



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 02:24 PM EST

PDB ID : 6V66
Title : EGFR(T790M/V948R) in complex with LN2899
Authors : Heppner, D.E.; Eck, M.J.
Deposited on : 2019-12-04
Resolution : 1.79 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 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 : 2.26
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) : 2.26

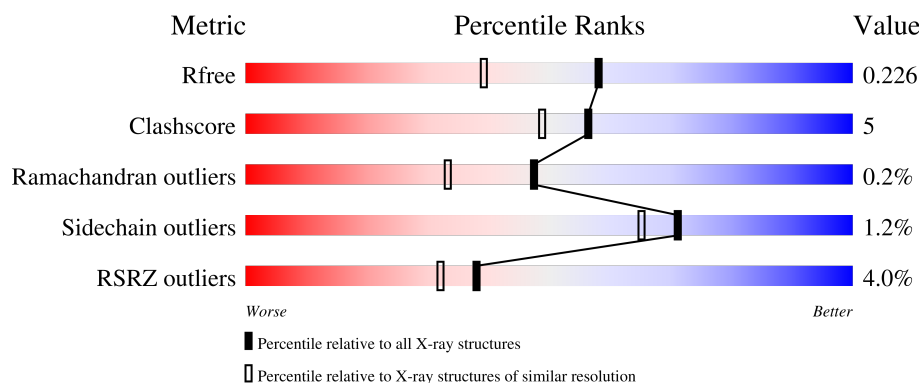
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	327	<div> <div>3%</div> <div>87%</div> <div>8%</div> <div>.</div> <div>.</div> </div>
1	B	327	<div> <div>5%</div> <div>83%</div> <div>10%</div> <div>8%</div> </div>
1	C	327	<div> <div>6%</div> <div>77%</div> <div>13%</div> <div>.</div> <div>9%</div> </div>
1	D	327	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	C	1102	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11049 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	D	314	Total	C	N	O	S	0	1	0
			2530	1619	428	464	19			
1	A	314	Total	C	N	O	S	0	0	0
			2521	1614	427	461	19			
1	B	302	Total	C	N	O	S	0	1	0
			2440	1566	413	441	20			
1	C	299	Total	C	N	O	S	0	0	0
			2410	1548	408	435	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

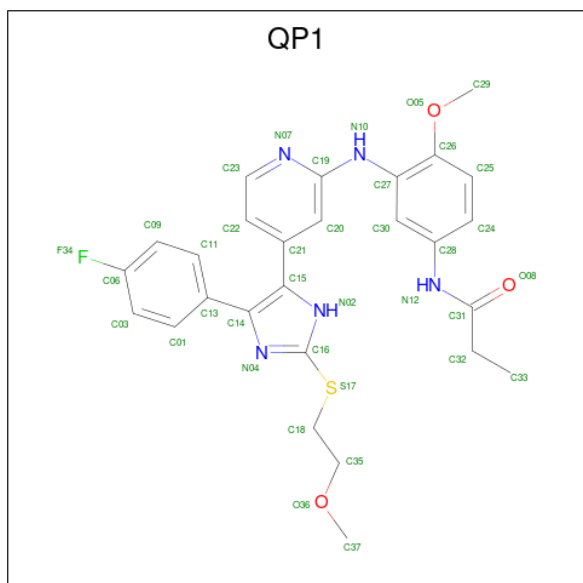
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is N-{3-[(4-{4-(4-fluorophenyl)-2-[(2-methoxyethyl)sulfanyl]-1H-imidazol-5-yl}pyridin-2-yl)amino]-4-methoxyphenyl}propanamide (three-letter code: QP1) (formula: $C_{27}H_{28}FN_5O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	S	0	0
			37	27	1	5	3	1		
4	A	1	Total	C	F	N	O	S	0	0
			37	27	1	5	3	1		
4	B	1	Total	C	F	N	O	S	0	0
			37	27	1	5	3	1		
4	C	1	Total	C	F	N	O	S	0	0
			37	27	1	5	3	1		

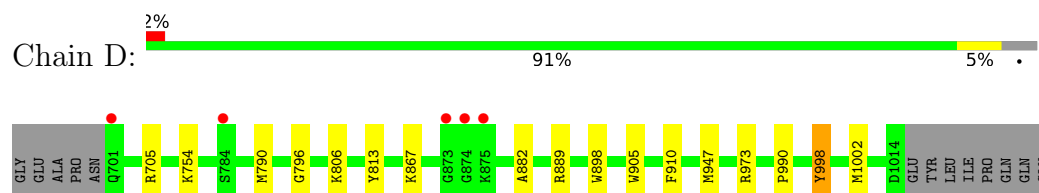
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	260	Total	O	0	0
			260	260		
5	A	301	Total	O	0	0
			301	301		
5	B	217	Total	O	0	0
			217	217		
5	C	210	Total	O	0	0
			210	210		

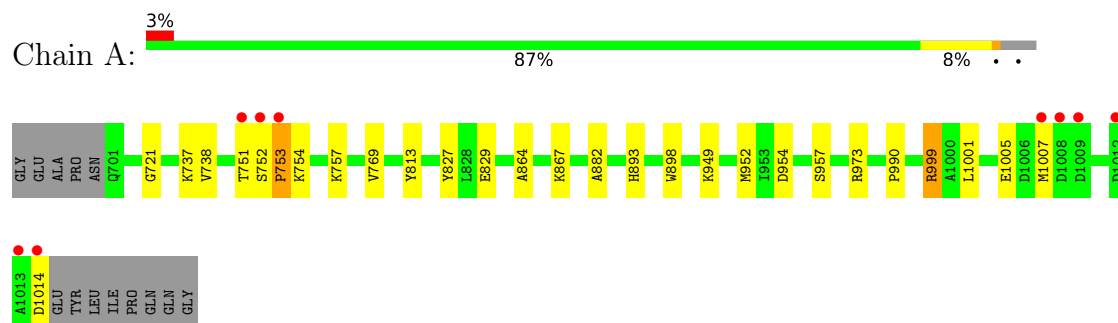
3 Residue-property plots [i](#)

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.

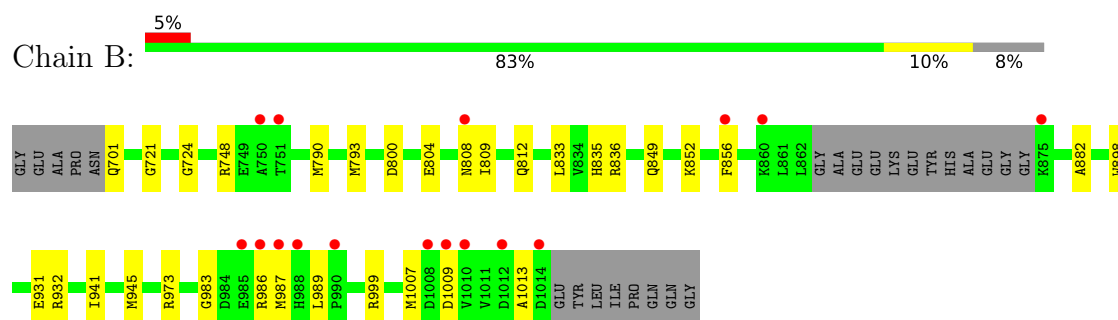
- Molecule 1: Epidermal growth factor receptor



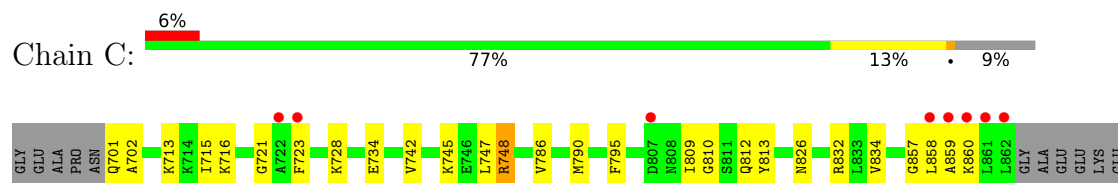
- Molecule 1: Epidermal growth factor receptor

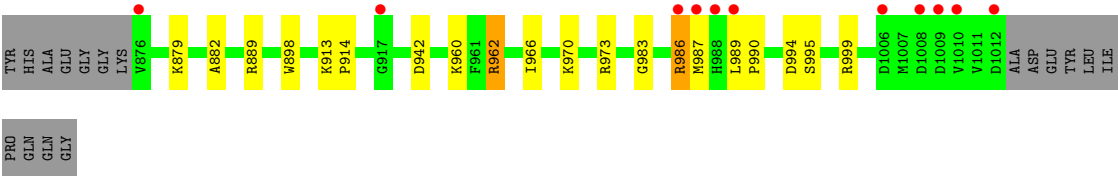


- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.48Å 102.45Å 87.42Å 90.00° 102.78° 90.00°	Depositor
Resolution (Å)	85.26 – 1.79 85.26 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (85.26-1.79) 99.0 (85.26-1.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.185 , 0.226 0.185 , 0.226	Depositor DCC
R_{free} test set	5744 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11049	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 22.66 % 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 5.4431e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, QP1, CL

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	0.33	0/2576	0.49	0/3483
1	B	0.32	0/2492	0.50	0/3369
1	C	0.31	0/2462	0.48	0/3330
1	D	0.33	0/2585	0.48	0/3495
All	All	0.32	0/10115	0.49	0/13677

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2521	0	2550	17	0
1	B	2440	0	2485	23	0
1	C	2410	0	2455	53	0
1	D	2530	0	2555	10	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
2	C	1	0	0	4	0
2	D	1	0	0	0	0
3	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	6	0	0
4	A	37	0	0	0	0
4	B	37	0	0	0	0
4	C	37	0	0	1	0
4	D	37	0	0	1	0
5	A	301	0	0	0	0
5	B	217	0	0	4	0
5	C	210	0	0	12	0
5	D	260	0	0	2	0
All	All	11049	0	10057	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 5.

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:C:790:MET:SD	5:C:1390:HOH:O	2.43	0.77
1:C:809:ILE:C	1:C:987:MET:CE	2.53	0.76
1:C:810:GLY:HA2	1:C:987:MET:HE2	1.69	0.73
1:B:986:ARG:HB3	1:B:987:MET:SD	2.31	0.71
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.26	0.70
1:B:812:GLN:HG2	1:B:989:LEU:HG	1.72	0.70
1:C:970:LYS:NZ	5:C:1201:HOH:O	2.20	0.70
1:B:790:MET:SD	5:B:1478:HOH:O	2.51	0.68
1:A:751:THR:O	1:A:753:PRO:HD3	1.95	0.66
1:B:983:GLY:O	1:B:986:ARG:HB2	1.96	0.66
1:D:889:ARG:NH1	5:D:1303:HOH:O	2.30	0.64
1:C:745:LYS:HD3	1:C:858:LEU:HD21	1.81	0.63
1:C:723:PHE:CD2	1:C:858:LEU:HB3	2.35	0.62
1:C:810:GLY:CA	1:C:987:MET:HE2	2.30	0.62
1:A:973:ARG:HB3	1:A:1014:ASP:HB3	1.82	0.61
1:D:973:ARG:NH2	5:D:1306:HOH:O	2.34	0.61
1:C:812:GLN:HG2	1:C:989:LEU:HG	1.81	0.60
1:C:962:ARG:NH1	5:C:1209:HOH:O	2.35	0.60
1:B:724:GLY:HA2	1:B:748:ARG:HG3	1.84	0.58
1:C:810:GLY:N	1:C:987:MET:CE	2.66	0.58
1:B:808:ASN:O	1:B:987:MET:HG2	2.04	0.58
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.69	0.57
1:C:983:GLY:HA3	1:C:986:ARG:NH1	2.20	0.56
1:A:751:THR:HG21	1:A:864:ALA:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:913:LYS:NZ	5:C:1211:HOH:O	2.37	0.56
1:B:849:GLN:NE2	5:B:1304:HOH:O	2.37	0.55
1:C:721:GLY:HA3	2:C:1102:CL:CL	2.45	0.54
1:B:748:ARG:HD2	1:C:832:ARG:HD3	1.89	0.54
1:B:833:LEU:HB3	1:B:856:PHE:CE1	2.42	0.54
1:C:826:ASN:ND2	1:C:962:ARG:HG2	2.23	0.53
1:C:973:ARG:NH2	5:C:1214:HOH:O	2.41	0.53
1:B:748:ARG:HG2	1:C:832:ARG:CZ	2.38	0.53
1:A:721:GLY:HA3	2:A:1201:CL:CL	2.46	0.52
1:D:905:TRP:CD1	1:D:947:MET:HE1	2.44	0.52
1:C:701:GLN:HG2	1:C:702:ALA:H	1.75	0.51
1:C:790:MET:HE3	5:C:1355:HOH:O	2.10	0.51
1:A:738:VAL:HG21	1:C:795:PHE:CZ	2.46	0.51
1:C:966:ILE:O	1:C:970:LYS:HG3	2.11	0.51
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.46	0.50
1:D:806:LYS:HG3	1:D:910:PHE:CG	2.46	0.50
1:C:810:GLY:N	1:C:987:MET:HE2	2.26	0.50
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.46	0.50
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.11	0.50
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.11	0.49
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.95	0.49
1:A:949:LYS:O	1:A:952:MET:HG3	2.13	0.49
1:B:973:ARG:NH2	5:B:1310:HOH:O	2.45	0.49
1:C:723:PHE:CE2	1:C:858:LEU:HB3	2.48	0.49
1:C:879:LYS:HD3	1:C:914:PRO:O	2.12	0.49
1:A:752:SER:O	1:A:754:LYS:N	2.45	0.49
1:A:769:VAL:HG13	1:A:827:TYR:HE2	1.78	0.48
1:C:701:GLN:HB3	5:C:1303:HOH:O	2.13	0.48
1:A:1001:LEU:HD21	1:C:742:VAL:HG12	1.96	0.47
1:A:751:THR:HG21	1:A:864:ALA:N	2.28	0.47
1:C:745:LYS:NZ	2:C:1102:CL:CL	2.75	0.47
1:C:960:LYS:NZ	5:C:1217:HOH:O	2.44	0.47
1:C:723:PHE:HD1	2:C:1102:CL:CL	2.35	0.47
1:C:713:LYS:HD2	1:C:715:ILE:HG22	1.96	0.47
1:C:723:PHE:HB2	2:C:1102:CL:CL	2.52	0.47
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.50	0.47
1:C:747:LEU:HD12	1:C:786:VAL:HB	1.96	0.47
4:C:1101:QP1:N12	5:C:1206:HOH:O	2.36	0.47
1:C:734:GLU:OE1	5:C:1202:HOH:O	2.20	0.46
1:A:954:ASP:OD2	1:A:957:SER:OG	2.32	0.46
1:B:941:ILE:HG13	1:B:945:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:ILE:O	1:B:987:MET:HE3	2.17	0.45
1:B:835:HIS:O	1:B:836:ARG:HB2	2.17	0.45
1:C:889:ARG:HD3	1:C:889:ARG:HA	1.76	0.45
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.52	0.45
1:A:829:GLU:HG3	1:A:893:HIS:CD2	2.51	0.45
1:A:1005:GLU:O	1:A:1007:MET:HG2	2.17	0.44
1:C:715:ILE:HG12	1:C:728:LYS:O	2.17	0.44
1:B:721:GLY:HA3	2:B:1203:CL:CL	2.55	0.44
1:B:931:GLU:HG2	1:B:932:ARG:N	2.33	0.43
1:C:826:ASN:HD21	1:C:962:ARG:HG2	1.82	0.43
1:C:834:VAL:O	1:C:860:LYS:HE3	2.17	0.43
1:B:800:ASP:O	1:B:804:GLU:HG3	2.17	0.43
1:B:833:LEU:HD13	1:B:856:PHE:CZ	2.53	0.43
1:B:701:GLN:NE2	5:B:1323:HOH:O	2.52	0.43
1:C:826:ASN:ND2	5:C:1209:HOH:O	2.49	0.42
1:C:716:LYS:HD2	5:C:1347:HOH:O	2.17	0.42
1:C:701:GLN:HG2	1:C:702:ALA:N	2.33	0.42
1:C:857:GLY:H	1:C:860:LYS:NZ	2.17	0.42
1:C:809:ILE:C	1:C:987:MET:HE1	2.39	0.42
1:C:857:GLY:H	1:C:860:LYS:HZ1	1.67	0.42
1:C:723:PHE:HE2	1:C:859:ALA:N	2.18	0.42
1:D:796:GLY:HA2	4:D:1203:QP1:C30	2.50	0.41
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.20	0.41
1:A:999:ARG:HH11	1:A:1007:MET:HE2	1.85	0.41
1:B:999:ARG:NH2	1:B:1007:MET:SD	2.93	0.41
1:C:857:GLY:HA2	1:C:860:LYS:HG2	2.02	0.41
1:D:867:LYS:HD2	1:D:867:LYS:H	1.86	0.41
1:D:998:TYR:HD1	1:D:1002:MET:HE3	1.85	0.41
1:C:810:GLY:N	1:C:987:MET:HE3	2.35	0.41
1:C:809:ILE:C	1:C:987:MET:HE3	2.39	0.41
1:B:941:ILE:HD12	1:B:941:ILE:HA	1.97	0.40
1:C:809:ILE:N	1:C:987:MET:HE1	2.36	0.40
1:B:793:MET:CE	1:B:852:LYS:HD3	2.51	0.40
1:C:721:GLY:O	1:C:748:ARG:NH2	2.47	0.40
1:C:995:SER:O	1:C:999:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/327 (95%)	305 (98%)	6 (2%)	1 (0%)	41	27
1	B	299/327 (91%)	292 (98%)	6 (2%)	1 (0%)	41	27
1	C	295/327 (90%)	288 (98%)	7 (2%)	0	100	100
1	D	313/327 (96%)	307 (98%)	6 (2%)	0	100	100
All	All	1219/1308 (93%)	1192 (98%)	25 (2%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1013	ALA
1	A	753	PRO

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	277/287 (96%)	273 (99%)	4 (1%)	67	59
1	B	271/287 (94%)	270 (100%)	1 (0%)	91	89
1	C	268/287 (93%)	264 (98%)	4 (2%)	65	56
1	D	278/287 (97%)	274 (99%)	4 (1%)	67	59
All	All	1094/1148 (95%)	1081 (99%)	13 (1%)	71	65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	705	ARG
1	D	754	LYS
1	D	790	MET
1	D	998	TYR
1	A	737	LYS
1	A	757	LYS
1	A	867	LYS
1	A	999	ARG
1	B	1009	ASP
1	C	748	ARG
1	C	942	ASP
1	C	962	ARG
1	C	986	ARG

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

Mol	Chain	Res	Type
1	C	826	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	QP1	B	1202	1	38,40,40	4.93	26 (68%)	45,54,54	1.56	6 (13%)
3	EDO	B	1201	-	3,3,3	0.47	0	2,2,2	0.16	0
4	QP1	A	1202	1	38,40,40	4.70	22 (57%)	45,54,54	1.75	10 (22%)
4	QP1	C	1101	1	38,40,40	4.78	26 (68%)	45,54,54	1.68	9 (20%)
3	EDO	D	1202	-	3,3,3	0.48	0	2,2,2	0.20	0
4	QP1	D	1203	1	38,40,40	4.94	26 (68%)	45,54,54	1.51	10 (22%)

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	QP1	B	1202	1	-	1/23/25/25	0/4/4/4
3	EDO	B	1201	-	-	1/1/1/1	-
4	QP1	A	1202	1	-	1/23/25/25	0/4/4/4
4	QP1	C	1101	1	-	1/23/25/25	0/4/4/4
3	EDO	D	1202	-	-	0/1/1/1	-
4	QP1	D	1203	1	-	3/23/25/25	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1202	QP1	C30-C27	8.25	1.52	1.39
4	D	1203	QP1	C30-C27	8.25	1.52	1.39
4	B	1202	QP1	C30-C28	8.22	1.52	1.39
4	A	1202	QP1	C24-C28	8.21	1.53	1.39
4	D	1203	QP1	C24-C28	7.97	1.52	1.39
4	D	1203	QP1	C03-C06	7.94	1.52	1.37
4	B	1202	QP1	C24-C28	7.93	1.52	1.39
4	B	1202	QP1	C25-C24	7.93	1.53	1.38
4	C	1101	QP1	C25-C24	7.87	1.53	1.38
4	C	1101	QP1	C24-C28	7.83	1.52	1.39
4	B	1202	QP1	C03-C06	7.80	1.52	1.37
4	C	1101	QP1	C30-C28	7.80	1.52	1.39
4	D	1203	QP1	C25-C24	7.79	1.52	1.38
4	C	1101	QP1	C09-C06	7.79	1.52	1.37
4	B	1202	QP1	C09-C06	7.76	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1203	QP1	C09-C06	7.70	1.52	1.37
4	D	1203	QP1	C03-C01	7.66	1.52	1.38
4	D	1203	QP1	C30-C28	7.63	1.51	1.39
4	A	1202	QP1	C09-C06	7.60	1.52	1.37
4	C	1101	QP1	C30-C27	7.60	1.51	1.39
4	B	1202	QP1	C09-C11	7.54	1.52	1.38
4	C	1101	QP1	C03-C06	7.50	1.51	1.37
4	A	1202	QP1	C25-C24	7.44	1.52	1.38
4	A	1202	QP1	C03-C06	7.42	1.51	1.37
4	D	1203	QP1	C09-C11	7.40	1.52	1.38
4	B	1202	QP1	C19-N07	7.39	1.48	1.34
4	A	1202	QP1	C19-N07	7.35	1.48	1.34
4	B	1202	QP1	C03-C01	7.30	1.52	1.38
4	C	1101	QP1	C09-C11	7.23	1.51	1.38
4	A	1202	QP1	C30-C27	7.21	1.50	1.39
4	A	1202	QP1	C09-C11	7.20	1.51	1.38
4	D	1203	QP1	C19-N07	7.16	1.47	1.34
4	A	1202	QP1	C03-C01	7.14	1.51	1.38
4	A	1202	QP1	C30-C28	7.03	1.50	1.39
4	C	1101	QP1	C19-N07	6.97	1.47	1.34
4	C	1101	QP1	C03-C01	6.75	1.51	1.38
4	B	1202	QP1	C11-C13	6.61	1.53	1.39
4	D	1203	QP1	C23-N07	6.58	1.48	1.34
4	D	1203	QP1	C11-C13	6.54	1.53	1.39
4	B	1202	QP1	C22-C23	6.54	1.51	1.38
4	B	1202	QP1	C25-C26	6.46	1.53	1.39
4	A	1202	QP1	C01-C13	6.40	1.53	1.39
4	D	1203	QP1	C25-C26	6.36	1.52	1.39
4	C	1101	QP1	C25-C26	6.34	1.52	1.39
4	C	1101	QP1	C11-C13	6.34	1.52	1.39
4	D	1203	QP1	C22-C23	6.28	1.51	1.38
4	C	1101	QP1	C23-N07	6.19	1.47	1.34
4	C	1101	QP1	C22-C23	6.19	1.51	1.38
4	D	1203	QP1	C01-C13	6.18	1.52	1.39
4	A	1202	QP1	C22-C23	6.18	1.51	1.38
4	A	1202	QP1	C25-C26	6.15	1.52	1.39
4	B	1202	QP1	C23-N07	6.14	1.47	1.34
4	C	1101	QP1	C01-C13	6.11	1.52	1.39
4	A	1202	QP1	C23-N07	6.03	1.47	1.34
4	A	1202	QP1	C11-C13	5.99	1.52	1.39
4	B	1202	QP1	C01-C13	5.83	1.51	1.39
4	C	1101	QP1	C27-C26	5.29	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1203	QP1	C27-C26	5.27	1.51	1.40
4	A	1202	QP1	C20-C19	5.17	1.52	1.39
4	B	1202	QP1	C20-C19	5.06	1.52	1.39
4	B	1202	QP1	C27-C26	4.99	1.51	1.40
4	C	1101	QP1	C20-C19	4.95	1.52	1.39
4	D	1203	QP1	C20-C19	4.86	1.51	1.39
4	D	1203	QP1	C20-C21	4.85	1.48	1.39
4	C	1101	QP1	C20-C21	4.76	1.48	1.39
4	A	1202	QP1	C22-C21	4.68	1.49	1.39
4	D	1203	QP1	C22-C21	4.67	1.49	1.39
4	A	1202	QP1	C27-C26	4.62	1.50	1.40
4	A	1202	QP1	C20-C21	4.59	1.47	1.39
4	B	1202	QP1	C20-C21	4.55	1.47	1.39
4	C	1101	QP1	C22-C21	4.37	1.48	1.39
4	D	1203	QP1	C31-N12	4.33	1.45	1.35
4	B	1202	QP1	C31-N12	4.23	1.45	1.35
4	B	1202	QP1	C22-C21	4.22	1.48	1.39
4	A	1202	QP1	C31-N12	4.18	1.44	1.35
4	C	1101	QP1	C31-N12	4.16	1.44	1.35
4	B	1202	QP1	C16-S17	3.24	1.81	1.75
4	B	1202	QP1	C15-C14	-3.24	1.35	1.44
4	A	1202	QP1	C15-C14	-3.22	1.36	1.44
4	D	1203	QP1	C19-N10	3.18	1.44	1.38
4	B	1202	QP1	C19-N10	3.14	1.44	1.38
4	D	1203	QP1	C16-S17	3.12	1.81	1.75
4	D	1203	QP1	C13-C14	3.11	1.52	1.49
4	D	1203	QP1	C15-C14	-3.07	1.36	1.44
4	C	1101	QP1	C15-C14	-3.04	1.36	1.44
4	A	1202	QP1	C14-N04	-2.96	1.30	1.37
4	B	1202	QP1	C13-C14	2.87	1.52	1.49
4	C	1101	QP1	C19-N10	2.87	1.43	1.38
4	C	1101	QP1	C15-N02	-2.86	1.30	1.37
4	B	1202	QP1	C15-N02	-2.63	1.30	1.37
4	A	1202	QP1	C15-N02	-2.57	1.31	1.37
4	C	1101	QP1	C14-N04	-2.52	1.31	1.37
4	D	1203	QP1	C15-N02	-2.44	1.31	1.37
4	D	1203	QP1	C14-N04	-2.39	1.31	1.37
4	D	1203	QP1	O08-C31	-2.27	1.18	1.23
4	C	1101	QP1	C16-S17	2.23	1.79	1.75
4	C	1101	QP1	C13-C14	2.17	1.51	1.49
4	C	1101	QP1	O08-C31	-2.09	1.19	1.23
4	B	1202	QP1	C14-N04	-2.05	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1202	QP1	O08-C31	-2.04	1.19	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1202	QP1	C22-C23-N07	-5.23	117.46	123.96
4	C	1101	QP1	C22-C23-N07	-4.82	117.97	123.96
4	B	1202	QP1	C18-S17-C16	4.46	108.97	102.90
4	B	1202	QP1	C22-C23-N07	-4.17	118.78	123.96
4	C	1101	QP1	C18-S17-C16	3.96	108.29	102.90
4	D	1203	QP1	O05-C26-C27	3.69	119.33	114.80
4	A	1202	QP1	C01-C13-C14	-3.62	114.88	120.61
4	C	1101	QP1	C01-C13-C14	-3.46	115.13	120.61
4	A	1202	QP1	C09-C11-C13	-3.42	116.21	121.13
4	C	1101	QP1	C23-N07-C19	3.31	121.91	117.22
4	B	1202	QP1	O05-C26-C27	3.24	118.77	114.80
4	D	1203	QP1	C22-C23-N07	-3.22	119.95	123.96
4	A	1202	QP1	C18-S17-C16	2.90	106.85	102.90
4	A	1202	QP1	C30-C27-C26	2.89	122.40	118.91
4	C	1101	QP1	O05-C26-C27	2.86	118.30	114.80
4	D	1203	QP1	C23-N07-C19	2.85	121.26	117.22
4	A	1202	QP1	C01-C13-C11	2.84	123.25	117.59
4	A	1202	QP1	C26-C27-N10	-2.81	111.89	117.78
4	D	1203	QP1	C18-S17-C16	2.69	106.56	102.90
4	B	1202	QP1	C23-N07-C19	2.69	121.04	117.22
4	D	1203	QP1	C20-C19-N07	-2.57	119.17	122.75
4	D	1203	QP1	C15-C14-N04	-2.44	107.17	113.76
4	B	1202	QP1	C15-C14-N04	-2.41	107.26	113.76
4	A	1202	QP1	C23-N07-C19	2.40	120.63	117.22
4	B	1202	QP1	C29-O05-C26	-2.37	113.95	117.53
4	D	1203	QP1	C20-C21-C15	-2.35	115.63	120.15
4	A	1202	QP1	C11-C09-C06	2.33	120.77	118.36
4	C	1101	QP1	C22-C21-C20	2.33	121.46	118.16
4	C	1101	QP1	C15-C14-N04	-2.23	107.73	113.76
4	A	1202	QP1	C30-C27-N10	2.23	125.69	121.05
4	D	1203	QP1	C22-C21-C20	2.22	121.30	118.16
4	D	1203	QP1	O05-C26-C25	-2.18	120.64	124.37
4	C	1101	QP1	C29-O05-C26	-2.14	114.29	117.53
4	C	1101	QP1	C01-C13-C11	2.09	121.76	117.59
4	D	1203	QP1	C29-O05-C26	-2.06	114.42	117.53

There are no chirality outliers.

All (7) torsion outliers are listed below:

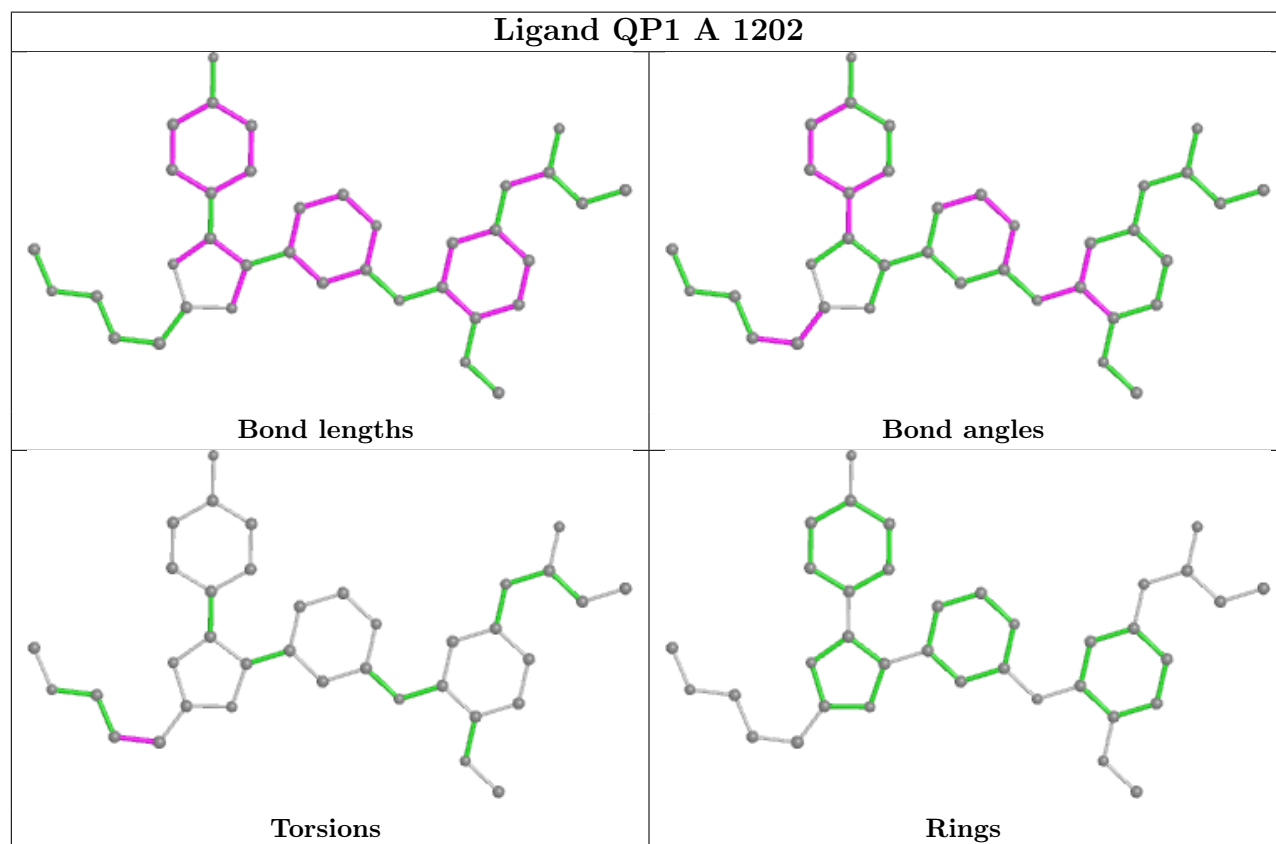
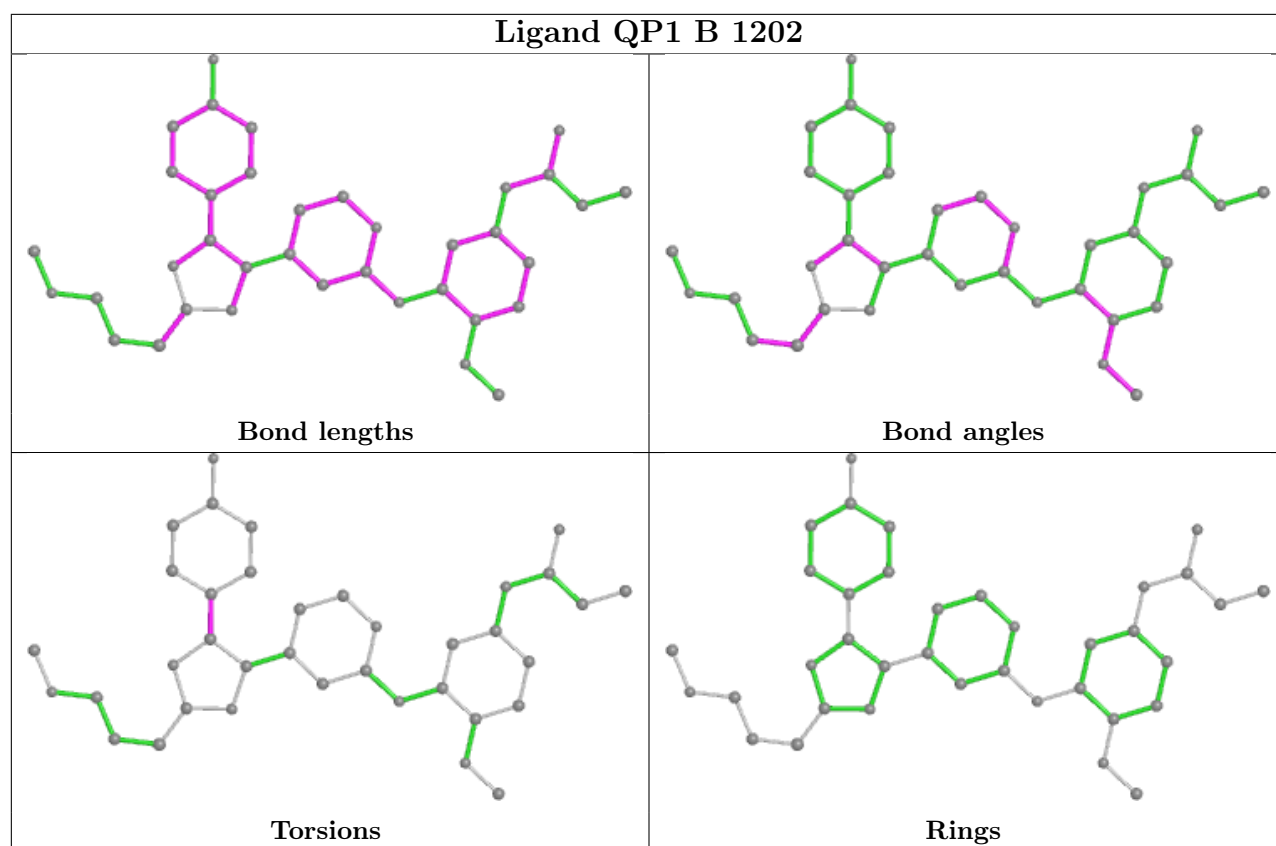
Mol	Chain	Res	Type	Atoms
4	C	1101	QP1	S17-C18-C35-O36
4	D	1203	QP1	C11-C13-C14-N04
4	D	1203	QP1	S17-C18-C35-O36
4	D	1203	QP1	C01-C13-C14-N04
4	B	1202	QP1	C11-C13-C14-N04
3	B	1201	EDO	O1-C1-C2-O2
4	A	1202	QP1	C35-C18-S17-C16

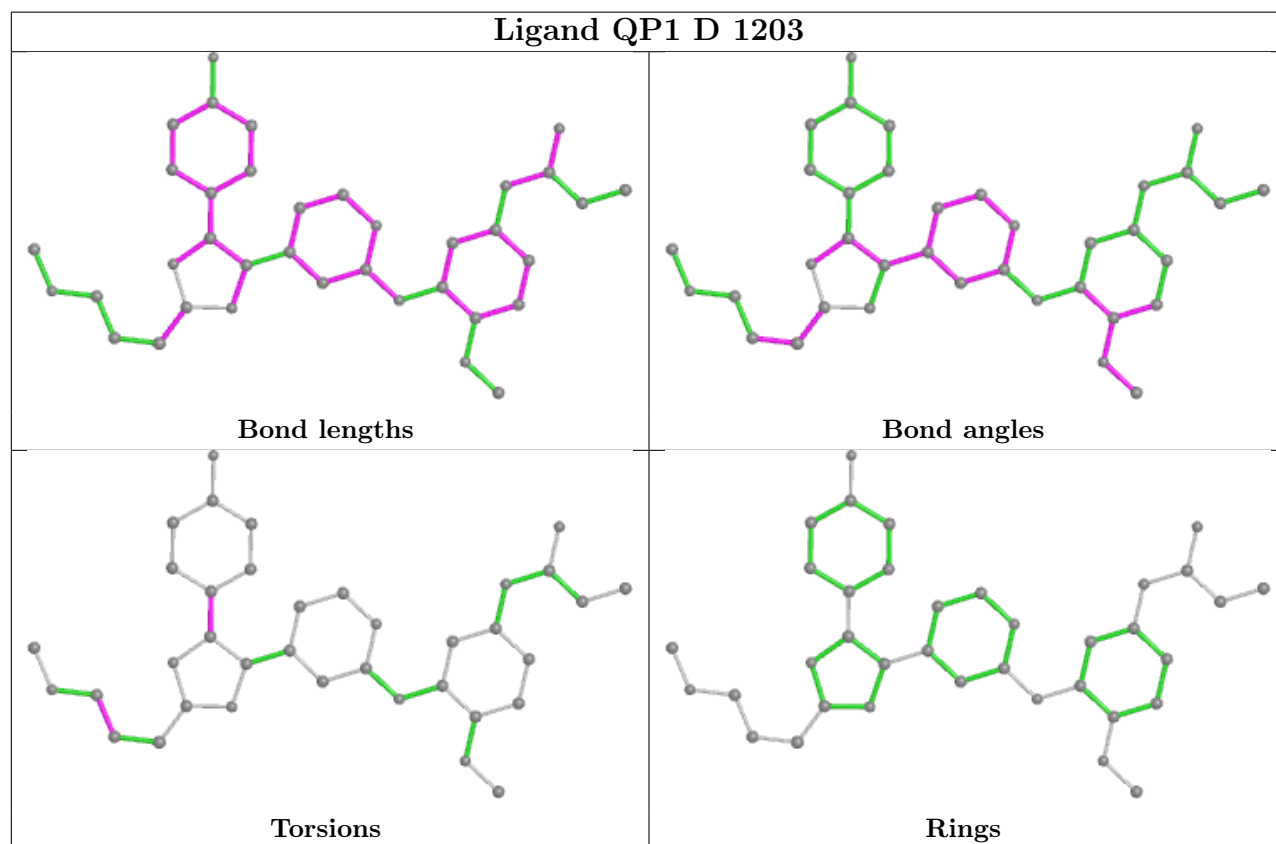
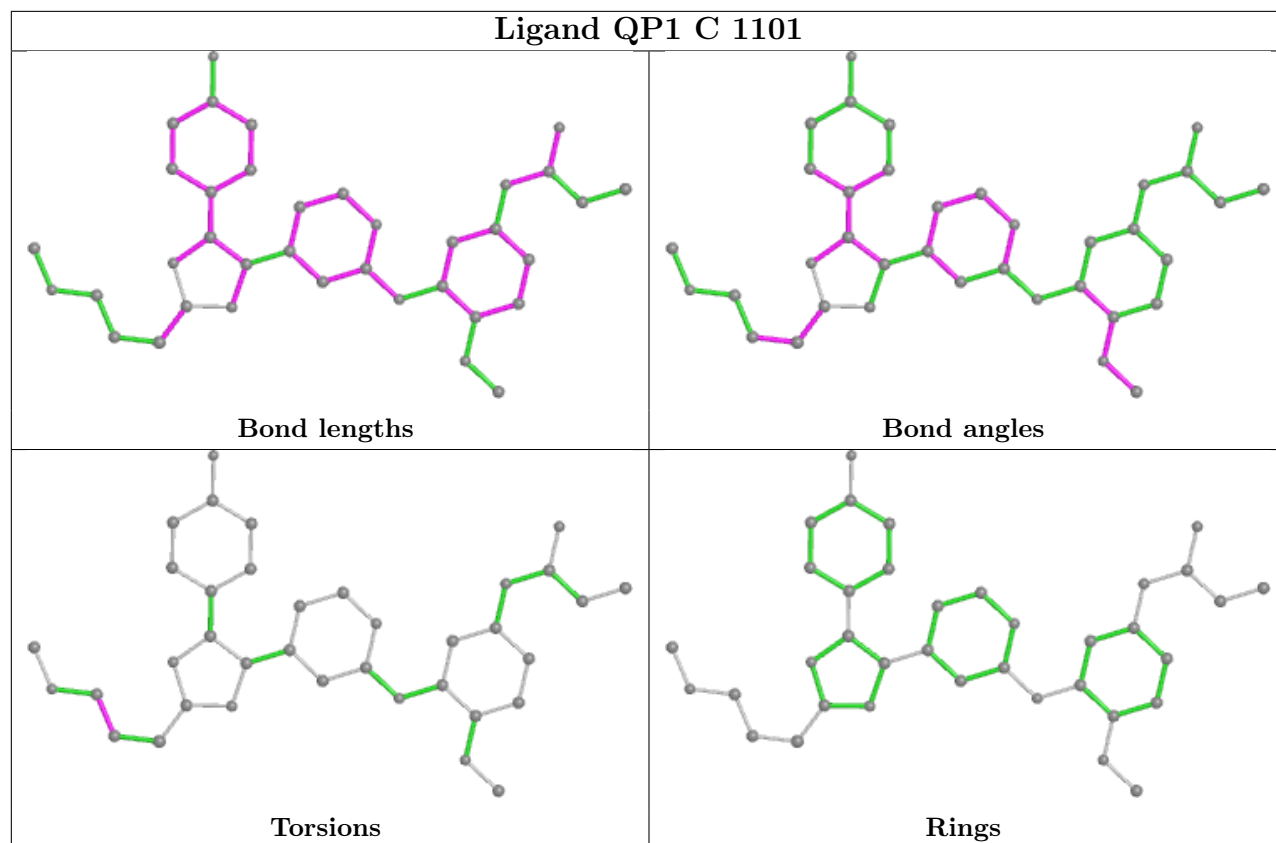
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1101	QP1	1	0
4	D	1203	QP1	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 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 ⓘ

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, 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	314/327 (96%)	-0.21	9 (2%)	51	46	12, 22, 49, 78	0
1	B	302/327 (92%)	-0.02	16 (5%)	26	21	14, 26, 56, 78	0
1	C	299/327 (91%)	0.08	19 (6%)	19	15	14, 27, 58, 80	0
1	D	314/327 (96%)	-0.18	5 (1%)	72	68	13, 26, 49, 72	0
All	All	1229/1308 (93%)	-0.09	49 (3%)	38	32	12, 25, 53, 80	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	723	PHE	8.2
1	D	873	GLY	7.1
1	B	1010	VAL	4.8
1	B	1014	ASP	4.8
1	A	753	PRO	4.5
1	A	1014	ASP	4.4
1	B	751	THR	4.4
1	C	862	LEU	4.3
1	C	859	ALA	4.3
1	C	988	HIS	4.1
1	C	722	ALA	4.0
1	A	751	THR	4.0
1	C	1010	VAL	3.9
1	A	752	SER	3.6
1	B	987	MET	3.5
1	C	858	LEU	3.4
1	C	989	LEU	3.4
1	B	750	ALA	3.4
1	C	917	GLY	3.3
1	C	1009	ASP	3.3
1	A	1013	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1012	ASP	3.2
1	C	876	VAL	3.2
1	B	988	HIS	3.1
1	B	1012	ASP	3.0
1	C	860	LYS	2.9
1	B	986	ARG	2.8
1	B	875	LYS	2.8
1	C	987	MET	2.8
1	C	807	ASP	2.7
1	C	861	LEU	2.6
1	B	1009	ASP	2.6
1	A	1008	ASP	2.5
1	C	1008	ASP	2.4
1	A	1007	MET	2.4
1	D	701	GLN	2.4
1	B	856	PHE	2.3
1	D	874	GLY	2.3
1	B	985	GLU	2.3
1	A	1009	ASP	2.3
1	B	860	LYS	2.3
1	C	1006	ASP	2.2
1	B	990	PRO	2.2
1	B	1008	ASP	2.2
1	A	1012	ASP	2.1
1	C	986	ARG	2.1
1	D	784	SER	2.1
1	D	875	LYS	2.0
1	B	808	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

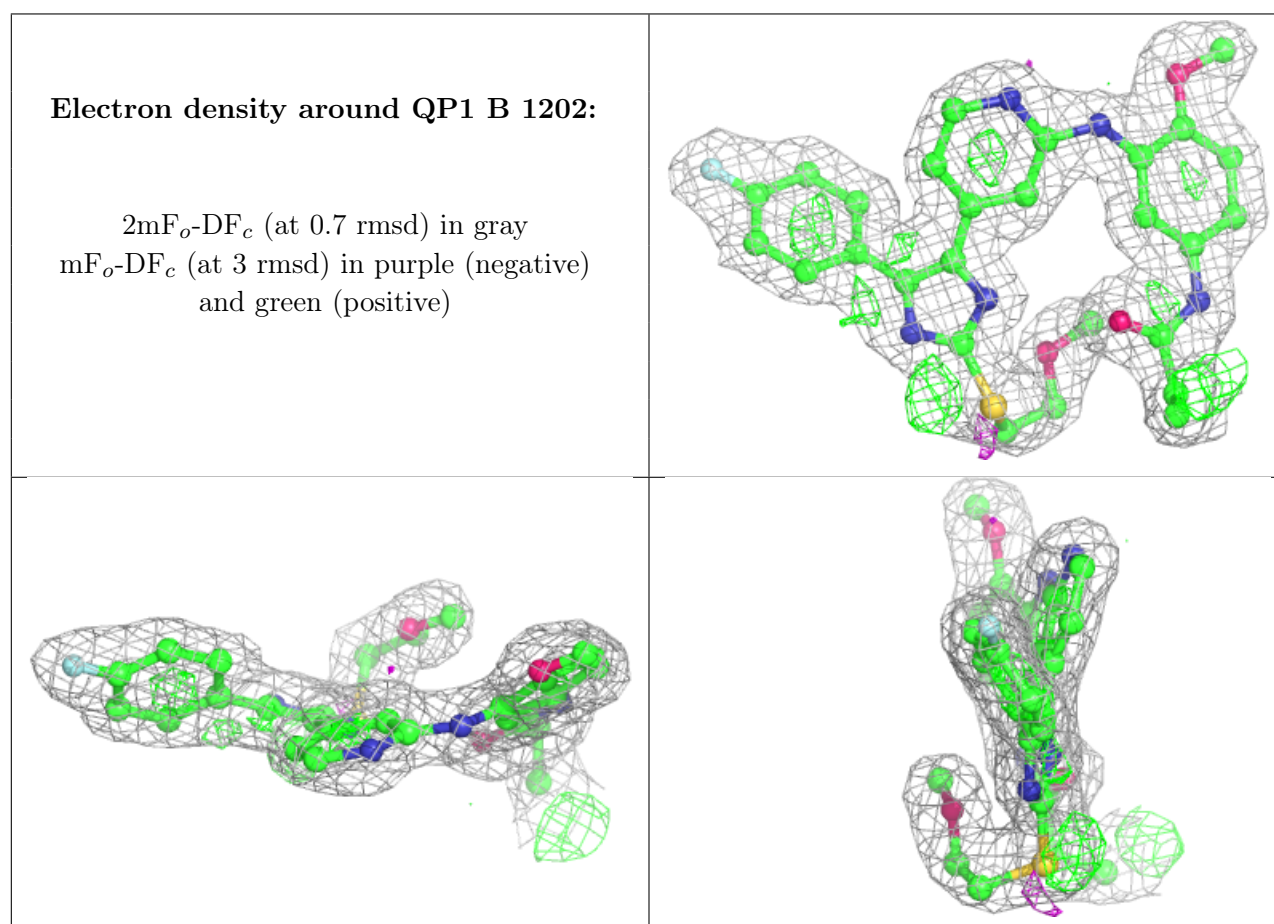
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

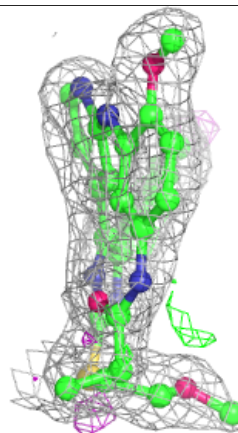
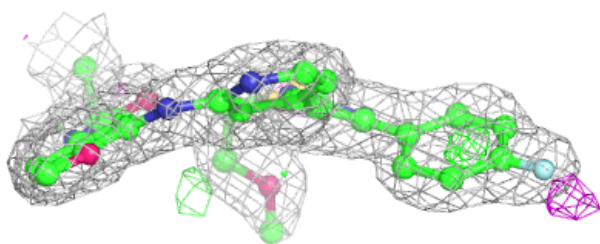
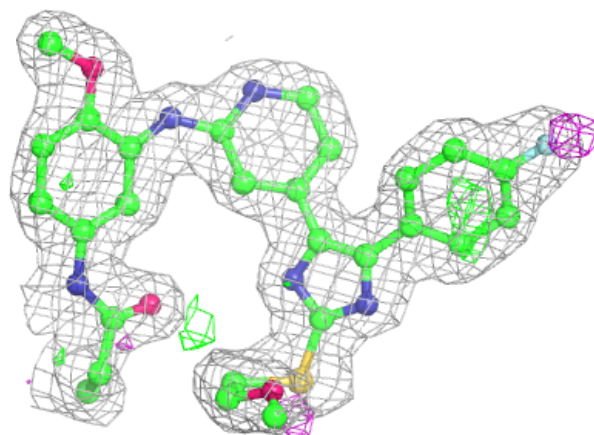
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	C	1102	1/1	0.53	0.31	73,73,73,73	0
3	EDO	B	1201	4/4	0.77	0.20	39,44,46,50	0
3	EDO	D	1202	4/4	0.88	0.14	21,29,30,36	0
4	QP1	B	1202	37/37	0.92	0.11	18,24,32,34	0
4	QP1	C	1101	37/37	0.92	0.10	17,22,34,39	0
4	QP1	D	1203	37/37	0.93	0.10	17,23,32,35	0
4	QP1	A	1202	37/37	0.96	0.09	10,16,19,20	0
2	CL	D	1201	1/1	0.98	0.04	27,27,27,27	0
2	CL	B	1203	1/1	0.99	0.03	40,40,40,40	0
2	CL	A	1201	1/1	0.99	0.05	21,21,21,21	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.



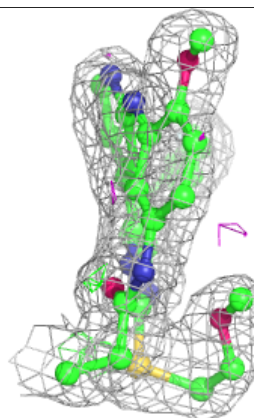
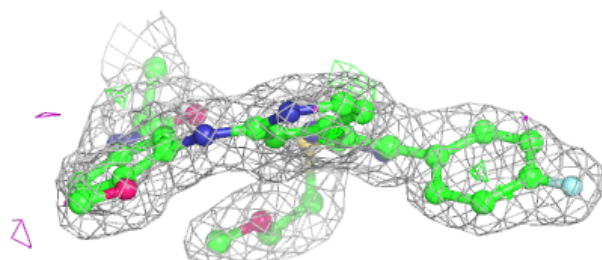
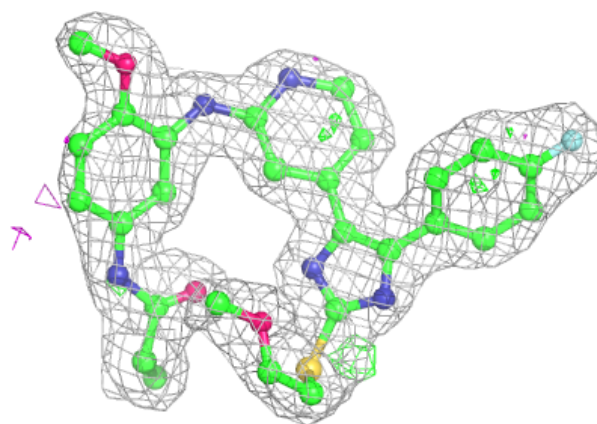
Electron density around QP1 C 1101:

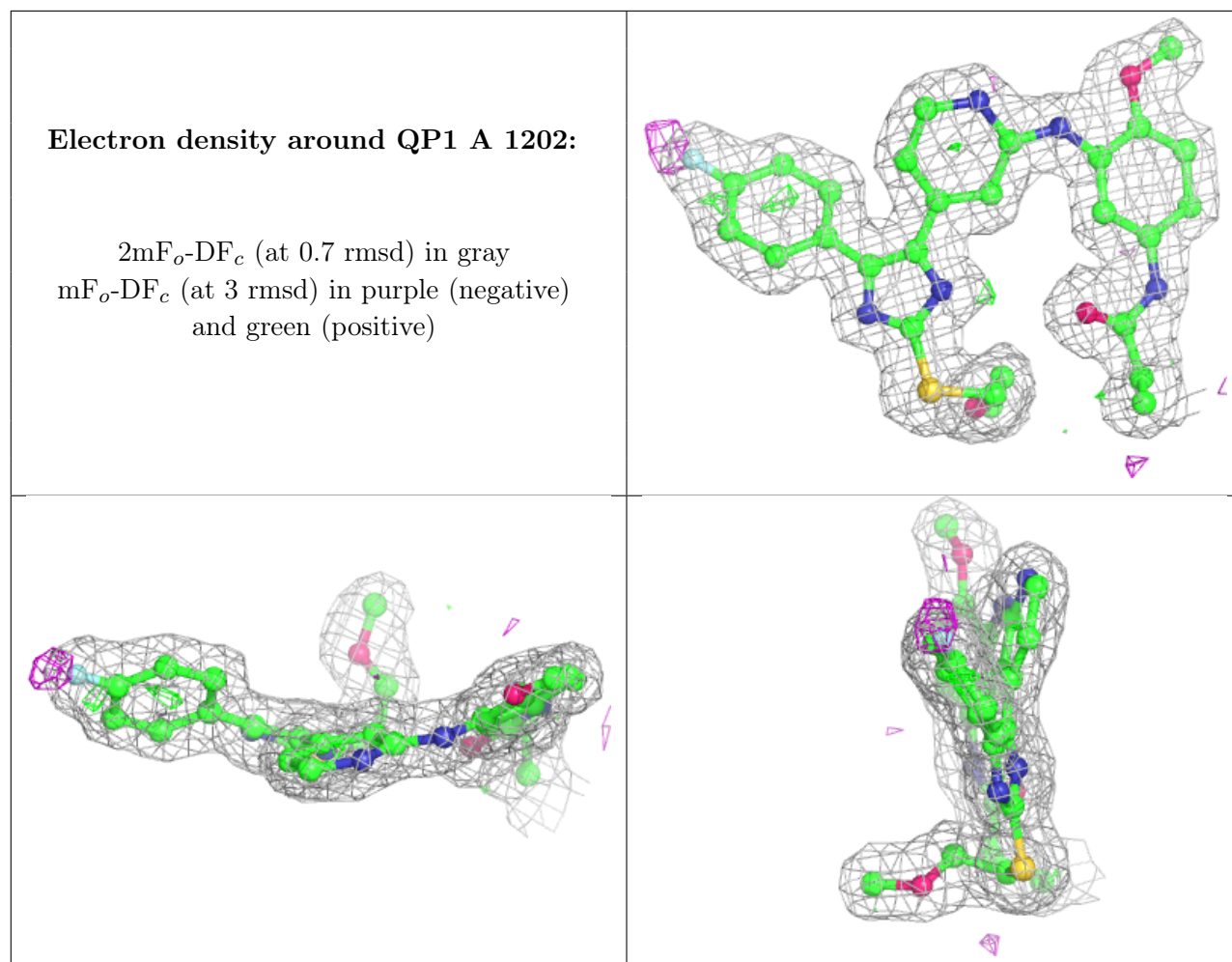
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around QP1 D 1203:

$2mF_o-DF_c$ (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.