1.46
1	B	48	ASP	N-CA	6.29	1.53	1.46
1	B	37	LEU	C-O	-6.24	1.16	1.23
1	B	76	GLU	C-O	-6.23	1.17	1.24
1	B	170	GLU	CA-CB	-6.22	1.44	1.53
1	A	249	VAL	CA-C	-6.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GLU	N-CA	-5.99	1.39	1.46
1	B	46	TYR	N-CA	5.95	1.53	1.46
1	B	39	LYS	CA-C	-5.93	1.44	1.52
1	B	199	ARG	C-N	-5.90	1.26	1.33
1	A	188	PRO	N-CA	-5.82	1.41	1.47
1	B	82	ILE	CA-CB	-5.81	1.47	1.54
1	A	61	GLN	CA-C	5.80	1.60	1.52
1	B	147	GLU	C-O	5.78	1.30	1.23
1	B	157	GLN	CD-OE1	5.75	1.34	1.23
1	A	212	VAL	N-CA	-5.73	1.39	1.46
1	B	252	GLU	CD-OE2	5.70	1.36	1.25
1	A	9	GLN	CD-NE2	5.70	1.45	1.33
1	B	184	VAL	CA-C	-5.67	1.47	1.52
1	A	89	PRO	C-O	-5.57	1.16	1.24
1	A	244	VAL	N-CA	5.56	1.52	1.46
1	A	212	VAL	CA-C	-5.56	1.45	1.52
1	B	64	ASN	N-CA	5.54	1.53	1.46
1	B	219	ILE	CA-CB	5.54	1.61	1.54
1	A	128	LYS	CA-C	-5.54	1.45	1.52
1	B	35	ALA	C-O	5.54	1.30	1.24
1	A	90	ASN	C-O	5.50	1.31	1.23
1	A	132	GLU	C-O	5.48	1.31	1.23
1	A	72	ILE	C-O	-5.45	1.18	1.24
1	A	92	CYS	C-N	5.44	1.40	1.33
1	B	215[A]	CYS	C-N	-5.43	1.26	1.33
1	B	215[B]	CYS	C-N	-5.43	1.26	1.33
1	A	198	VAL	CA-CB	5.41	1.60	1.54
1	B	210	PRO	C-N	-5.36	1.27	1.33
1	B	218	GLY	N-CA	5.32	1.52	1.45
1	A	85	GLN	CD-OE1	5.31	1.33	1.23
1	B	198	VAL	CA-CB	5.29	1.61	1.54
1	B	156	ARG	CD-NE	5.29	1.53	1.46
1	B	181	ASP	C-O	5.29	1.30	1.24
1	B	263	THR	C-O	5.28	1.30	1.23
1	A	77	ALA	C-O	-5.27	1.17	1.24
1	B	46	TYR	CA-C	5.26	1.58	1.52
1	B	184	VAL	N-CA	5.17	1.52	1.46
1	B	24	ARG	N-CA	-5.17	1.40	1.46
1	B	41	LYS	C-O	-5.17	1.18	1.24
1	B	29	ASP	CA-CB	-5.16	1.45	1.53
1	A	224	THR	N-CA	5.15	1.52	1.46
1	B	77	ALA	CA-C	-5.15	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	LYS	CA-CB	-5.14	1.46	1.53
1	B	286	SER	CA-C	5.10	1.59	1.52
1	B	69	ALA	CA-C	-5.10	1.46	1.52
1	B	59	LEU	CA-C	5.09	1.59	1.52
1	B	262	GLN	CD-NE2	5.07	1.43	1.33
1	B	145	ILE	CA-C	5.06	1.59	1.52
1	B	45	ARG	C-O	5.04	1.30	1.24
1	B	27	ALA	C-O	-5.02	1.17	1.23
1	A	222	SER	CA-CB	5.00	1.61	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLN	CB-CA-C	8.73	123.86	109.89
1	B	235	MET	CG-SD-CE	-8.47	82.26	100.90
1	A	62	GLU	N-CA-C	-7.89	99.90	110.55
1	B	79	ARG	NE-CZ-NH2	7.72	126.15	119.20
1	B	262	GLN	CA-CB-CG	7.14	128.39	114.10
1	A	2	GLU	CA-C-O	6.63	128.60	121.44
1	B	205	SER	CB-CA-C	6.35	118.64	109.11
1	B	147	GLU	N-CA-CB	-6.06	100.62	110.81
1	B	105	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	B	33	ARG	CA-C-O	-5.95	114.24	120.55
1	B	33	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	A	33	ARG	CG-CD-NE	-5.78	99.27	112.00
1	B	34	VAL	N-CA-C	-5.61	105.06	110.72
1	B	36	LYS	CG-CD-CE	5.48	123.90	111.30
1	A	233	LEU	CB-CA-C	-5.47	102.26	110.90
1	B	61	GLN	CB-CG-CD	-5.42	103.39	112.60
1	B	86	GLY	O-C-N	-5.42	116.35	121.77
1	A	266	GLN	CA-C-O	5.34	126.22	120.55
1	A	64	ASN	N-CA-C	-5.32	98.98	108.13
1	B	8	GLU	CA-CB-CG	-5.30	103.50	114.10
1	A	280	PHE	N-CA-C	5.19	117.02	111.36
1	A	9	GLN	O-C-N	5.17	127.60	122.12
1	B	147	GLU	CA-C-O	-5.16	113.93	120.28
1	B	29	ASP	CA-CB-CG	-5.16	107.44	112.60
1	A	231	CYS	N-CA-C	-5.11	105.71	111.28
1	A	262	GLN	CA-CB-CG	-5.08	103.94	114.10
1	B	275	ILE	N-CA-C	5.07	115.29	110.42
1	B	30	PHE	CA-C-N	-5.04	115.04	120.03
1	B	30	PHE	C-N-CA	-5.04	115.04	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2318	0	2300	19	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	3	0
7	A	153	0	0	3	3
7	B	212	0	0	14	2
All	All	5136	0	4722	50	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 (50) 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	1.57
1:B:215[B]:CYS:SG	7:B:544:HOH:O	2.03	1.17
1:B:43:ARG:HD3	7:B:404:HOH:O	1.43	1.16
1:B:226[B]:CYS:SG	1:B:253[B]:MET:HE1	1.91	1.11
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:262:GLN:CD	1:B:262:GLN:CB	2.71	0.62
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
6:B:302:DMS:H13	7:B:508:HOH:O	2.04	0.56
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
1:B:197:LYS:HZ2	1:B:200[B]:GLU:CD	2.15	0.54
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: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:B:42:ASN:ND2	6:B:302:DMS:H12	2.28	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:A:186[B]:GLU:H	1:A:186[B]:GLU:CD	2.25	0.45
6:B:302:DMS:C1	7:B:508:HOH:O	2.64	0.44
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	6
1	B	298/298 (100%)	287 (96%)	9 (3%)	2 (1%)	18	6
All	All	581/596 (98%)	562 (97%)	15 (3%)	4 (1%)	18	6

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%)	252 (97%)	7 (3%)	39	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	273/271 (101%)	268 (98%)	5 (2%)	51	28
All	All	532/542 (98%)	520 (98%)	12 (2%)	44	20

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
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
1	B	118	SER
1	B	237	LYS
1	B	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	111	ASN
1	B	21	GLN
1	B	42	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	PGE	A	303	-	9,9,9	0.50	0	8,8,8	0.80	0
3	ZD5	A	302	-	25,25,25	0.89	0	31,37,37	2.39	9 (29%)
2	ZD3	A	301	-	25,25,25	0.89	1 (4%)	31,37,37	2.16	6 (19%)
6	DMS	B	302	-	3,3,3	0.53	0	3,3,3	1.44	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
4	PGE	A	303	-	-	2/7/7/7	-
3	ZD5	A	302	-	-	3/12/34/34	0/3/3/3
2	ZD3	A	301	-	-	2/12/34/34	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ZD3	C7-N6	2.12	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	ZD5	CA-CB-N10	8.51	116.89	110.19
2	A	301	ZD3	CA-CB-N10	5.81	114.76	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ZD3	C-CA-N	5.32	114.77	109.17
2	A	301	ZD3	C8-C9-N10	-5.10	111.58	120.67
2	A	301	ZD3	C13-C9-N10	4.21	129.26	119.20
2	A	301	ZD3	C15-C7-N6	3.79	120.50	114.79
3	A	302	ZD5	F17-C15-C7	3.64	118.84	112.43
3	A	302	ZD5	C15-C7-N6	3.62	120.24	114.79
3	A	302	ZD5	C8-C7-N6	-3.58	121.54	125.47
3	A	302	ZD5	F18-C15-C7	-3.47	106.32	112.43
3	A	302	ZD5	C8-C9-N10	-3.30	114.80	120.67
3	A	302	ZD5	CB-CA-N	3.28	116.31	110.85
3	A	302	ZD5	C13-C9-N10	3.15	126.73	119.20
3	A	302	ZD5	C11-N10-C9	2.84	124.69	116.32
2	A	301	ZD3	C8-C7-C15	-2.55	116.21	120.09
6	B	302	DMS	O-S-C1	2.31	118.06	106.49

There are no chirality outliers.

All (7) 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
4	A	303	PGE	O3-C5-C6-O4
3	A	302	ZD5	C13-C9-N10-CB
3	A	302	ZD5	O-C-CA-CB
3	A	302	ZD5	C8-C9-N10-CB
4	A	303	PGE	C1-C2-O2-C3

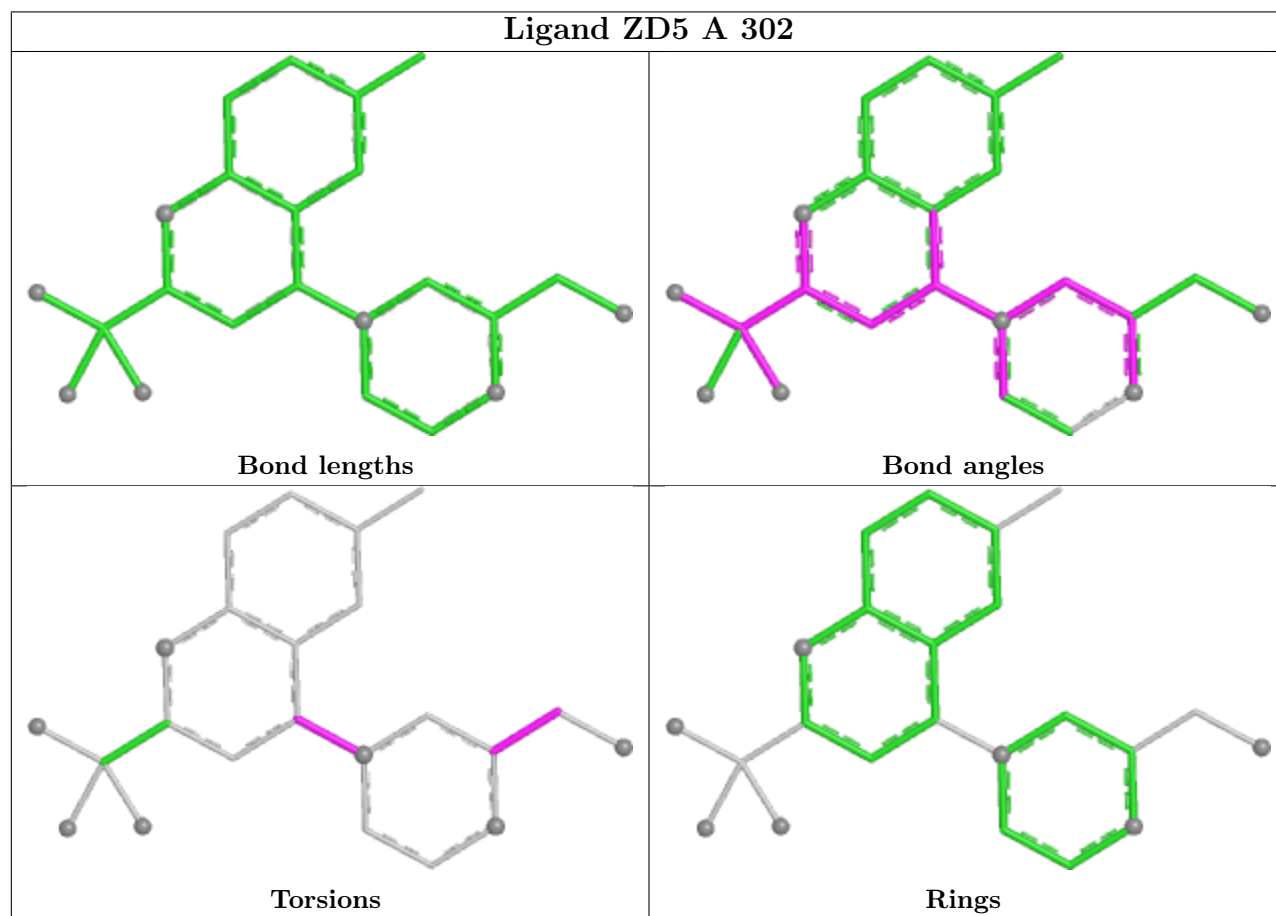
There are no ring outliers.

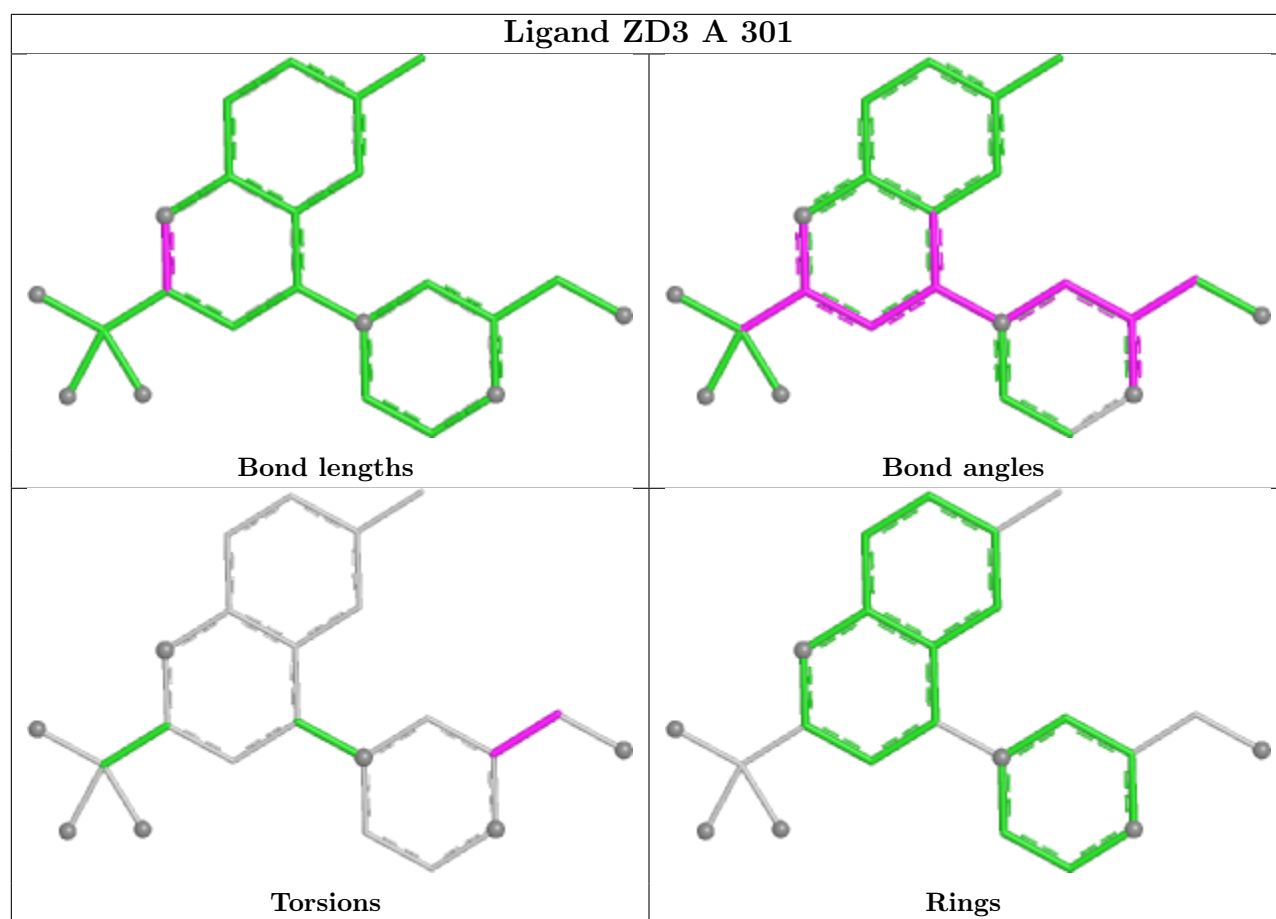
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	PGE	1	0
6	B	302	DMS	3	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 [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	281/298 (94%)	0.23	11 (3%) 43 47	19, 32, 56, 90	4 (1%)
1	B	287/298 (96%)	-0.03	6 (2%) 63 68	12, 25, 52, 77	13 (4%)
All	All	568/596 (95%)	0.10	17 (2%) 52 56	12, 28, 55, 90	17 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ALA	4.0
1	A	281	ILE	3.5
1	B	46	TYR	3.3
1	A	63	ASP	3.1
1	A	1	MET	2.9
1	A	196	PHE	2.8
1	A	182	PHE	2.7
1	B	119	LEU	2.6
1	A	241	PRO	2.6
1	A	280	PHE	2.5
1	B	287	VAL	2.5
1	A	46	TYR	2.4
1	B	117	GLY	2.4
1	B	48	ASP	2.3
1	A	62	GLU	2.1
1	A	61	GLN	2.0
1	A	152	TYR	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](#)

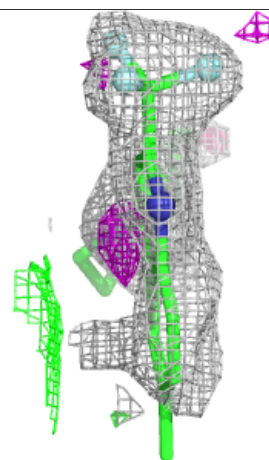
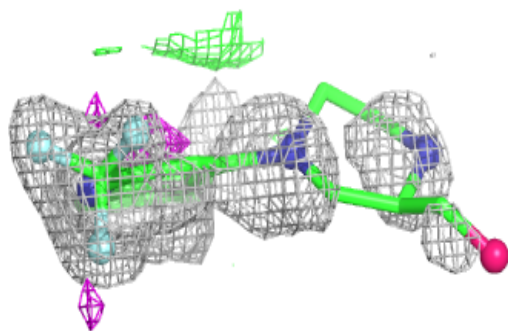
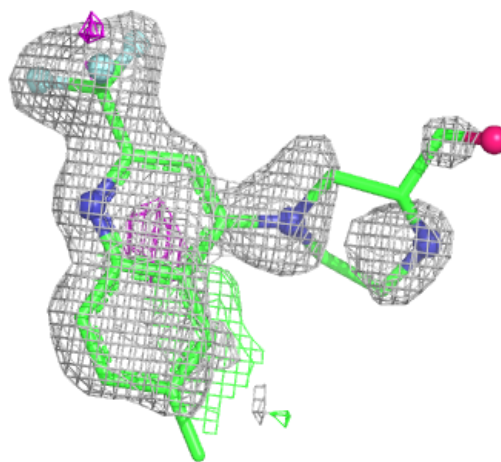
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZD5	A	302	23/23	0.76	0.17	46,86,100,104	0
2	ZD3	A	301	23/23	0.78	0.15	47,61,69,71	0
4	PGE	A	303	10/10	0.78	0.15	48,54,63,63	0
6	DMS	B	302	4/4	0.87	0.18	40,45,49,52	0
5	MG	B	301	1/1	0.92	0.09	52,52,52,52	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.

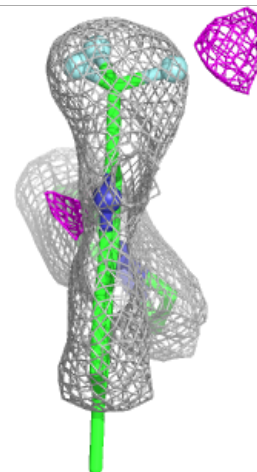
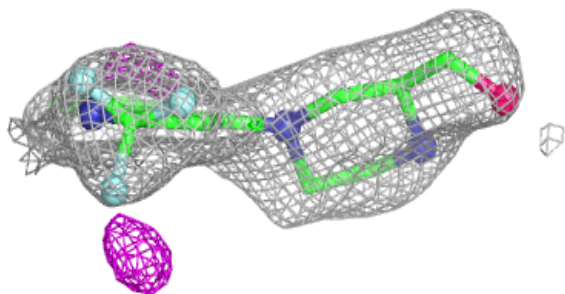
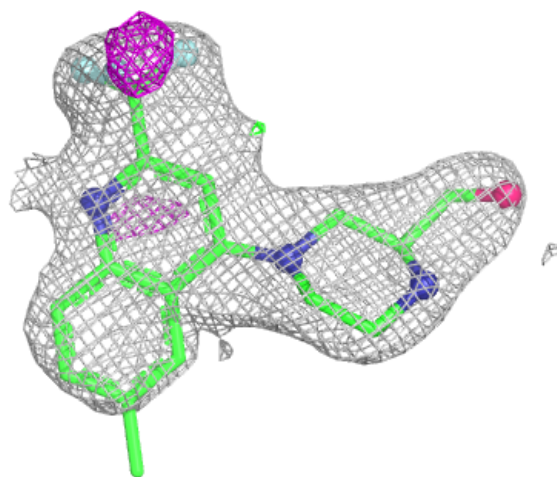
Electron density around ZD5 A 302:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.