



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 1Q6T / pdb_00001q6t
Title : THE STRUCTURE OF PHOSPHOTYROSINE PHOSPHATASE 1B IN
COMPLEX WITH COMPOUND 11
Authors : Scapin, G.; Patel, S.B.; Becker, J.W.; Wang, Q.; Desponts, C.; Waddleton,
D.; Skorey, K.; Cromlish, W.; Bayly, C.; Therien, M.; Gauthier, J.Y.; Li, C.S.;
Lau, C.K.; Ramachandran, C.; Kennedy, B.P.; Asante-Appiah, E.
Deposited on : 2003-08-13
Resolution : 2.30 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](#) ①) 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

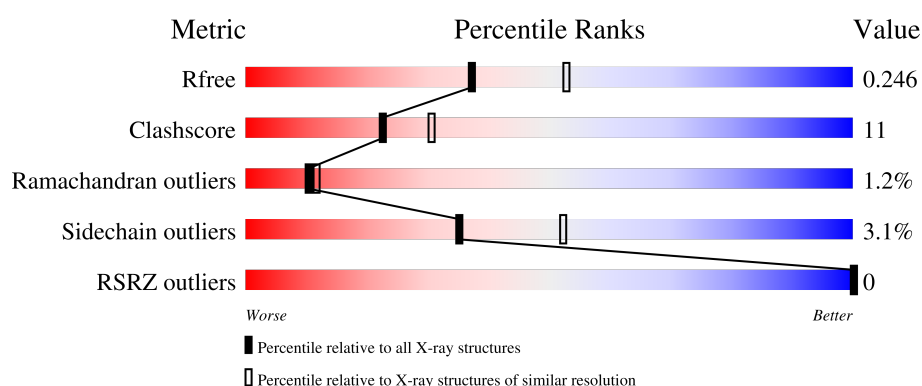
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	310	
1	B	310	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5018 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 Protein-tyrosine phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2349	1490	404	439	16			
1	B	289	Total	C	N	O	S	0	0	0
			2346	1488	404	439	15			

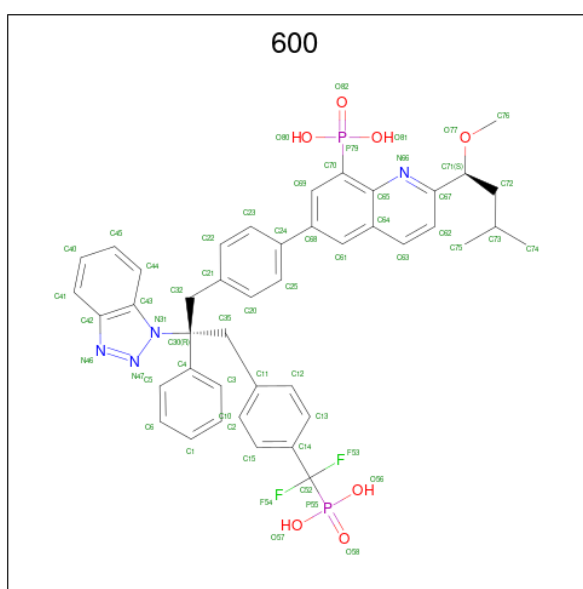
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	MET	-	cloning artifact	UNP P18031
A	490	ASP	-	cloning artifact	UNP P18031
A	491	TYR	-	cloning artifact	UNP P18031
A	492	LYS	-	cloning artifact	UNP P18031
A	493	ASP	-	cloning artifact	UNP P18031
A	494	ASP	-	cloning artifact	UNP P18031
A	495	ASP	-	cloning artifact	UNP P18031
A	496	ASP	-	cloning artifact	UNP P18031
A	497	LYS	-	cloning artifact	UNP P18031
A	498	LEU	-	cloning artifact	UNP P18031
A	499	GLU	-	cloning artifact	UNP P18031
A	500	PHE	-	cloning artifact	UNP P18031
B	989	MET	-	cloning artifact	UNP P18031
B	990	ASP	-	cloning artifact	UNP P18031
B	991	TYR	-	cloning artifact	UNP P18031
B	992	LYS	-	cloning artifact	UNP P18031
B	993	ASP	-	cloning artifact	UNP P18031
B	994	ASP	-	cloning artifact	UNP P18031
B	995	ASP	-	cloning artifact	UNP P18031
B	996	ASP	-	cloning artifact	UNP P18031
B	997	LYS	-	cloning artifact	UNP P18031
B	998	LEU	-	cloning artifact	UNP P18031
B	999	GLU	-	cloning artifact	UNP P18031
B	1000	PHE	-	cloning artifact	UNP P18031

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

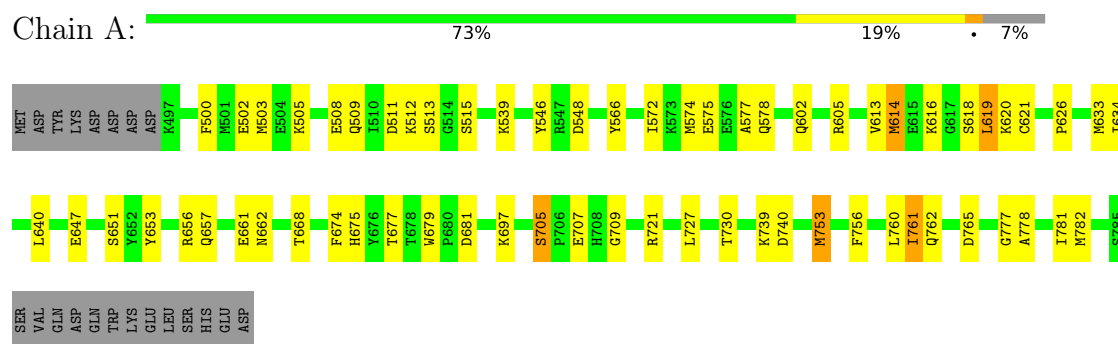
- Molecule 3 is 6-[4-((2S)-2-(1H-1,2,3-BENZOTRIAZOL-1-YL)-3-{4-[DIFLUORO(PHOSPHONO)METHYL]PHENYL}-2-PHENYLPROPYL)PHENYL]-2-[(1S)-1-METHOXY-3-METHYLBUTYL]QUINOLIN-8-YLPHOSPHONIC ACID (CCD ID: 600) (formula: C₄₃H₄₂F₂N₄O₇P₂).



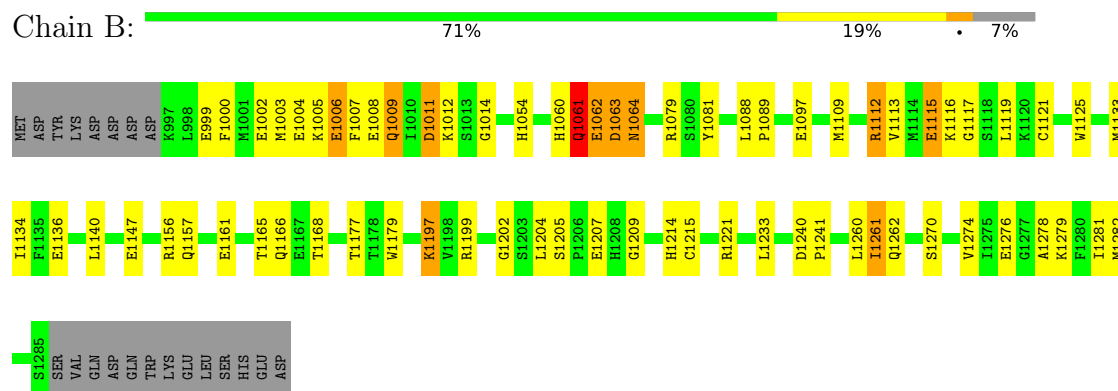
3 Residue-property plots

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: Protein-tyrosine phosphatase, non-receptor type 1



- Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.03Å 87.83Å 138.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.30 12.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (12.00-2.30) 97.4 (12.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.96Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.214 , 0.246 0.215 , 0.246	Depositor DCC
R_{free} test set	3519 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.063 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 600

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	0.57	0/2402	0.91	6/3237 (0.2%)
1	B	0.65	3/2399 (0.1%)	1.06	13/3234 (0.4%)
All	All	0.61	3/4801 (0.1%)	0.99	19/6471 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1119	LEU	C-N	-9.17	1.20	1.33
1	B	1062	GLU	CA-C	-5.23	1.46	1.53
1	B	1064	ASN	N-CA	5.08	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1063	ASP	CA-CB-CG	-21.96	90.64	112.60
1	B	1061	GLN	OE1-CD-NE2	-9.93	112.67	122.60
1	A	762	GLN	N-CA-C	7.79	122.98	113.17
1	B	1262	GLN	N-CA-C	7.40	122.31	113.28
1	A	705	SER	CA-C-N	7.16	126.80	119.56
1	A	705	SER	C-N-CA	7.16	126.80	119.56
1	B	1061	GLN	CG-CD-NE2	7.14	127.11	116.40
1	A	566	TYR	N-CA-C	7.04	121.78	109.96
1	B	1054	HIS	N-CA-C	6.36	119.03	111.71
1	B	1209	GLY	N-CA-C	-6.01	104.79	112.00
1	A	651	SER	N-CA-C	5.74	117.21	111.07
1	B	1240	ASP	CA-C-N	5.51	125.60	119.32
1	B	1240	ASP	C-N-CA	5.51	125.60	119.32
1	B	1215	CYS	N-CA-C	-5.43	99.23	110.80
1	A	677	THR	N-CA-C	5.37	119.93	113.17
1	B	1063	ASP	N-CA-C	5.26	122.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1177	THR	N-CA-C	5.08	119.48	113.28
1	B	1125	TRP	CA-C-N	5.01	124.77	119.76
1	B	1125	TRP	C-N-CA	5.01	124.77	119.76

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	2349	0	2306	50	0
1	B	2346	0	2299	55	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	58	0	37	2	0
3	B	58	0	37	0	0
4	A	97	0	0	2	0
4	B	108	0	0	2	0
All	All	5018	0	4679	100	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 11.

All (100) 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:1161:GLU:HG3	1:B:1168:THR:HG22	1.56	0.88
1:A:500:PHE:HA	1:A:503:MET:HE3	1.63	0.79
1:B:1002:GLU:HG3	1:B:1005:LYS:HE2	1.64	0.78
1:B:1112:ARG:HB2	1:B:1112:ARG:NH1	2.00	0.76
1:B:1011:ASP:O	1:B:1012:LYS:HG3	1.85	0.76
1:A:619:LEU:HD12	1:A:619:LEU:H	1.52	0.74
1:B:1000:PHE:HA	1:B:1003:MET:HE3	1.69	0.74
1:A:674:PHE:HE2	1:A:697:LYS:HD2	1.57	0.69
1:B:1000:PHE:HE2	1:B:1278:ALA:HB1	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:GLU:HG2	1:B:1003:MET:HE2	1.75	0.69
1:B:1064:ASN:OD1	1:B:1064:ASN:C	2.34	0.69
1:A:513:SER:HB2	1:B:1117:GLY:H	1.58	0.67
1:A:508:GLU:O	1:A:512:LYS:HG3	1.95	0.67
1:A:508:GLU:HB3	1:A:512:LYS:NZ	2.09	0.67
1:A:513:SER:HB2	1:B:1117:GLY:N	2.10	0.67
1:A:626:PRO:HG3	1:A:633:MET:HG3	1.77	0.66
1:A:502:GLU:HG3	1:A:505:LYS:HZ2	1.62	0.65
1:A:605:ARG:HH11	1:A:605:ARG:HG2	1.64	0.63
1:B:1270:SER:O	1:B:1274:VAL:HG23	1.99	0.62
1:A:778:ALA:HA	1:A:781:ILE:HG22	1.82	0.62
1:A:502:GLU:HG3	1:A:505:LYS:NZ	2.16	0.61
1:A:613:VAL:HG13	1:A:621:CYS:O	2.00	0.60
1:B:1003:MET:O	1:B:1006:GLU:HG3	2.01	0.60
1:B:1002:GLU:O	1:B:1005:LYS:HG2	2.00	0.60
1:B:1113:VAL:HA	1:B:1121:CYS:HB3	1.84	0.60
1:B:1063:ASP:OD1	1:B:1063:ASP:C	2.44	0.59
1:B:1079:ARG:CZ	1:B:1233:LEU:HD11	2.33	0.59
1:A:502:GLU:HA	1:A:505:LYS:HG2	1.85	0.59
1:A:727:LEU:HA	1:A:753:MET:HE1	1.85	0.59
1:B:1112:ARG:HB2	1:B:1112:ARG:HH11	1.66	0.58
1:A:508:GLU:HB3	1:A:512:LYS:HZ3	1.70	0.56
1:A:619:LEU:H	1:A:619:LEU:CD1	2.16	0.56
1:B:1161:GLU:CG	1:B:1168:THR:HG22	2.34	0.56
1:B:1205:SER:OG	1:B:1207:GLU:HG2	2.06	0.55
1:A:705:SER:OG	1:A:707:GLU:HG2	2.07	0.55
1:B:1062:GLU:HA	1:B:1062:GLU:OE1	2.06	0.54
1:B:1281:ILE:HG13	1:B:1282:MET:SD	2.47	0.54
1:B:1179:TRP:CE2	1:B:1221:ARG:HG2	2.42	0.54
1:A:619:LEU:HD12	1:A:619:LEU:N	2.20	0.54
1:A:661:GLU:HG3	1:A:668:THR:HG22	1.87	0.54
1:B:1109:MET:HE1	1:B:1113:VAL:HG13	1.90	0.54
1:B:1136:GLU:HG2	4:B:190:HOH:O	2.09	0.53
1:A:778:ALA:HA	1:A:781:ILE:CG2	2.39	0.53
1:B:1112:ARG:HG2	1:B:1115:GLU:OE2	2.09	0.52
1:A:697:LYS:O	1:A:697:LYS:HD3	2.11	0.51
1:A:739:LYS:HG3	1:A:740:ASP:H	1.75	0.51
1:A:653:TYR:HB2	1:A:675:HIS:O	2.12	0.50
1:A:679:TRP:CE2	1:A:721:ARG:HG2	2.46	0.50
1:A:640:LEU:HD23	1:A:662:ASN:HA	1.93	0.50
1:A:616:LYS:NZ	1:B:1014:GLY:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1133:MET:C	1:B:1134:ILE:HD12	2.37	0.49
1:B:1165:THR:O	1:B:1166:GLN:HB2	2.13	0.49
1:B:1005:LYS:HG3	1:B:1006:GLU:N	2.27	0.49
1:A:513:SER:HB2	1:B:1117:GLY:CA	2.43	0.48
1:B:1109:MET:HG3	1:B:1214:HIS:CE1	2.49	0.48
1:A:574:MET:HE2	1:A:730:THR:HG21	1.95	0.48
1:A:697:LYS:HD3	1:A:697:LYS:C	2.39	0.48
1:A:548:ASP:O	3:A:801:600:H61	2.15	0.47
1:B:1197:LYS:HE2	1:B:1197:LYS:CA	2.45	0.47
1:B:1005:LYS:HA	1:B:1008:GLU:CD	2.40	0.47
1:A:572:ILE:HG13	1:A:756:PHE:HB2	1.97	0.46
1:B:1005:LYS:CG	1:B:1006:GLU:N	2.78	0.46
1:B:1112:ARG:HG2	1:B:1115:GLU:CD	2.41	0.46
1:B:1060:HIS:O	1:B:1061:GLN:O	2.34	0.46
1:A:614:MET:HG2	1:A:619:LEU:HG	1.98	0.45
1:B:1005:LYS:HA	1:B:1008:GLU:OE2	2.17	0.45
1:B:1063:ASP:OD1	1:B:1063:ASP:O	2.33	0.45
1:A:539:LYS:HE3	4:A:36:HOH:O	2.17	0.45
1:A:515:SER:HA	4:A:29:HOH:O	2.17	0.45
1:B:1202:GLY:O	1:B:1205:SER:HB3	2.17	0.44
1:A:781:ILE:HG23	1:A:782:MET:SD	2.57	0.44
1:B:1004:GLU:O	1:B:1008:GLU:HG3	2.18	0.44
1:B:1112:ARG:HB2	1:B:1112:ARG:CZ	2.48	0.44
1:B:1276:GLU:OE1	1:B:1279:LYS:HE2	2.18	0.44
1:A:739:LYS:HG3	1:A:740:ASP:N	2.33	0.43
1:A:546:TYR:HB3	3:A:801:600:N47	2.34	0.43
1:A:513:SER:HB2	1:B:1117:GLY:HA3	2.01	0.43
1:B:999:GLU:OE2	1:B:1241:PRO:HB2	2.18	0.43
1:A:727:LEU:CA	1:A:753:MET:HE1	2.48	0.43
1:A:605:ARG:HG2	1:A:605:ARG:NH1	2.31	0.42
1:B:1147:GLU:CB	1:B:1156:ARG:HG2	2.49	0.42
1:B:1278:ALA:O	1:B:1282:MET:HB2	2.19	0.42
1:B:1147:GLU:O	1:B:1147:GLU:HG3	2.19	0.42
1:B:1079:ARG:HG2	1:B:1081:TYR:CZ	2.55	0.42
1:B:1088:LEU:O	1:B:1089:PRO:C	2.62	0.42
1:A:647:GLU:HB2	1:A:656:ARG:HG2	2.02	0.42
1:A:777:GLY:O	1:A:781:ILE:HG22	2.20	0.42
1:A:577:ALA:O	1:A:578:GLN:HB2	2.20	0.42
1:A:634:ILE:HD12	1:A:634:ILE:N	2.35	0.42
1:A:602:GLN:O	1:A:709:GLY:HA3	2.19	0.42
1:A:778:ALA:CA	1:A:781:ILE:HG22	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:GLU:O	1:B:1007:PHE:HB3	2.21	0.41
1:A:618:SER:O	1:A:620:LYS:HG3	2.21	0.41
1:B:1009:GLN:HE21	1:B:1009:GLN:HB3	1.69	0.41
1:B:1097:GLU:HA	1:B:1140:LEU:HD11	2.03	0.41
1:B:1199:ARG:HG2	1:B:1204:LEU:HD12	2.03	0.40
1:A:674:PHE:CE2	1:A:697:LYS:HD2	2.47	0.40
1:B:1064:ASN:HA	4:B:91:HOH:O	2.21	0.40
1:B:1079:ARG:NE	1:B:1233:LEU:HD11	2.36	0.40
1:A:616:LYS:HE3	1:A:681:ASP:OD1	2.22	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	287/310 (93%)	270 (94%)	14 (5%)	3 (1%)	12	15
1	B	287/310 (93%)	270 (94%)	13 (4%)	4 (1%)	9	9
All	All	574/620 (93%)	540 (94%)	27 (5%)	7 (1%)	10	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1061	GLN
1	B	1116	LYS
1	A	619	LEU
1	B	1011	ASP
1	A	575	GLU
1	A	761	ILE
1	B	1261	ILE

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	259/283 (92%)	251 (97%)	8 (3%)	35	52
1	B	258/283 (91%)	250 (97%)	8 (3%)	35	52
All	All	517/566 (91%)	501 (97%)	16 (3%)	35	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	511	ASP
1	A	614	MET
1	A	657	GLN
1	A	753	MET
1	A	760	LEU
1	A	761	ILE
1	A	765	ASP
1	B	1006	GLU
1	B	1009	GLN
1	B	1112	ARG
1	B	1115	GLU
1	B	1157	GLN
1	B	1197	LYS
1	B	1260	LEU
1	B	1261	ILE

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	560	HIS
1	A	561	GLN
1	A	708	HIS
1	A	762	GLN
1	B	1009	GLN
1	B	1025	HIS

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Mol	Chain	Res	Type
1	B	1123	GLN
1	B	1139	ASN
1	B	1166	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	600	B	1301	-	61,64,64	2.99	37 (60%)	77,97,97	5.08	23 (29%)
3	600	A	801	-	61,64,64	2.99	42 (68%)	77,97,97	5.19	20 (25%)

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	600	B	1301	-	-	6/52/57/57	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	600	A	801	-	-	8/52/57/57	0/7/7/7

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	600	C32-C21	6.38	1.61	1.51
3	B	1301	600	C35-C30	6.37	1.62	1.55
3	B	1301	600	C30-C4	5.92	1.60	1.52
3	B	1301	600	C64-C65	5.65	1.49	1.42
3	A	801	600	C30-C4	5.64	1.60	1.52
3	B	1301	600	C5-C4	5.55	1.48	1.39
3	A	801	600	C32-C21	5.53	1.60	1.51
3	A	801	600	C67-N66	5.39	1.37	1.32
3	A	801	600	C64-C65	5.34	1.49	1.42
3	B	1301	600	C43-N31	5.23	1.45	1.38
3	A	801	600	C35-C30	5.19	1.61	1.55
3	A	801	600	C5-C4	4.96	1.47	1.39
3	B	1301	600	C43-C42	4.88	1.48	1.40
3	A	801	600	C3-C4	4.77	1.47	1.39
3	A	801	600	O77-C76	-4.59	1.26	1.42
3	B	1301	600	C62-C67	4.41	1.47	1.38
3	B	1301	600	O77-C76	-4.33	1.27	1.42
3	A	801	600	C43-N31	4.21	1.43	1.38
3	A	801	600	C13-C14	4.17	1.46	1.39
3	B	1301	600	C3-C4	4.16	1.46	1.39
3	A	801	600	C43-C42	4.09	1.47	1.40
3	A	801	600	C62-C67	3.90	1.46	1.38
3	B	1301	600	C45-C44	3.75	1.45	1.38
3	A	801	600	C12-C11	3.63	1.46	1.38
3	B	1301	600	P79-O81	-3.61	1.45	1.54
3	B	1301	600	C20-C21	3.54	1.45	1.38
3	B	1301	600	C67-N66	3.51	1.35	1.32
3	B	1301	600	C35-C11	3.37	1.56	1.51
3	B	1301	600	C45-C40	3.37	1.45	1.38
3	A	801	600	P79-O81	-3.35	1.46	1.54
3	A	801	600	C63-C62	3.32	1.43	1.36
3	A	801	600	C68-C24	3.31	1.56	1.49
3	A	801	600	C10-C11	3.30	1.45	1.38
3	B	1301	600	P55-O57	-3.23	1.46	1.54
3	A	801	600	C61-C68	3.13	1.46	1.38
3	A	801	600	C13-C12	3.11	1.43	1.38
3	B	1301	600	C63-C62	3.11	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	600	C13-C12	3.07	1.43	1.38
3	A	801	600	P79-O82	3.07	1.55	1.49
3	B	1301	600	C10-C11	3.05	1.44	1.38
3	A	801	600	C45-C44	3.01	1.44	1.38
3	B	1301	600	C6-C5	3.00	1.44	1.38
3	A	801	600	C20-C21	2.99	1.44	1.38
3	B	1301	600	C44-C43	2.98	1.44	1.39
3	B	1301	600	C61-C68	2.96	1.46	1.38
3	A	801	600	C70-C65	2.92	1.44	1.42
3	A	801	600	C6-C5	2.88	1.43	1.38
3	A	801	600	C40-C41	2.84	1.43	1.38
3	A	801	600	C15-C14	2.78	1.44	1.39
3	B	1301	600	C13-C14	2.77	1.43	1.39
3	A	801	600	P55-O57	-2.77	1.47	1.54
3	B	1301	600	C12-C11	2.77	1.44	1.38
3	A	801	600	C45-C40	2.77	1.44	1.38
3	A	801	600	C25-C24	2.75	1.44	1.39
3	B	1301	600	N46-N47	2.73	1.34	1.30
3	B	1301	600	C40-C41	2.70	1.43	1.38
3	B	1301	600	C2-C1	2.69	1.44	1.38
3	A	801	600	C32-C30	2.68	1.58	1.55
3	A	801	600	C22-C21	2.66	1.44	1.38
3	A	801	600	C44-C43	2.63	1.43	1.39
3	B	1301	600	C23-C24	2.62	1.44	1.39
3	A	801	600	O77-C71	-2.58	1.29	1.42
3	B	1301	600	C22-C21	2.57	1.44	1.38
3	A	801	600	C2-C1	2.55	1.43	1.38
3	A	801	600	N46-N47	2.53	1.34	1.30
3	B	1301	600	C25-C24	2.48	1.44	1.39
3	B	1301	600	O77-C71	-2.47	1.30	1.42
3	B	1301	600	C2-C3	2.46	1.43	1.38
3	B	1301	600	C25-C20	2.45	1.42	1.38
3	A	801	600	C25-C20	2.42	1.42	1.38
3	A	801	600	C2-C3	2.35	1.42	1.38
3	B	1301	600	C42-N46	-2.35	1.34	1.38
3	A	801	600	C69-C68	2.33	1.43	1.39
3	A	801	600	C6-C1	2.16	1.43	1.38
3	B	1301	600	C23-C22	2.13	1.42	1.38
3	B	1301	600	C6-C1	2.12	1.42	1.38
3	A	801	600	C23-C24	2.11	1.43	1.39
3	A	801	600	C35-C11	2.11	1.54	1.51
3	A	801	600	C61-C64	2.07	1.46	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	600	C73-C72-C71	26.44	154.66	115.26
3	B	1301	600	C73-C72-C71	25.53	153.31	115.26
3	A	801	600	N31-N47-N46	-23.94	101.08	109.03
3	B	1301	600	N31-N47-N46	-23.03	101.38	109.03
3	A	801	600	C43-N31-N47	15.84	114.30	109.86
3	B	1301	600	C42-N46-N47	14.00	119.43	108.41
3	B	1301	600	C43-N31-N47	13.66	113.69	109.86
3	A	801	600	C42-N46-N47	13.06	118.69	108.41
3	B	1301	600	C72-C71-C67	-10.85	96.32	111.74
3	A	801	600	C72-C71-C67	-9.91	97.65	111.74
3	B	1301	600	O77-C71-C67	7.70	124.87	110.69
3	A	801	600	O77-C71-C67	7.23	124.00	110.69
3	B	1301	600	C43-C42-N46	-6.50	103.29	108.70
3	A	801	600	C43-C42-N46	-6.00	103.71	108.70
3	B	1301	600	C42-C43-N31	-4.69	102.20	103.89
3	A	801	600	C42-C43-N31	-4.64	102.22	103.89
3	A	801	600	C30-C32-C21	4.55	124.60	115.52
3	B	1301	600	C30-C32-C21	4.03	123.55	115.52
3	A	801	600	C64-C65-N66	-3.79	117.91	122.68
3	A	801	600	C74-C73-C72	3.58	123.95	111.08
3	B	1301	600	O77-C71-C72	3.50	122.63	107.48
3	B	1301	600	C41-C42-N46	3.42	134.96	130.50
3	B	1301	600	C44-C43-C42	-3.35	118.36	122.23
3	A	801	600	O77-C71-C72	3.35	121.97	107.48
3	B	1301	600	C64-C65-N66	-3.30	118.53	122.68
3	A	801	600	O58-P55-C52	-3.28	104.67	111.78
3	B	1301	600	C76-O77-C71	3.23	123.38	113.72
3	A	801	600	C62-C67-N66	-3.18	119.92	122.97
3	A	801	600	C41-C42-N46	3.16	134.62	130.50
3	B	1301	600	C62-C67-N66	-3.14	119.95	122.97
3	A	801	600	C44-C43-C42	-3.12	118.63	122.23
3	A	801	600	C76-O77-C71	3.07	122.91	113.72
3	B	1301	600	C74-C73-C72	2.99	121.84	111.08
3	B	1301	600	C44-C43-N31	2.96	139.43	133.54
3	A	801	600	C44-C43-N31	2.82	139.15	133.54
3	B	1301	600	C69-C68-C24	-2.70	116.31	120.84
3	A	801	600	C30-C35-C11	2.45	120.40	115.52
3	B	1301	600	O58-P55-C52	-2.44	106.50	111.78
3	B	1301	600	C32-C21-C20	-2.38	117.87	121.06
3	B	1301	600	C25-C24-C68	-2.17	117.51	121.25
3	B	1301	600	C30-C35-C11	2.07	119.64	115.52
3	B	1301	600	C68-C61-C64	-2.02	118.02	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	600	O81-P79-C70	2.00	110.57	106.81

There are no chirality outliers.

All (14) torsion outliers are listed below:

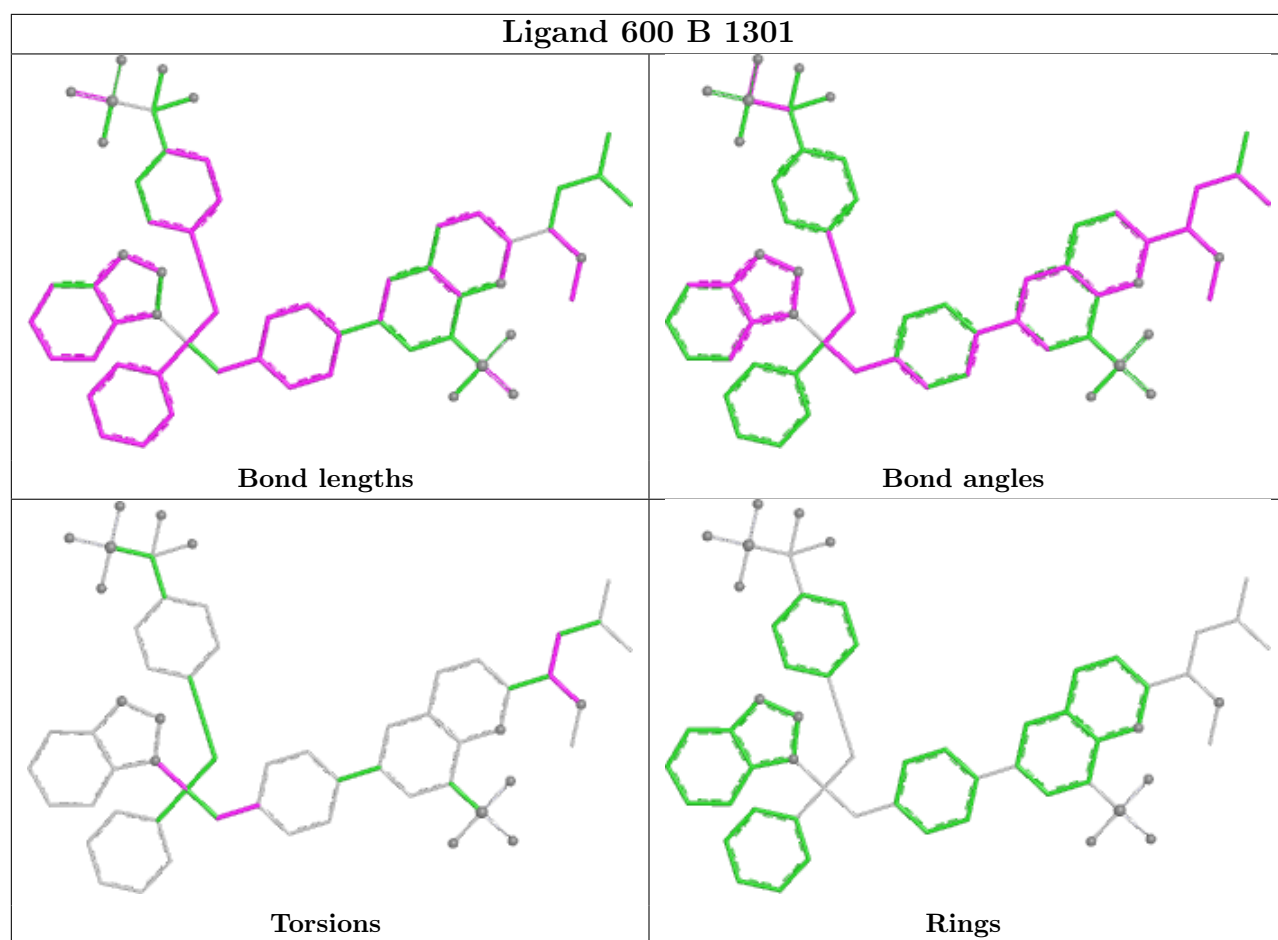
Mol	Chain	Res	Type	Atoms
3	A	801	600	C67-C71-O77-C76
3	A	801	600	C72-C71-O77-C76
3	A	801	600	C67-C71-C72-C73
3	B	1301	600	C67-C71-O77-C76
3	B	1301	600	C72-C71-O77-C76
3	B	1301	600	C67-C71-C72-C73
3	A	801	600	C62-C67-C71-O77
3	A	801	600	C20-C21-C32-C30
3	A	801	600	C22-C21-C32-C30
3	B	1301	600	C20-C21-C32-C30
3	B	1301	600	C22-C21-C32-C30
3	A	801	600	C4-C30-N31-N47
3	B	1301	600	C4-C30-N31-N47
3	A	801	600	N66-C67-C71-O77

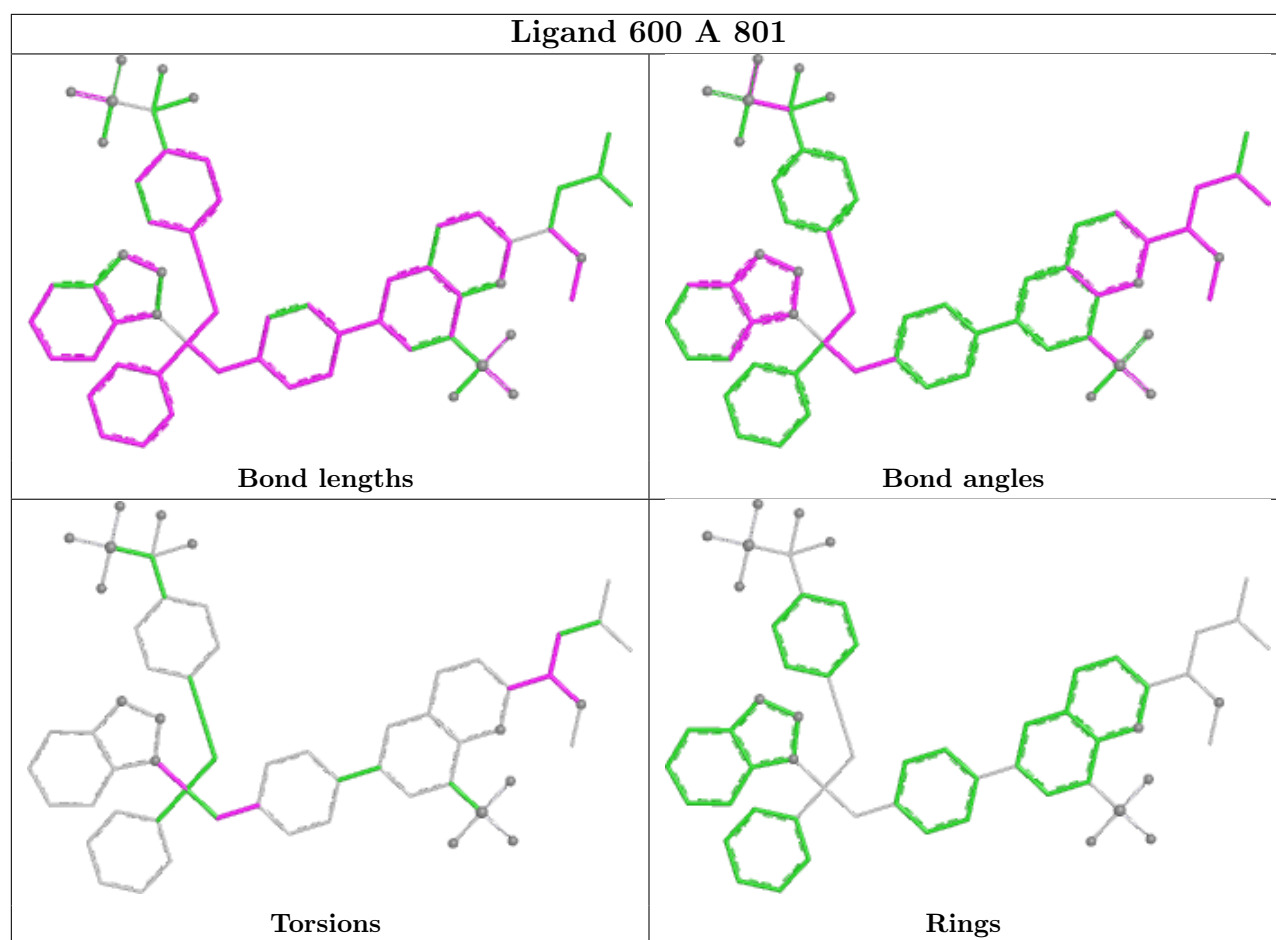
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	600	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 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	289/310 (93%)	-1.38	0 100 100	23, 38, 68, 76	0
1	B	289/310 (93%)	-1.38	0 100 100	21, 38, 70, 78	0
All	All	578/620 (93%)	-1.38	0 100 100	21, 39, 70, 78	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

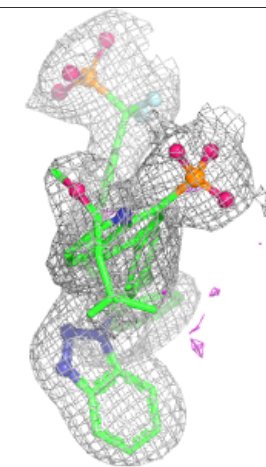
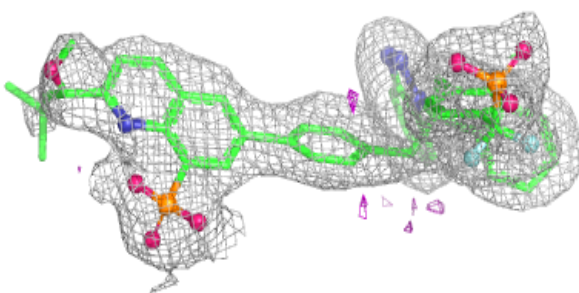
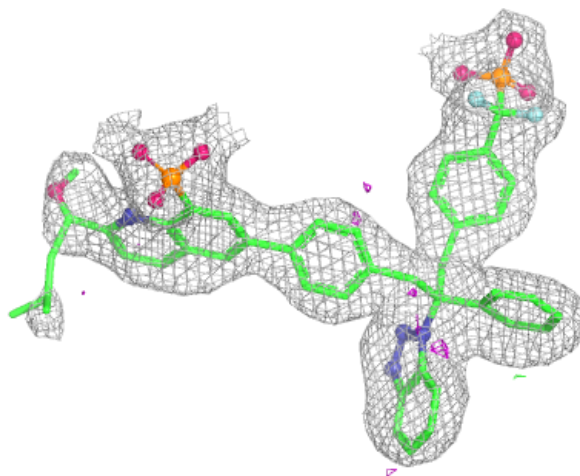
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	6000	1/1	0.98	0.10	32,32,32,32	1
2	MG	B	5000	1/1	0.99	0.05	26,26,26,26	1
3	600	A	801	58/58	1.00	0.03	22,28,55,59	0
3	600	B	1301	58/58	1.00	0.03	19,28,44,47	0

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.

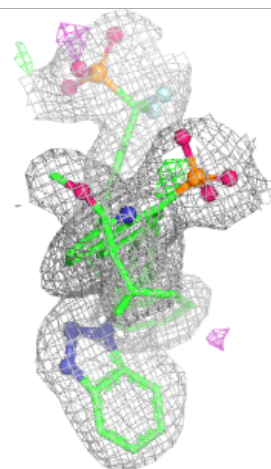
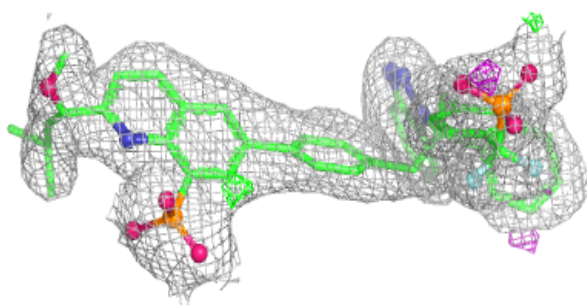
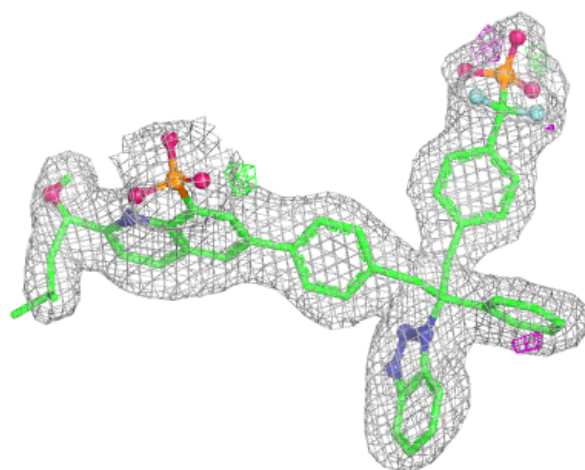
Electron density around 600 A 801:

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



Electron density around 600 B 1301:

$2mF_o-DF_c$ (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.