Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 02:18 AM JST

PDB ID	:	5YU9
Title	:	Crystal structure of EGFR 696-1022 T790M in complex with Ibrutinib
Authors	:	Yan, X.E.; Yun, C.H.
Deposited on	:	2017-11-21
Resolution	:	1.95 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:

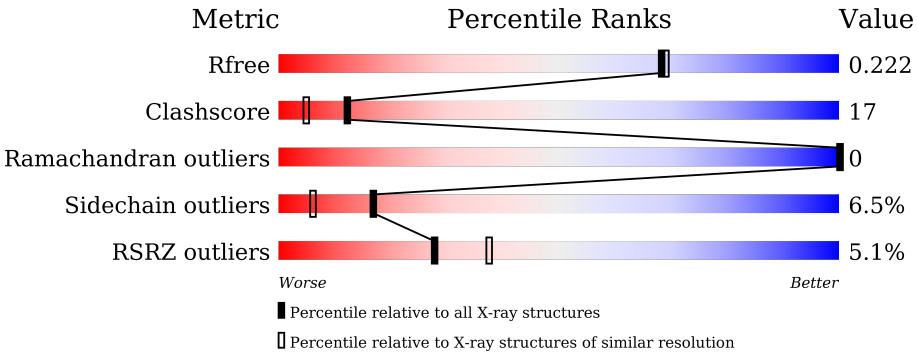
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	331	5% 70% 18% • 9%
1	B	331	4% 63% 23% • 11%
1	C	331	5% 68% 23% • 8%
1	D	331	5% 70% 17% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10782 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.

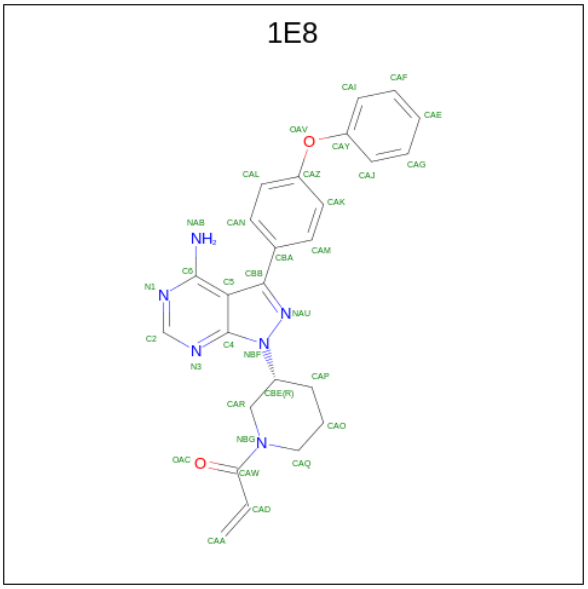
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	5	0
			2440	1570	410	440	20			
1	B	295	Total	C	N	O	S	0	6	0
			2395	1547	400	429	19			
1	C	306	Total	C	N	O	S	0	3	0
			2454	1584	413	437	20			
1	D	300	Total	C	N	O	S	0	4	0
			2408	1553	401	434	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	ALA	-	expression tag	UNP P00533
A	694	MET	-	expression tag	UNP P00533
A	695	GLY	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	ALA	-	expression tag	UNP P00533
B	694	MET	-	expression tag	UNP P00533
B	695	GLY	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	ALA	-	expression tag	UNP P00533
C	694	MET	-	expression tag	UNP P00533
C	695	GLY	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	ALA	-	expression tag	UNP P00533
D	694	MET	-	expression tag	UNP P00533
D	695	GLY	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533

- Molecule 2 is 1-{(3R)-3-[4-amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]piperidin-1-yl}prop-2-en-1-one (three-letter code: 1E8) (formula: $C_{25}H_{24}N_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 33 25 6 2	0	0
2	B	1	Total C N O 33 25 6 2	0	0
2	C	1	Total C N O 33 25 6 2	0	0
2	D	1	Total C N O 33 25 6 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	259	Total O 259 259	0	0
4	B	259	Total O 259 259	0	0

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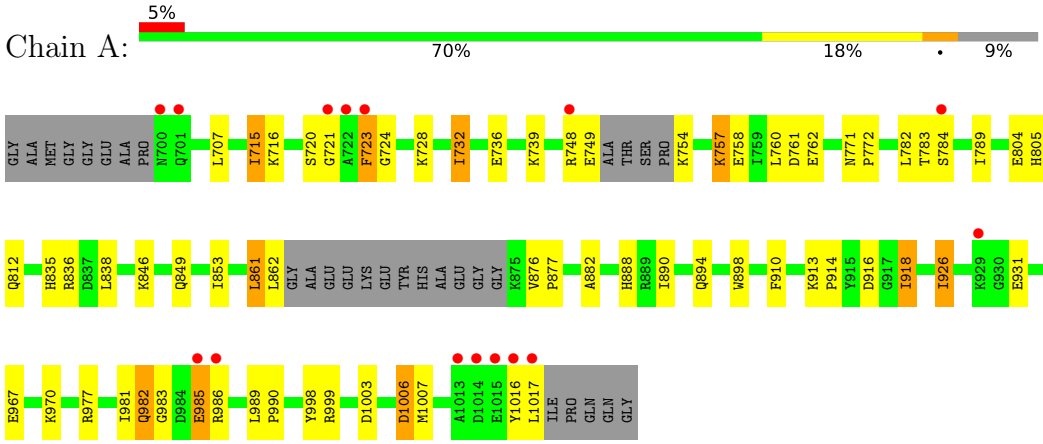
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	225	Total O 225 225	0	0
4	D	207	Total O 207 207	0	0

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.

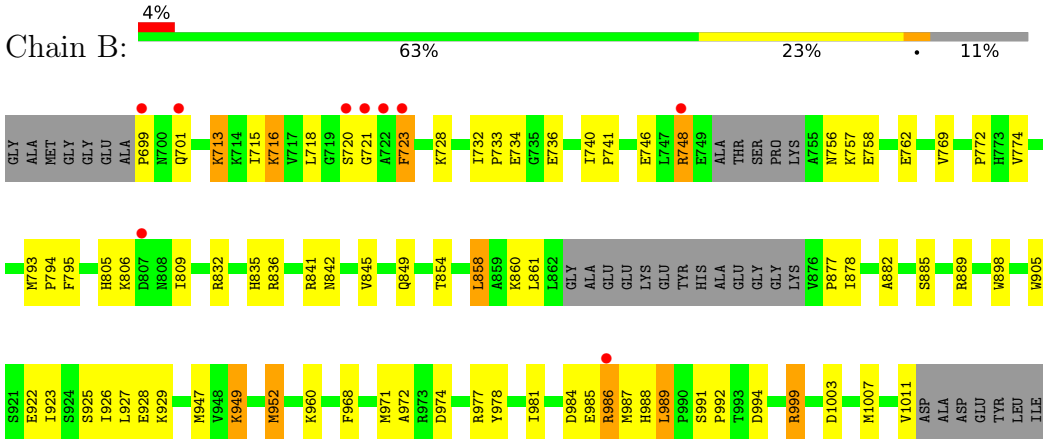
• Molecule 1: Epidermal growth factor receptor

Chain A:



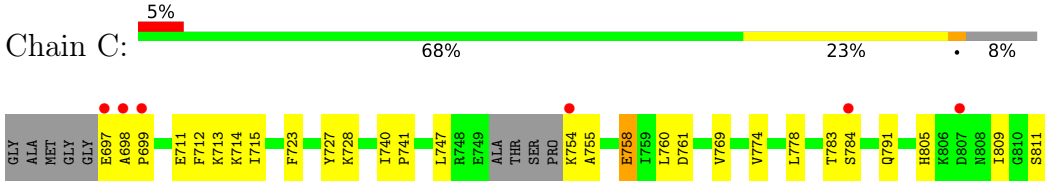
• Molecule 1: Epidermal growth factor receptor

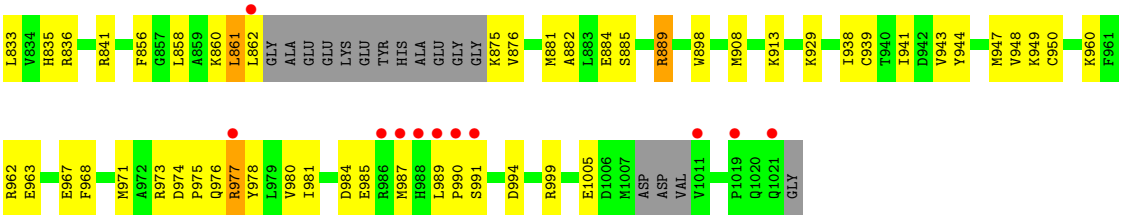
Chain B:



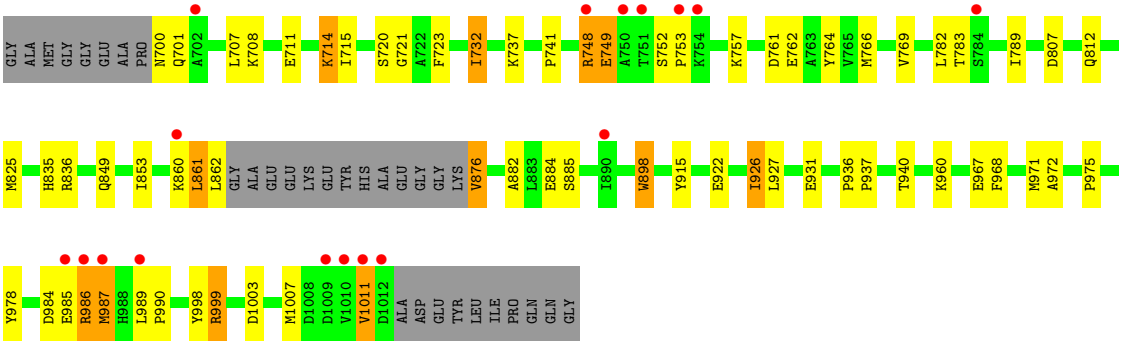
• Molecule 1: Epidermal growth factor receptor

Chain C:





• Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.19Å 74.39Å 120.46Å 90.00° 118.32° 90.00°	Depositor
Resolution (Å)	41.63 – 1.95 46.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.63-1.95) 99.5 (46.56-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 1.95Å)	Xtriage
Refinement program	PHENIX (dev_2400)	Depositor
R, R_{free}	0.202 , 0.222 0.202 , 0.222	Depositor DCC
R_{free} test set	4748 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10782	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1879e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL, 1E8

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.55	0/2508	0.64	0/3391
1	B	0.56	0/2466	0.60	0/3338
1	C	0.54	0/2515	0.60	0/3402
1	D	0.57	0/2475	0.59	0/3352
All	All	0.55	0/9964	0.60	0/13483

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

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	2440	0	2474	74	0
1	B	2395	0	2443	109	0
1	C	2454	0	2484	77	0
1	D	2408	0	2456	88	0
2	A	33	0	22	1	0
2	B	33	0	23	1	0
2	C	33	0	23	0	0
2	D	33	0	23	0	0
3	C	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	259	0	0	24	0
4	B	259	0	0	29	0
4	C	225	0	0	13	0
4	D	207	0	0	10	0
All	All	10782	0	9948	337	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 17.

All (337) 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:985:GLU:HB2	4:C:1308:HOH:O	1.36	1.22
1:B:989:LEU:HG	4:B:1201:HOH:O	1.37	1.21
1:A:732[A]:ILE:HD12	4:A:1201:HOH:O	1.40	1.21
1:A:723:PHE:CD1	1:A:862:LEU:HD12	1.81	1.17
1:B:832:ARG:NH2	1:D:748:ARG:HD3	1.57	1.16
1:B:919:PRO:HG2	1:B:922:GLU:HG3	1.23	1.15
1:D:999:ARG:HG2	1:D:999:ARG:HH11	1.04	1.14
1:A:914:PRO:HG2	4:A:1356:HOH:O	1.49	1.13
1:C:943:VAL:HB	4:C:1252:HOH:O	1.46	1.11
1:A:982[A]:GLN:CD	1:A:982[A]:GLN:H	1.53	1.10
1:C:697:GLU:HA	4:C:1259:HOH:O	1.48	1.09
1:C:861:LEU:HD23	1:C:861:LEU:O	1.53	1.06
1:B:832:ARG:HH21	1:D:748:ARG:HD3	0.88	1.04
1:B:748:ARG:HG3	4:B:1306:HOH:O	1.56	1.04
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.08	1.04
1:B:832:ARG:NH2	1:D:748:ARG:HB3	1.72	1.02
1:D:812:GLN:HG2	1:D:989:LEU:CG	1.91	1.01
1:B:999:ARG:HH11	1:B:999:ARG:HG2	0.88	1.00
1:B:783:THR:HG22	1:B:784:SER:H	1.25	1.00
1:C:861:LEU:HD22	1:C:862:LEU:CD2	1.91	1.00
1:B:949:LYS:HE3	4:B:1403:HOH:O	1.61	0.99
1:B:832:ARG:HD2	1:D:748:ARG:NH1	1.77	0.98
1:D:701:GLN:HG2	1:D:764:TYR:CE1	1.97	0.98
1:C:758:GLU:OE1	1:C:758:GLU:HA	1.61	0.98
1:B:999:ARG:HG2	1:B:999:ARG:NH1	1.69	0.97
1:B:746:GLU:OE1	1:B:785:THR:HG21	1.63	0.97
1:B:732[A]:ILE:HD12	1:B:733:PRO:HD2	1.46	0.97
1:D:999:ARG:HG2	1:D:999:ARG:NH1	1.69	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:PHE:HD1	1:A:862:LEU:HD12	1.18	0.96
1:B:723:PHE:HB2	4:B:1380:HOH:O	1.65	0.96
1:D:812:GLN:CG	1:D:989:LEU:HG	1.95	0.95
1:B:715:ILE:HD11	1:B:728:LYS:HE2	1.49	0.94
1:B:832:ARG:HH21	1:D:748:ARG:CD	1.81	0.94
1:B:999:ARG:HH11	1:B:999:ARG:CG	1.79	0.94
1:A:1016:TYR:O	1:A:1017:LEU:CB	2.14	0.93
1:D:849:GLN:HG2	1:D:990:PRO:HG2	1.51	0.92
1:C:861:LEU:HD22	1:C:862:LEU:HD23	1.51	0.91
1:B:832:ARG:HH22	1:D:748:ARG:HB3	1.36	0.90
1:C:783:THR:O	1:C:784:SER:OG	1.91	0.87
1:B:732[A]:ILE:HD12	1:B:733:PRO:CD	2.04	0.86
1:D:999:ARG:HH11	1:D:999:ARG:CG	1.85	0.86
1:D:737:LYS:HE3	4:D:1374:HOH:O	1.74	0.86
3:C:1102:CL:CL	4:C:1411:HOH:O	2.32	0.84
1:D:849:GLN:CG	1:D:990:PRO:HG2	2.08	0.83
1:B:832:ARG:NH2	1:D:748:ARG:CD	2.40	0.82
1:B:832:ARG:HD2	1:D:748:ARG:HH11	1.44	0.82
1:D:752:SER:HB2	1:D:753:PRO:HD2	1.62	0.81
1:D:989:LEU:HD22	1:D:990:PRO:CD	2.11	0.81
1:D:849:GLN:HE21	1:D:990:PRO:HG3	1.46	0.81
1:C:698:ALA:N	1:C:699:PRO:HD2	1.98	0.79
1:B:919:PRO:HG2	1:B:922:GLU:CG	2.09	0.79
1:A:723:PHE:HB2	4:A:1361:HOH:O	1.83	0.79
1:C:758:GLU:OE1	1:C:758:GLU:CA	2.30	0.79
1:D:989:LEU:CD2	1:D:990:PRO:HD3	2.15	0.77
1:A:723:PHE:HD1	1:A:862:LEU:CD1	1.96	0.77
1:B:756:ASN:HB3	4:B:1382:HOH:O	1.84	0.76
1:D:989:LEU:HD22	1:D:990:PRO:HD3	1.67	0.76
1:C:861:LEU:HD23	1:C:861:LEU:C	2.06	0.75
1:C:861:LEU:CD2	1:C:862:LEU:HD23	2.16	0.75
1:B:783:THR:HG22	1:B:784:SER:N	2.02	0.74
1:D:723:PHE:CD1	1:D:862:LEU:HD12	2.23	0.74
1:B:925:SER:O	1:B:929:LYS:HG2	1.87	0.73
1:C:832:ARG:NH2	1:C:832:ARG:HG3	2.05	0.72
1:A:748:ARG:O	1:A:749:GLU:CB	2.39	0.70
1:B:713:LYS:NZ	1:B:732[A]:ILE:HG22	2.06	0.70
1:C:861:LEU:C	1:C:861:LEU:CD2	2.61	0.70
1:A:723:PHE:CE1	1:A:862:LEU:HD12	2.27	0.69
1:C:962:ARG:HD2	4:C:1332:HOH:O	1.92	0.69
1:C:754:LYS:O	1:C:755:ALA:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:ARG:NH2	1:D:860:LYS:HD3	2.08	0.68
1:C:861:LEU:O	1:C:861:LEU:CD2	2.38	0.68
1:B:832:ARG:CD	1:D:748:ARG:NH1	2.56	0.67
1:D:701:GLN:HG2	1:D:764:TYR:CZ	2.29	0.67
1:D:989:LEU:HD22	1:D:990:PRO:HD2	1.77	0.66
1:C:747:LEU:HD13	1:C:862:LEU:HD11	1.77	0.66
1:A:723:PHE:CB	4:A:1361:HOH:O	2.41	0.66
1:C:832:ARG:HG3	1:C:832:ARG:HH21	1.60	0.66
1:A:762:GLU:OE1	1:A:861:LEU:HA	1.96	0.65
1:B:732[A]:ILE:HD11	1:B:736:GLU:O	1.96	0.65
1:B:721:GLY:HA3	4:B:1379:HOH:O	1.96	0.65
1:C:861:LEU:HD22	1:C:862:LEU:HD21	1.76	0.64
1:C:758:GLU:OE1	1:C:761:ASP:HB2	1.98	0.64
1:C:714:LYS:HD3	1:C:727:TYR:CG	2.32	0.63
1:A:967:GLU:HG2	4:A:1383:HOH:O	1.98	0.63
1:B:762[A]:GLU:CD	4:B:1224:HOH:O	2.37	0.63
1:A:715:ILE:HD11	1:A:728:LYS:HG2	1.79	0.63
1:A:804:GLU:HB3	4:A:1336:HOH:O	1.99	0.63
1:C:832:ARG:HH21	1:C:832:ARG:CG	2.12	0.63
1:A:962:ARG:NE	4:A:1202:HOH:O	2.32	0.62
1:B:716:LYS:NZ	4:B:1203:HOH:O	2.31	0.62
1:B:919:PRO:CG	1:B:922:GLU:HG3	2.15	0.62
1:C:714:LYS:HD3	1:C:727:TYR:CD2	2.34	0.62
1:A:985:GLU:HG2	1:A:986:ARG:N	2.14	0.62
1:C:944:TYR:O	1:C:948:VAL:HG23	1.99	0.62
1:B:748:ARG:CG	4:B:1306:HOH:O	2.30	0.61
1:C:698:ALA:N	1:C:699:PRO:CD	2.64	0.61
1:D:1003:ASP:OD2	1:D:1007[B]:MET:HE1	2.00	0.61
1:B:732[A]:ILE:HD12	1:B:733:PRO:N	2.15	0.61
1:B:926:ILE:HG13	1:B:927:LEU:N	2.15	0.61
1:A:962:ARG:CZ	4:A:1202:HOH:O	2.48	0.61
1:C:999:ARG:NH2	1:C:1005:GLU:O	2.34	0.60
1:B:723:PHE:CB	4:B:1380:HOH:O	2.36	0.60
1:B:715:ILE:HD11	1:B:728:LYS:CE	2.29	0.60
1:A:723:PHE:HE1	1:A:862:LEU:HB2	1.65	0.60
1:A:838:LEU:HD13	4:A:1333:HOH:O	2.01	0.60
1:C:968:PHE:HA	1:C:971:MET:HE3	1.84	0.60
1:A:894:GLN:HG2	4:A:1349:HOH:O	2.02	0.60
1:B:949:LYS:CE	4:B:1403:HOH:O	2.32	0.60
1:B:968:PHE:CD1	1:B:971:MET:CE	2.85	0.60
1:C:941:ILE:HG22	4:C:1344:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:ASP:OD1	1:A:1006:ASP:N	2.30	0.59
1:B:786:VAL:HG23	4:B:1205:HOH:O	2.00	0.59
1:D:984:ASP:HA	1:D:987:MET:HG3	1.83	0.59
1:A:757:LYS:HE3	4:A:1397:HOH:O	2.01	0.59
1:D:1007[A]:MET:HE3	4:D:1353:HOH:O	2.02	0.59
1:B:734:GLU:HB2	4:B:1402:HOH:O	2.02	0.59
1:A:918:ILE:N	1:A:918:ILE:CD1	2.66	0.59
1:A:949:LYS:NZ	4:A:1204:HOH:O	2.35	0.59
1:C:861:LEU:CD2	1:C:862:LEU:CD2	2.75	0.59
1:B:713:LYS:HZ2	1:B:732[A]:ILE:HG22	1.67	0.58
1:B:746:GLU:OE1	1:B:785:THR:CG2	2.47	0.58
1:C:723:PHE:CG	1:C:858:LEU:HD13	2.38	0.58
1:D:915:TYR:CE1	1:D:926[A]:ILE:HD11	2.38	0.58
1:D:926[A]:ILE:HD12	1:D:931:GLU:O	2.03	0.58
1:A:981:ILE:HA	1:A:982[A]:GLN:OE1	2.04	0.58
1:C:769:VAL:HG11	1:C:774:VAL:HG11	1.86	0.58
1:D:968:PHE:CD1	1:D:971:MET:CE	2.87	0.57
1:D:985:GLU:HG2	1:D:986:ARG:N	2.20	0.57
1:B:832:ARG:NH2	1:D:748:ARG:CB	2.60	0.57
1:D:968:PHE:CD1	1:D:971:MET:HE3	2.39	0.57
1:A:732[B]:ILE:HG23	4:A:1201:HOH:O	2.03	0.57
1:B:716:LYS:HD3	4:B:1203:HOH:O	2.02	0.57
1:A:918:ILE:N	1:A:918:ILE:HD13	2.19	0.57
1:D:849:GLN:CG	1:D:990:PRO:CG	2.82	0.57
1:B:981:ILE:O	1:B:984:ASP:HB2	2.05	0.57
1:B:835:HIS:O	1:B:836:ARG:HB2	2.05	0.57
1:D:989:LEU:CD2	1:D:990:PRO:CD	2.80	0.57
1:B:949:LYS:O	1:B:952:MET:HG3	2.05	0.56
1:C:989:LEU:HD11	4:C:1263:HOH:O	2.04	0.56
1:A:926:ILE:C	1:A:926:ILE:HD12	2.25	0.56
1:C:723:PHE:CD2	1:C:858:LEU:HD13	2.40	0.56
1:B:728:LYS:NZ	4:B:1217:HOH:O	2.39	0.56
1:D:812:GLN:HG2	1:D:989:LEU:CD1	2.35	0.56
1:D:720:SER:HB2	1:D:748:ARG:HH22	1.70	0.56
1:A:962:ARG:NH1	4:A:1202:HOH:O	2.39	0.56
1:A:715:ILE:CD1	1:A:728:LYS:HG2	2.36	0.56
1:C:769:VAL:HG11	1:C:774:VAL:CG1	2.36	0.55
1:C:835:HIS:O	1:C:836:ARG:HB2	2.06	0.55
1:C:805:HIS:O	1:C:809:ILE:HG13	2.06	0.55
1:A:716:LYS:HG3	4:A:1434:HOH:O	2.07	0.54
1:A:977:ARG:HE	1:D:926[A]:ILE:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:LYS:NZ	1:B:718:LEU:HD23	2.23	0.54
1:B:762[A]:GLU:CG	4:B:1224:HOH:O	2.56	0.54
1:D:721:GLY:HA3	4:D:1344:HOH:O	2.07	0.54
1:D:876:VAL:N	4:D:1209:HOH:O	2.41	0.54
1:C:977:ARG:HD3	1:C:977:ARG:C	2.27	0.54
1:A:1007[A]:MET:HE3	4:A:1290:HOH:O	2.08	0.54
1:B:805:HIS:ND1	4:B:1210:HOH:O	2.33	0.54
1:D:835:HIS:O	1:D:836:ARG:HB2	2.08	0.54
1:B:885:SER:O	1:B:889:ARG:HD3	2.08	0.54
1:B:991:SER:OG	1:B:992:PRO:HD2	2.07	0.54
1:D:700:ASN:N	4:D:1208:HOH:O	2.40	0.53
1:C:963:GLU:O	1:C:967:GLU:HG3	2.08	0.53
1:B:849:GLN:NE2	4:B:1213:HOH:O	2.35	0.53
1:A:977:ARG:NE	1:D:926[A]:ILE:HD13	2.24	0.53
1:D:989:LEU:HD23	1:D:990:PRO:HD3	1.90	0.53
1:C:962:ARG:HG3	4:C:1354:HOH:O	2.08	0.53
1:C:984:ASP:HA	1:C:987:MET:HG2	1.91	0.53
1:D:807:ASP:HB2	4:D:1284:HOH:O	2.08	0.53
1:B:985:GLU:HG2	1:B:986:ARG:N	2.23	0.53
2:B:1101:1E8:CAN	2:B:1101:1E8:HNAA	2.22	0.53
1:D:1003:ASP:OD2	1:D:1007[B]:MET:CE	2.57	0.53
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.44	0.53
1:A:805:HIS:O	1:A:809:ILE:HG13	2.09	0.52
1:C:939:CYS:CB	4:C:1252:HOH:O	2.57	0.52
1:B:968:PHE:CD1	1:B:971:MET:HE3	2.45	0.52
1:B:783:THR:CG2	1:B:784:SER:H	2.07	0.52
1:A:835:HIS:O	1:A:836:ARG:HB2	2.10	0.52
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.45	0.52
1:B:805:HIS:HB3	4:B:1210:HOH:O	2.09	0.52
1:D:1003:ASP:CG	1:D:1007[B]:MET:HE1	2.30	0.52
1:C:715:ILE:HD11	1:C:728:LYS:HE2	1.92	0.51
1:C:813:TYR:CE1	1:C:990:PRO:HD3	2.45	0.51
1:D:749:GLU:HG2	4:D:1317:HOH:O	2.09	0.51
1:D:985:GLU:HG2	1:D:986:ARG:HG2	1.93	0.51
1:C:754:LYS:O	1:C:755:ALA:CB	2.57	0.51
1:B:806:LYS:HE2	4:B:1327:HOH:O	2.10	0.51
1:C:791:GLN:HB2	4:C:1311:HOH:O	2.10	0.51
1:D:940:THR:HG23	1:D:978:TYR:O	2.10	0.50
1:B:769:VAL:HG11	1:B:774:VAL:CG1	2.41	0.50
1:C:758:GLU:OE1	1:C:758:GLU:O	2.30	0.50
1:C:811:SER:OG	1:C:975:PRO:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:720:SER:HB2	1:D:748:ARG:NH2	2.27	0.50
1:A:758:GLU:OE1	1:A:762:GLU:OE2	2.30	0.50
1:D:708:LYS:O	1:D:711:GLU:HG2	2.12	0.49
1:A:728:LYS:NZ	4:A:1213:HOH:O	2.46	0.49
1:A:1006:ASP:C	1:A:1007[B]:MET:HG3	2.32	0.49
1:B:832:ARG:CG	1:D:748:ARG:NH1	2.76	0.49
1:A:804:GLU:HG3	4:A:1306:HOH:O	2.12	0.49
1:C:876:VAL:HG12	1:C:881:MET:SD	2.52	0.49
1:B:713:LYS:HZ1	1:B:732[A]:ILE:CG2	2.26	0.49
1:B:878:ILE:HD13	1:B:920:ALA:HB1	1.95	0.49
1:B:926:ILE:HA	1:B:929:LYS:HG3	1.95	0.49
1:B:723:PHE:HD2	4:B:1380:HOH:O	1.96	0.48
1:D:849:GLN:NE2	1:D:990:PRO:HG3	2.22	0.48
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.79	0.48
1:D:714:LYS:O	1:D:715:ILE:HD13	2.13	0.48
1:D:762:GLU:HG2	1:D:861:LEU:HG	1.95	0.48
1:A:732[B]:ILE:HD11	1:A:739:LYS:HG2	1.96	0.48
1:B:716:LYS:CD	4:B:1203:HOH:O	2.59	0.48
1:B:999:ARG:NH1	1:B:999:ARG:CG	2.49	0.48
1:A:724:GLY:HA2	1:A:748:ARG:HG2	1.96	0.47
1:D:700:ASN:N	4:D:1218:HOH:O	2.46	0.47
1:A:789:ILE:HD12	1:A:789:ILE:N	2.29	0.47
1:B:923:ILE:O	1:B:926:ILE:HG13	2.15	0.47
1:C:938:ILE:HG12	4:C:1304:HOH:O	2.14	0.47
1:A:721:GLY:N	1:A:724:GLY:O	2.46	0.47
1:A:762:GLU:HG2	4:A:1276:HOH:O	2.15	0.47
1:B:841:ARG:HH12	1:B:877:PRO:HB3	1.80	0.47
1:A:835:HIS:CD2	4:A:1333:HOH:O	2.68	0.47
1:A:853:ILE:HG21	4:A:1333:HOH:O	2.14	0.47
1:C:747:LEU:HD13	1:C:862:LEU:HD21	1.97	0.47
1:C:976:GLN:HE22	1:C:985:GLU:HG3	1.80	0.47
1:D:986:ARG:HG2	1:D:986:ARG:H	1.45	0.47
1:C:813:TYR:OH	1:C:990:PRO:HB3	2.14	0.47
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.50	0.47
1:A:715:ILE:HD11	1:A:728:LYS:HE2	1.96	0.46
1:C:908:MET:HG3	1:C:939:CYS:SG	2.56	0.46
1:A:849:GLN:HE21	1:A:990:PRO:HG3	1.81	0.46
1:B:926:ILE:HG13	1:B:927:LEU:H	1.80	0.46
1:A:888:HIS:HB2	1:A:890:ILE:HD12	1.96	0.46
1:D:757:LYS:NZ	4:D:1213:HOH:O	2.44	0.46
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:ARG:HD2	1:C:978:TYR:CE1	2.50	0.46
1:D:884:GLU:HG2	1:D:885:SER:N	2.31	0.46
2:A:1101:1E8:CAN	2:A:1101:1E8:HNAA	2.27	0.46
1:B:974:ASP:O	1:B:977:ARG:HB3	2.16	0.46
1:B:762[A]:GLU:HG2	4:B:1224:HOH:O	2.15	0.46
1:D:766:MET:O	1:D:769:VAL:HG22	2.15	0.46
1:D:1003:ASP:CG	1:D:1007[B]:MET:CE	2.85	0.46
1:A:783:THR:O	1:A:784:SER:OG	2.29	0.45
1:B:988:HIS:C	4:B:1201:HOH:O	2.54	0.45
1:D:967:GLU:O	1:D:971:MET:HG3	2.15	0.45
1:A:849:GLN:HG2	1:A:990:PRO:HG2	1.98	0.45
1:A:853:ILE:CG2	4:A:1333:HOH:O	2.65	0.45
1:B:713:LYS:NZ	1:B:732[A]:ILE:CG2	2.76	0.45
1:B:713:LYS:HZ1	1:B:732[A]:ILE:HG22	1.78	0.45
1:D:825:MET:SD	1:D:853:ILE:HD13	2.56	0.45
1:D:849:GLN:HG3	1:D:990:PRO:HG2	1.95	0.45
1:C:876:VAL:HG11	1:C:889:ARG:HH22	1.81	0.45
1:B:748:ARG:H	1:B:748:ARG:HG2	1.21	0.45
1:A:806:LYS:HB2	1:A:910:PHE:HB3	1.98	0.45
1:A:977:ARG:HD3	1:D:926[B]:ILE:HG12	1.98	0.45
1:C:723:PHE:CB	1:C:858:LEU:HD13	2.46	0.45
1:A:723:PHE:CD1	1:A:862:LEU:CD1	2.73	0.45
1:A:926:ILE:HD13	1:A:931:GLU:HB2	1.98	0.45
1:C:783:THR:C	1:C:784:SER:HG	2.05	0.44
1:A:849:GLN:NE2	1:A:990:PRO:HG3	2.33	0.44
1:B:758:GLU:O	1:B:762[B]:GLU:HG3	2.18	0.44
1:C:723:PHE:CD2	1:C:858:LEU:CD1	3.00	0.44
1:B:960:LYS:HB3	1:B:960:LYS:HE3	1.76	0.44
1:C:939:CYS:CA	4:C:1252:HOH:O	2.66	0.44
1:A:999[B]:ARG:HG2	1:A:1003:ASP:O	2.18	0.44
1:B:806:LYS:HB3	1:B:806:LYS:HE3	1.72	0.44
1:B:977:ARG:NE	1:B:978:TYR:OH	2.50	0.44
1:D:972:ALA:CB	1:D:1011:VAL:HG22	2.48	0.44
1:D:926[A]:ILE:HG13	1:D:927:LEU:N	2.32	0.43
4:A:1335:HOH:O	1:B:949:LYS:HD2	2.17	0.43
1:B:793:MET:HA	1:B:794:PRO:HD2	1.85	0.43
1:B:740[B]:ILE:HA	1:B:741:PRO:HD3	1.82	0.43
1:B:793:MET:HE1	4:B:1259:HOH:O	2.17	0.43
1:D:707:LEU:HD12	1:D:789:ILE:HD13	2.01	0.43
1:D:732:ILE:HD13	4:D:1242:HOH:O	2.19	0.43
1:B:699:PRO:HG2	4:B:1328:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:936:PRO:HA	1:D:937:PRO:HD3	1.88	0.43
1:C:898:TRP:CD1	1:C:898:TRP:C	2.92	0.43
1:D:812:GLN:CG	1:D:989:LEU:CD1	2.97	0.43
1:B:968:PHE:CE1	1:B:971:MET:HE1	2.54	0.43
1:C:884:GLU:HG2	1:C:885:SER:N	2.32	0.43
1:A:707:LEU:HD12	1:A:789:ILE:HD13	1.99	0.42
1:A:876:VAL:CG1	1:A:877:PRO:HD2	2.49	0.42
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.54	0.42
1:C:698:ALA:HB3	1:C:699:PRO:HD3	2.01	0.42
1:D:926[A]:ILE:CD1	1:D:931:GLU:O	2.66	0.42
1:B:860:LYS:HE3	4:B:1412:HOH:O	2.19	0.42
1:C:984:ASP:O	1:C:987:MET:HG2	2.19	0.42
1:D:960:LYS:HA	1:D:960:LYS:HD2	1.83	0.42
1:A:771:ASN:ND2	1:A:772:PRO:HD2	2.34	0.42
1:C:949:LYS:NZ	4:C:1224:HOH:O	2.47	0.42
1:C:976:GLN:HE22	1:C:985:GLU:CG	2.32	0.42
1:A:736:GLU:C	4:A:1201:HOH:O	2.57	0.42
1:C:740:ILE:HA	1:C:741:PRO:HD3	1.88	0.42
1:C:811:SER:HB3	1:C:981:ILE:HD12	2.01	0.42
1:A:898:TRP:CD1	1:A:898:TRP:C	2.93	0.42
1:B:769:VAL:HG11	1:B:774:VAL:HG11	2.02	0.42
1:B:842:ASN:O	1:B:854:THR:HG22	2.19	0.42
1:D:915:TYR:HE1	1:D:926[A]:ILE:HD11	1.82	0.42
1:B:732[A]:ILE:CD1	1:B:733:PRO:HD2	2.33	0.42
1:B:805:HIS:O	1:B:809:ILE:HG13	2.19	0.42
1:A:983:GLY:HA2	1:A:985:GLU:OE2	2.21	0.41
1:C:833:LEU:HD13	1:C:856:PHE:CZ	2.55	0.41
1:B:716:LYS:HZ1	1:B:718:LEU:HD23	1.84	0.41
1:B:968:PHE:HA	1:B:971:MET:HE2	2.03	0.41
1:D:861:LEU:HD23	1:D:861:LEU:HA	1.86	0.41
1:C:977:ARG:HD2	1:C:978:TYR:CZ	2.55	0.41
1:B:793:MET:CE	4:B:1259:HOH:O	2.68	0.41
1:B:841:ARG:NH1	1:B:877:PRO:HB3	2.35	0.41
1:D:732:ILE:HD12	1:D:732:ILE:N	2.35	0.41
1:D:987:MET:H	1:D:987:MET:HG2	1.55	0.41
1:A:913:LYS:HE2	1:A:916:ASP:OD1	2.20	0.41
1:C:712:PHE:C	1:C:713:LYS:HG2	2.40	0.41
1:B:905:TRP:HD1	1:B:947:MET:CE	2.34	0.41
1:C:980:VAL:O	1:C:980:VAL:HG12	2.21	0.41
1:A:849:GLN:CG	1:A:990:PRO:HG2	2.50	0.41
1:B:985:GLU:HG2	1:B:986:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:ARG:HA	1:B:1003:ASP:HB3	2.01	0.41
1:C:778:LEU:N	1:C:778:LEU:HD23	2.36	0.41
1:A:783:THR:O	1:A:784:SER:CB	2.69	0.41
1:B:795:PHE:HB2	1:B:845:VAL:O	2.21	0.41
1:B:987:MET:O	4:B:1201:HOH:O	2.21	0.41
1:C:783:THR:O	1:C:784:SER:CB	2.69	0.41
1:C:947:MET:O	1:C:950:CYS:HB2	2.21	0.41
1:D:836:ARG:CZ	1:D:860:LYS:HD3	2.50	0.41
1:D:984:ASP:HA	1:D:987:MET:CG	2.48	0.41
1:B:972:ALA:HB3	1:B:1011:VAL:HG11	2.02	0.41
1:D:757:LYS:O	1:D:761:ASP:OD2	2.39	0.40
1:B:858:LEU:HD12	1:B:858:LEU:HA	1.78	0.40
1:B:772:PRO:HB3	1:B:1007:MET:HB3	2.02	0.40
1:C:960:LYS:HD2	1:C:960:LYS:HA	1.91	0.40
1:A:812:GLN:NE2	1:A:989:LEU:H	2.19	0.40
1:D:972:ALA:O	1:D:975:PRO:HD3	2.20	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	301/331 (91%)	297 (99%)	4 (1%)	0	100	100
1	B	295/331 (89%)	289 (98%)	6 (2%)	0	100	100
1	C	301/331 (91%)	293 (97%)	8 (3%)	0	100	100
1	D	300/331 (91%)	296 (99%)	4 (1%)	0	100	100
All	All	1197/1324 (90%)	1175 (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	269/288 (93%)	246 (91%)	23 (9%)	10	3
1	B	267/288 (93%)	249 (93%)	18 (7%)	16	5
1	C	267/288 (93%)	250 (94%)	17 (6%)	17	6
1	D	268/288 (93%)	251 (94%)	17 (6%)	18	7
All	All	1071/1152 (93%)	996 (93%)	75 (7%)	17	5

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	715	ILE
1	A	720	SER
1	A	723	PHE
1	A	732[A]	ILE
1	A	732[B]	ILE
1	A	754	LYS
1	A	757	LYS
1	A	760	LEU
1	A	761	ASP
1	A	782	LEU
1	A	806	LYS
1	A	846	LYS
1	A	861	LEU
1	A	918	ILE
1	A	926	ILE
1	A	962	ARG
1	A	970[A]	LYS
1	A	970[B]	LYS
1	A	982[A]	GLN
1	A	982[B]	GLN
1	A	985	GLU
1	A	998	TYR
1	A	1006	ASP
1	B	701	GLN

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Mol	Chain	Res	Type
1	B	713	LYS
1	B	716	LYS
1	B	720[A]	SER
1	B	720[B]	SER
1	B	723	PHE
1	B	748	ARG
1	B	757	LYS
1	B	858	LEU
1	B	861	LEU
1	B	928[A]	GLU
1	B	928[B]	GLU
1	B	949	LYS
1	B	952	MET
1	B	986	ARG
1	B	989	LEU
1	B	994	ASP
1	B	999	ARG
1	C	711	GLU
1	C	758	GLU
1	C	760	LEU
1	C	832	ARG
1	C	841[A]	ARG
1	C	841[B]	ARG
1	C	860	LYS
1	C	861	LEU
1	C	875	LYS
1	C	889	ARG
1	C	913	LYS
1	C	929	LYS
1	C	973	ARG
1	C	974	ASP
1	C	977	ARG
1	C	991	SER
1	C	994	ASP
1	D	714	LYS
1	D	732	ILE
1	D	748	ARG
1	D	749	GLU
1	D	782	LEU
1	D	783	THR
1	D	861	LEU
1	D	876	VAL

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Mol	Chain	Res	Type
1	D	898	TRP
1	D	922	GLU
1	D	926[A]	ILE
1	D	926[B]	ILE
1	D	986	ARG
1	D	987	MET
1	D	998	TYR
1	D	999	ARG
1	D	1011	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	773	HIS
1	A	812	GLN
1	C	976	GLN
1	D	812	GLN
1	D	849	GLN

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 7 ligands modelled in this entry, 3 are 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	1E8	A	1101	1	35,37,37	4.47	7 (20%)	41,52,52	2.13	6 (14%)
2	1E8	D	1101	1	35,37,37	4.69	7 (20%)	41,52,52	2.38	12 (29%)
2	1E8	C	1101	1	35,37,37	4.63	8 (22%)	41,52,52	2.39	11 (26%)
2	1E8	B	1101	1	35,37,37	4.45	7 (20%)	41,52,52	2.15	6 (14%)

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	1E8	A	1101	1	-	2/14/28/28	0/5/5/5
2	1E8	D	1101	1	-	4/14/28/28	0/5/5/5
2	1E8	C	1101	1	-	4/14/28/28	0/5/5/5
2	1E8	B	1101	1	-	2/14/28/28	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	1E8	NAU-NBF	-23.66	1.08	1.37
2	C	1101	1E8	NAU-NBF	-23.18	1.09	1.37
2	A	1101	1E8	NAU-NBF	-22.28	1.10	1.37
2	B	1101	1E8	NAU-NBF	-22.28	1.10	1.37
2	C	1101	1E8	CBA-CBB	-11.10	1.33	1.49
2	D	1101	1E8	CBA-CBB	-11.02	1.33	1.49
2	A	1101	1E8	CBA-CBB	-10.84	1.34	1.49
2	B	1101	1E8	CBA-CBB	-10.63	1.34	1.49
2	B	1101	1E8	CAA-CAD	4.96	1.54	1.30
2	C	1101	1E8	C2-N3	4.66	1.39	1.32
2	C	1101	1E8	CAA-CAD	4.55	1.52	1.30
2	A	1101	1E8	CAA-CAD	4.50	1.52	1.30
2	D	1101	1E8	CAA-CAD	4.45	1.52	1.30
2	A	1101	1E8	C2-N3	4.33	1.39	1.32
2	D	1101	1E8	C2-N3	4.19	1.38	1.32
2	B	1101	1E8	C2-N3	4.03	1.38	1.32
2	B	1101	1E8	C5-C4	-3.95	1.32	1.43
2	D	1101	1E8	C5-C4	-3.85	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	1E8	C5-C4	-3.79	1.32	1.43
2	C	1101	1E8	C5-C4	-3.77	1.33	1.43
2	D	1101	1E8	CBB-NAU	-3.38	1.32	1.35
2	A	1101	1E8	CBB-NAU	-2.92	1.32	1.35
2	A	1101	1E8	C2-N1	2.78	1.39	1.33
2	B	1101	1E8	C2-N1	2.69	1.38	1.33
2	D	1101	1E8	C2-N1	2.60	1.38	1.33
2	C	1101	1E8	CBB-NAU	-2.58	1.33	1.35
2	C	1101	1E8	C2-N1	2.45	1.38	1.33
2	C	1101	1E8	OAV-CAY	-2.13	1.35	1.39
2	B	1101	1E8	CBB-NAU	-2.05	1.33	1.35

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	1E8	CBB-NAU-NBF	8.01	111.57	105.17
2	D	1101	1E8	CBB-NAU-NBF	7.75	111.36	105.17
2	A	1101	1E8	CBB-NAU-NBF	7.59	111.23	105.17
2	C	1101	1E8	CAA-CAD-CAW	-7.57	105.84	121.33
2	B	1101	1E8	CBB-NAU-NBF	7.15	110.88	105.17
2	D	1101	1E8	CAA-CAD-CAW	-6.96	107.09	121.33
2	B	1101	1E8	N3-C2-N1	-6.83	118.00	128.68
2	D	1101	1E8	N3-C2-N1	-6.78	118.09	128.68
2	A	1101	1E8	N3-C2-N1	-6.74	118.14	128.68
2	C	1101	1E8	N3-C2-N1	-6.67	118.25	128.68
2	B	1101	1E8	CAA-CAD-CAW	-6.51	108.01	121.33
2	A	1101	1E8	CAA-CAD-CAW	-5.75	109.57	121.33
2	C	1101	1E8	CAQ-NBG-CAR	3.28	119.63	113.06
2	D	1101	1E8	CAD-CAW-NBG	-3.23	113.91	117.66
2	C	1101	1E8	CBE-CAR-NBG	3.06	113.69	109.57
2	D	1101	1E8	CBE-CAR-NBG	3.00	113.62	109.57
2	A	1101	1E8	CAQ-NBG-CAR	2.92	118.90	113.06
2	A	1101	1E8	C5-C6-NAB	-2.84	117.55	122.67
2	D	1101	1E8	CAQ-NBG-CAR	2.82	118.70	113.06
2	C	1101	1E8	CBB-C5-C4	-2.63	101.60	106.55
2	D	1101	1E8	CAM-CBA-CBB	2.62	124.94	120.65
2	D	1101	1E8	CAO-CAQ-NBG	-2.57	105.59	110.66
2	D	1101	1E8	CBB-C5-C4	-2.53	101.78	106.55
2	D	1101	1E8	OAC-CAW-NBG	2.50	124.73	121.13
2	B	1101	1E8	CBB-C5-C4	-2.46	101.92	106.55
2	B	1101	1E8	CAQ-NBG-CAR	2.45	117.96	113.06
2	C	1101	1E8	CAM-CBA-CBB	2.41	124.59	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1101	1E8	CAN-CBA-CBB	-2.40	116.72	120.65
2	A	1101	1E8	CBB-C5-C4	-2.27	102.28	106.55
2	D	1101	1E8	C5-C6-NAB	-2.24	118.63	122.67
2	C	1101	1E8	C5-C6-NAB	-2.23	118.65	122.67
2	C	1101	1E8	CAD-CAW-NBG	-2.20	115.11	117.66
2	C	1101	1E8	OAC-CAW-NBG	2.15	124.23	121.13
2	C	1101	1E8	CAN-CBA-CBB	-2.14	117.15	120.65
2	B	1101	1E8	C5-C6-NAB	-2.01	119.04	122.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	1E8	CAM-CBA-CBB-NAU
2	A	1101	1E8	CAN-CBA-CBB-NAU
2	B	1101	1E8	CAM-CBA-CBB-NAU
2	B	1101	1E8	CAN-CBA-CBB-NAU
2	C	1101	1E8	CAA-CAD-CAW-OAC
2	C	1101	1E8	CAA-CAD-CAW-NBG
2	C	1101	1E8	CAM-CBA-CBB-NAU
2	C	1101	1E8	CAN-CBA-CBB-NAU
2	D	1101	1E8	CAA-CAD-CAW-NBG
2	D	1101	1E8	CAM-CBA-CBB-NAU
2	D	1101	1E8	CAN-CBA-CBB-NAU
2	D	1101	1E8	CAA-CAD-CAW-OAC

There are no ring outliers.

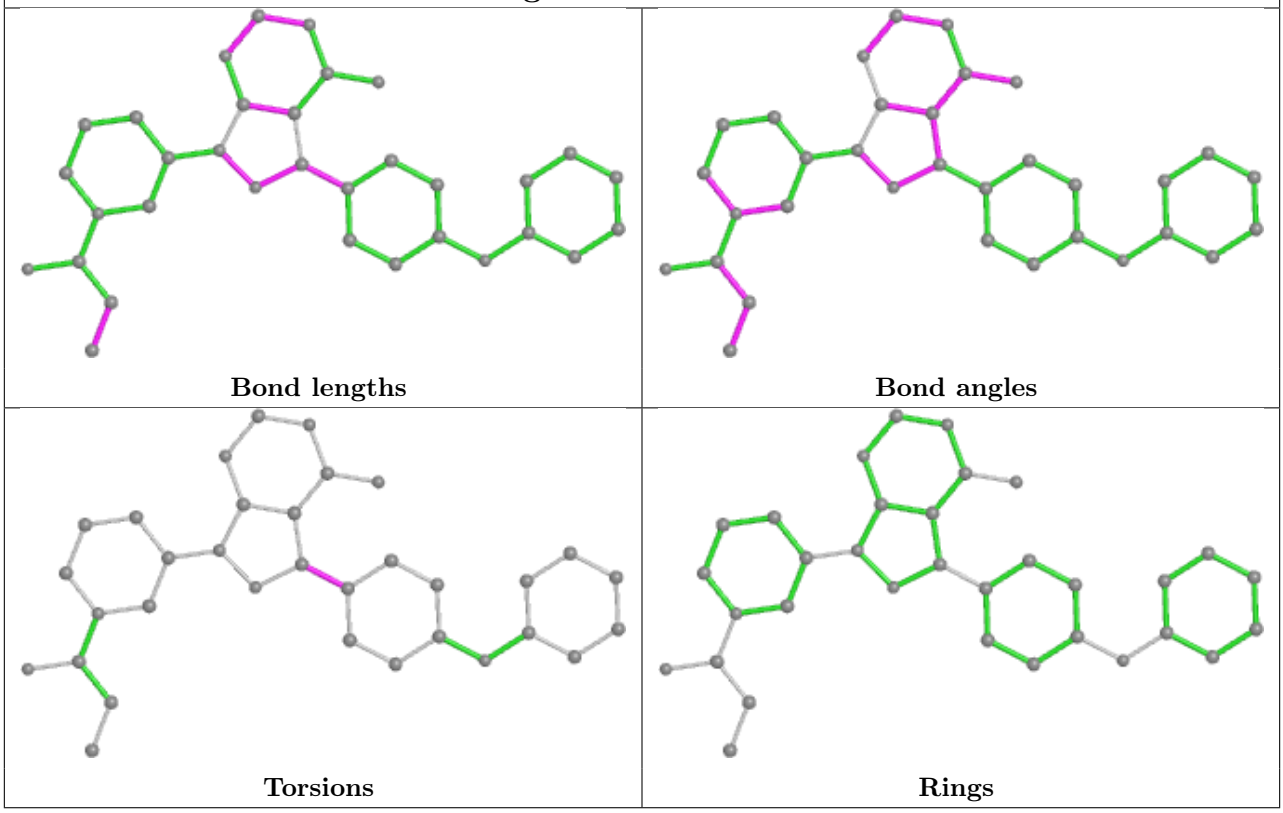
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	1E8	1	0
2	B	1101	1E8	1	0

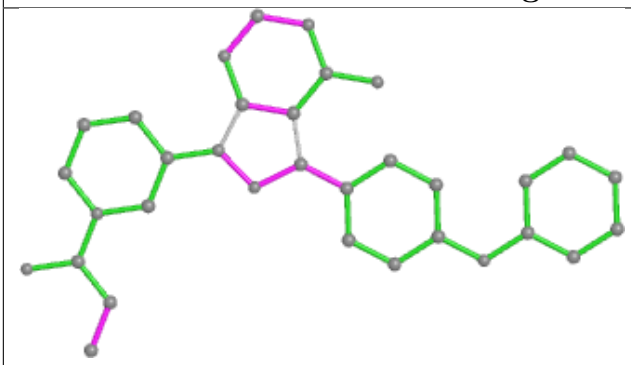
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

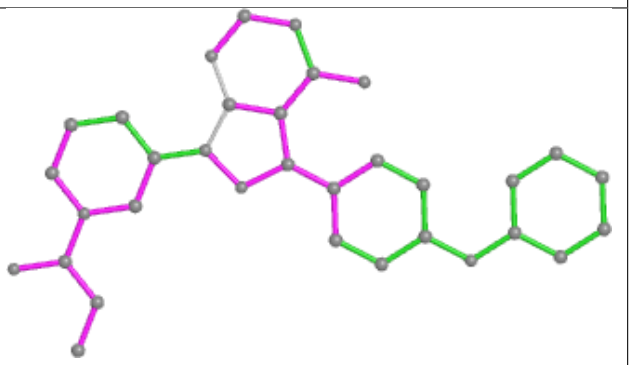
Ligand 1E8 A 1101



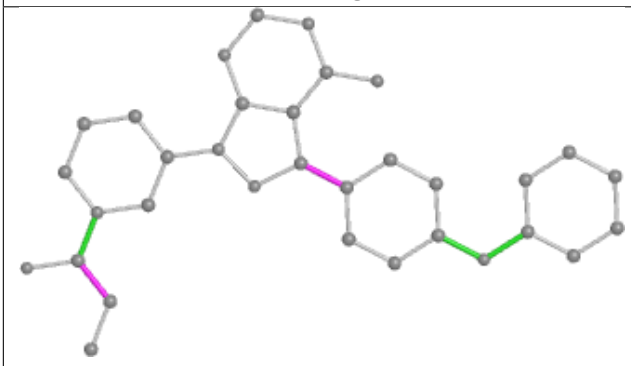
Ligand 1E8 D 1101



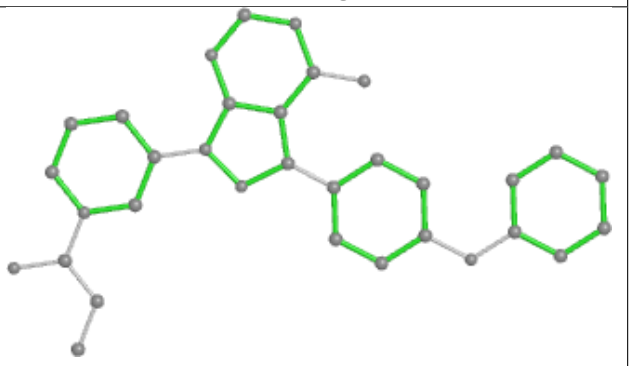
Bond lengths



Bond angles

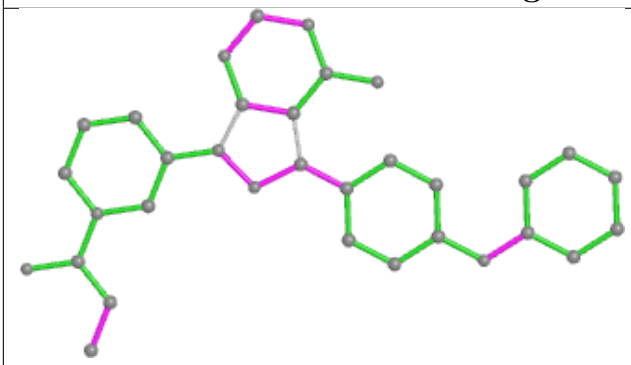


Torsions

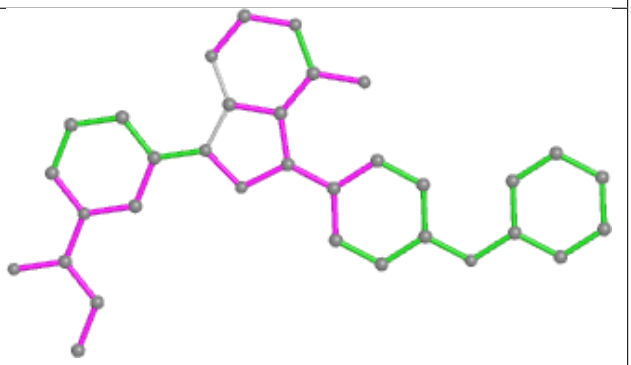


Rings

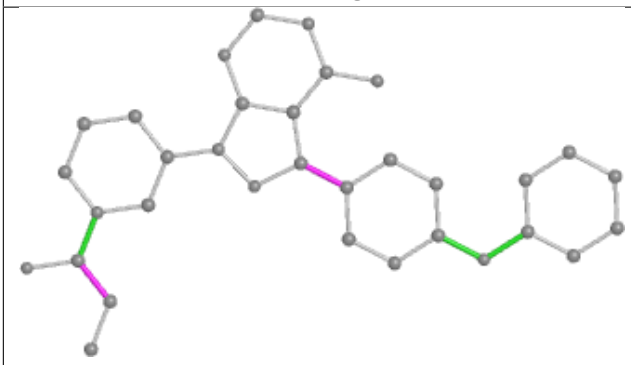
Ligand 1E8 C 1101



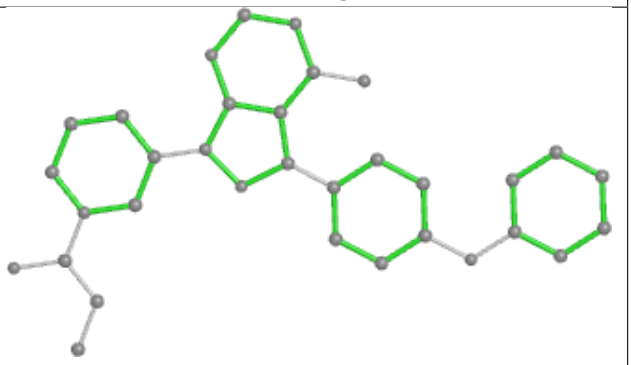
Bond lengths



Bond angles

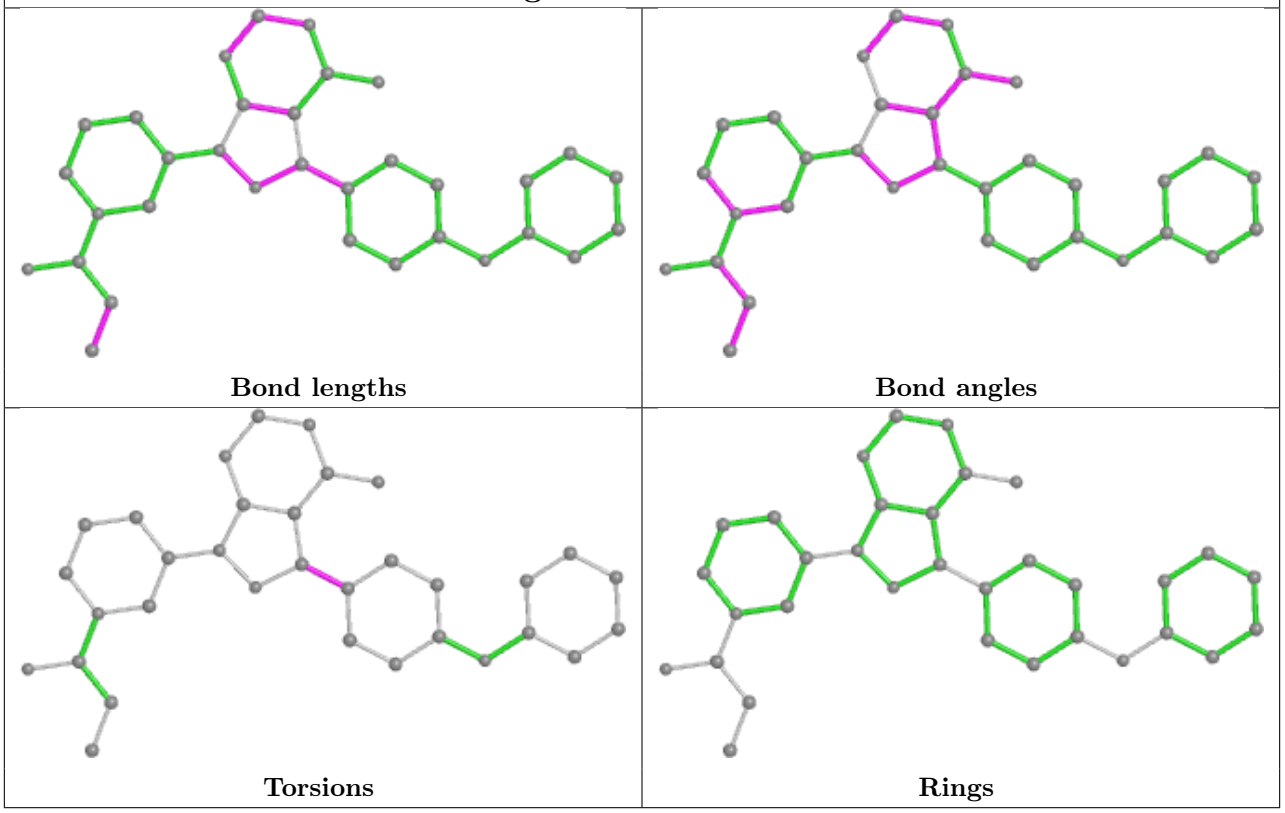


Torsions



Rings

Ligand 1E8 B 1101



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	302/331 (91%)	0.10	15 (4%)	28	39	13, 25, 48, 58	4 (1%)
1	B	295/331 (89%)	0.16	12 (4%)	37	46	13, 25, 51, 66	4 (1%)
1	C	306/331 (92%)	0.24	17 (5%)	24	33	15, 27, 52, 70	2 (0%)
1	D	300/331 (90%)	0.14	17 (5%)	23	32	14, 26, 51, 64	1 (0%)
All	All	1203/1324 (90%)	0.16	61 (5%)	28	37	13, 26, 51, 70	11 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	722	ALA	8.2
1	C	697	GLU	7.8
1	B	721	GLY	7.8
1	C	986	ARG	6.1
1	B	723	PHE	5.7
1	C	784	SER	4.8
1	C	699	PRO	4.4
1	A	1016	TYR	4.1
1	A	1017	LEU	4.1
1	A	721	GLY	4.0
1	B	986	ARG	3.8
1	A	722	ALA	3.7
1	A	1014	ASP	3.7
1	C	1021	GLN	3.5
1	C	988	HIS	3.4
1	A	784	SER	3.3
1	B	748	ARG	3.3
1	D	784	SER	3.2
1	D	754	LYS	3.2
1	B	720[A]	SER	3.2
1	A	700	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	701	GLN	3.1
1	C	698	ALA	3.1
1	A	723	PHE	3.1
1	C	989	LEU	3.0
1	B	785	THR	3.0
1	D	986	ARG	3.0
1	D	985	GLU	2.9
1	D	750	ALA	2.9
1	D	751	THR	2.8
1	C	1011	VAL	2.8
1	D	1010	VAL	2.8
1	C	807	ASP	2.8
1	A	1015	GLU	2.8
1	A	986	ARG	2.7
1	D	989	LEU	2.7
1	D	987	MET	2.7
1	C	990	PRO	2.7
1	A	701	GLN	2.6
1	B	699	PRO	2.6
1	D	753	PRO	2.6
1	A	748	ARG	2.6
1	D	1012	ASP	2.6
1	D	1011	VAL	2.5
1	A	985	GLU	2.5
1	C	754	LYS	2.4
1	D	748	ARG	2.4
1	C	1019	PRO	2.4
1	D	890	ILE	2.3
1	C	987	MET	2.3
1	A	1013	ALA	2.3
1	C	862	LEU	2.3
1	D	702	ALA	2.2
1	B	784	SER	2.2
1	B	918	ILE	2.2
1	A	929	LYS	2.2
1	C	977	ARG	2.2
1	C	991	SER	2.1
1	D	1009	ASP	2.1
1	B	807	ASP	2.0
1	D	860	LYS	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)

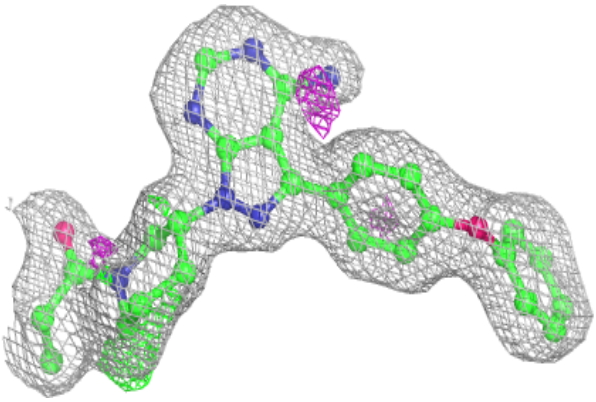
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

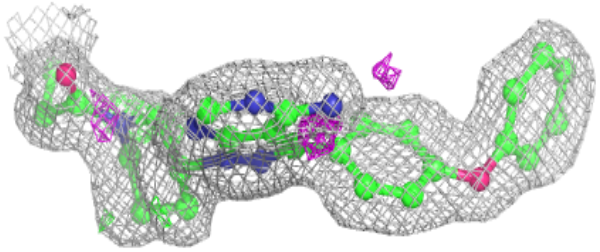
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	D	1102	1/1	0.76	0.09	62,62,62,62	0
3	CL	C	1103	1/1	0.92	0.07	62,62,62,62	1
2	1E8	D	1101	33/33	0.92	0.12	17,23,31,34	0
2	1E8	C	1101	33/33	0.93	0.10	15,22,29,34	0
2	1E8	A	1101	33/33	0.95	0.09	17,21,30,36	0
2	1E8	B	1101	33/33	0.95	0.09	17,24,36,44	0
3	CL	C	1102	1/1	0.98	0.12	43,43,43,43	0

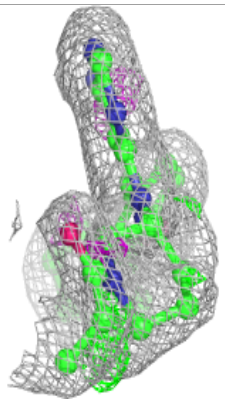
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1E8 D 1101:

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

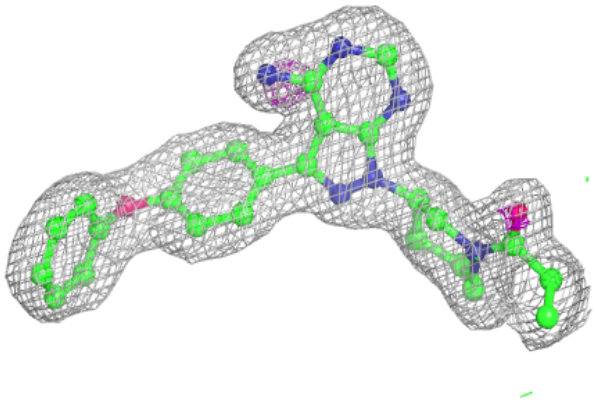


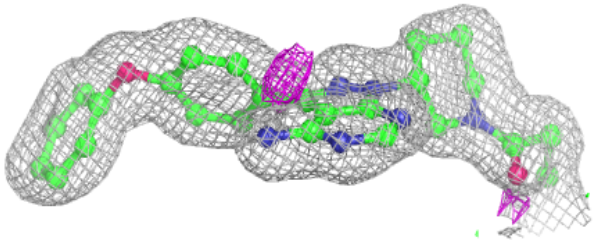


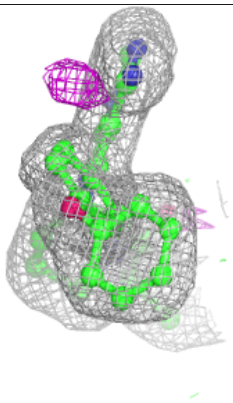


Electron density around 1E8 C 1101:

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

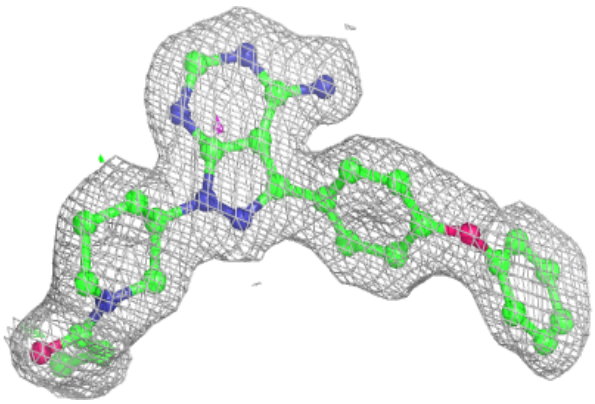


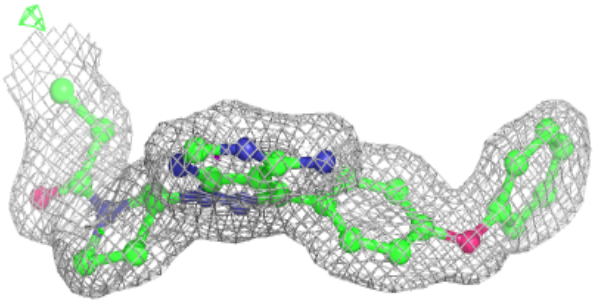


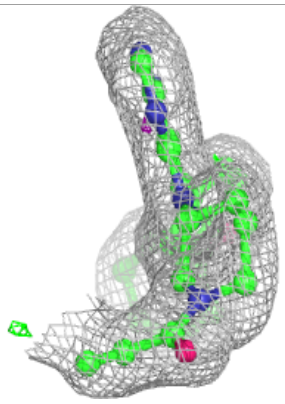


Electron density around 1E8 A 1101:

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

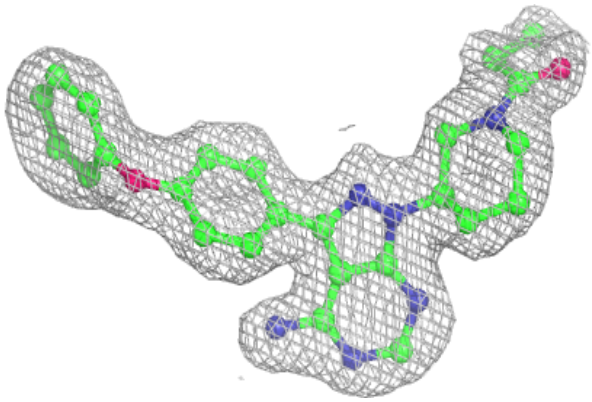


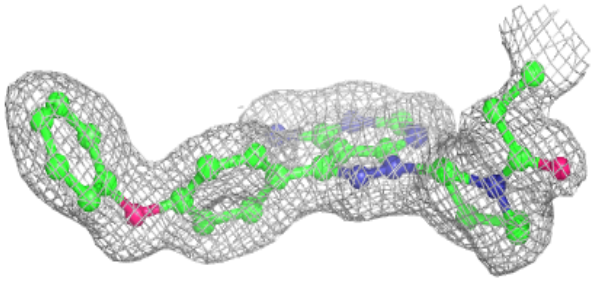


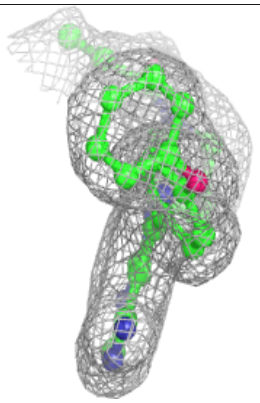


Electron density around 1E8 B 1101:

$2mF_o$-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.