



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 04:54 PM EST

PDB ID : 6V6O
Title : EGFR(T790M/V948R) in complex with LN2380
Authors : Heppner, D.E.; Eck, M.J.
Deposited on : 2019-12-05
Resolution : 2.10 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

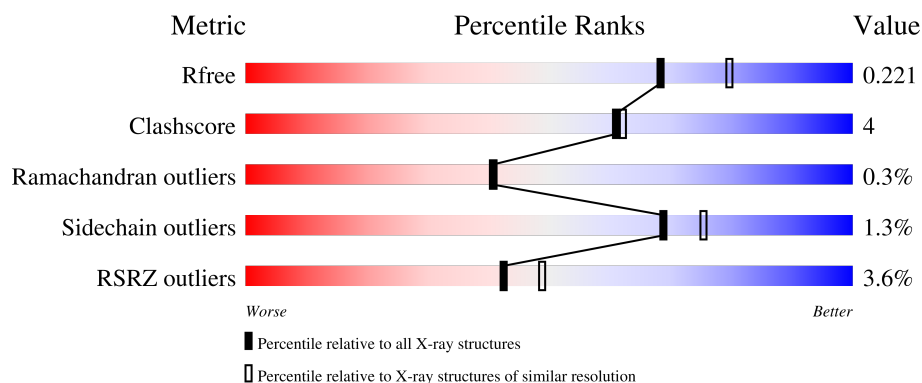
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	327	<div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	C	327	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	D	327	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	327	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>. 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	327	<div><div></div><div>6%</div><div>77%</div><div>13%</div><div>•</div><div>9%</div></div>
1	G	327	<div><div></div><div>5%</div><div>80%</div><div>10%</div><div>10%</div></div>
1	H	327	<div><div></div><div>3%</div><div>83%</div><div>9%</div><div>9%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21480 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	307	Total	C	N	O	S	0	0	0
			2470	1585	420	446	19			
1	B	314	Total	C	N	O	S	0	0	0
			2521	1614	427	461	19			
1	C	297	Total	C	N	O	S	0	0	0
			2390	1538	406	427	19			
1	E	303	Total	C	N	O	S	0	1	0
			2445	1568	414	444	19			
1	F	299	Total	C	N	O	S	0	1	0
			2419	1553	409	438	19			
1	G	294	Total	C	N	O	S	0	1	0
			2378	1526	404	429	19			
1	H	299	Total	C	N	O	S	0	1	0
			2413	1550	408	437	18			

There are 16 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
E	790	MET	THR	engineered mutation	UNP P00533
E	948	ARG	VAL	engineered mutation	UNP P00533
F	790	MET	THR	engineered mutation	UNP P00533
F	948	ARG	VAL	engineered mutation	UNP P00533
G	790	MET	THR	engineered mutation	UNP P00533

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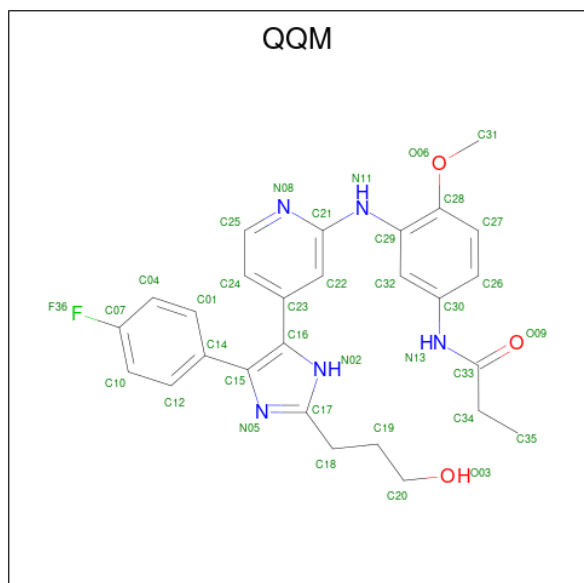
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Chain	Residue	Modelled	Actual	Comment	Reference
G	948	ARG	VAL	engineered mutation	UNP P00533
H	790	MET	THR	engineered mutation	UNP P00533
H	948	ARG	VAL	engineered mutation	UNP P00533

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0

- Molecule 3 is N-[3-(4-[4-(4-fluorophenyl)-2-(3-hydroxypropyl)-1H-imidazol-5-yl]pyridin-2-yl)amino)-4-methoxyphenyl]propanamide (three-letter code: QQM) (formula: C₂₇H₂₈FN₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	A	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	B	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	C	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	E	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	F	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	G	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	H	1	Total	C	F	N	O	0	0
			36	27	1	5	3		

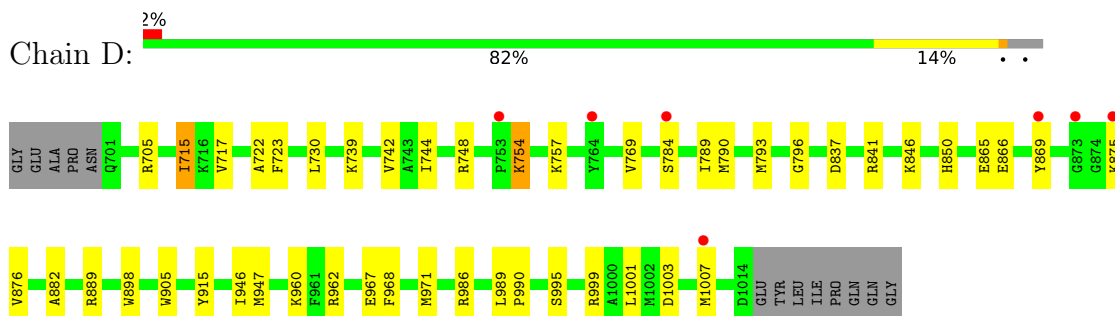
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	196	Total	O	0	0
			196	196		
4	A	172	Total	O	0	0
			172	172		
4	B	286	Total	O	0	0
			286	286		
4	C	219	Total	O	0	0
			219	219		
4	E	212	Total	O	0	0
			212	212		
4	F	156	Total	O	0	0
			156	156		
4	G	188	Total	O	0	0
			188	188		
4	H	189	Total	O	0	0
			189	189		

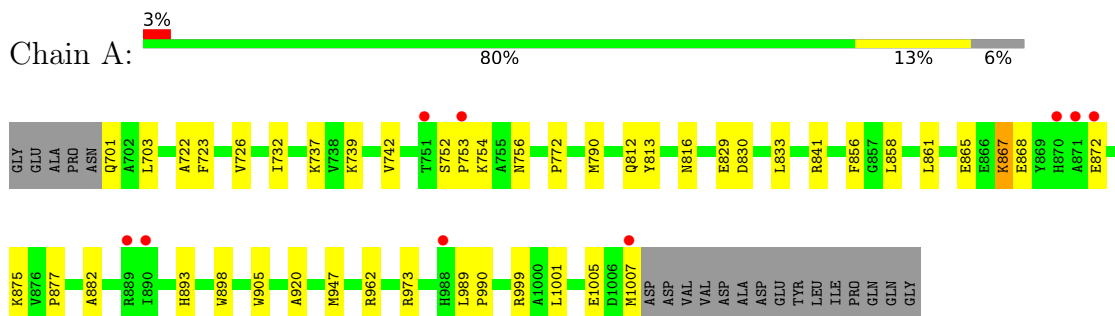
3 Residue-property plots [i](#)

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.

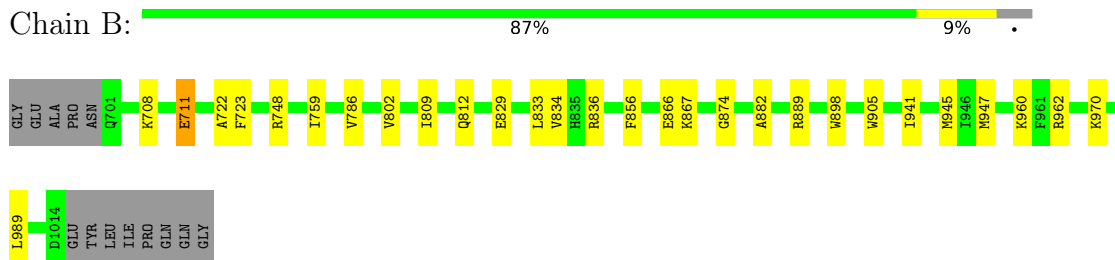
- Molecule 1: Epidermal growth factor receptor



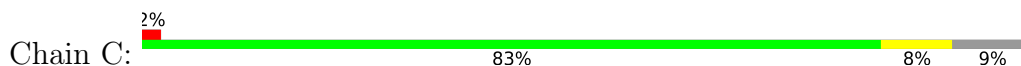
- Molecule 1: Epidermal growth factor receptor

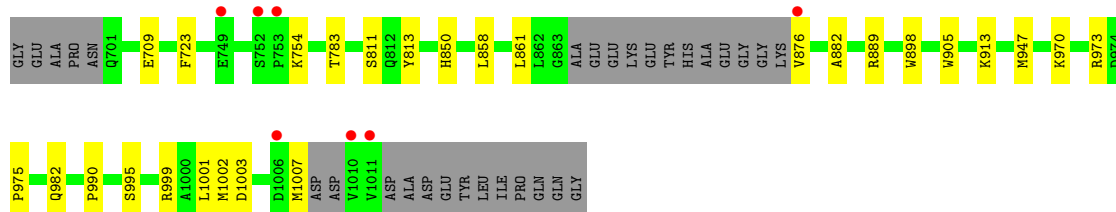


- Molecule 1: Epidermal growth factor receptor

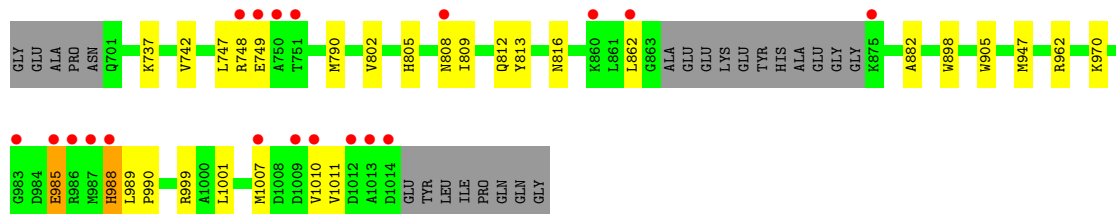
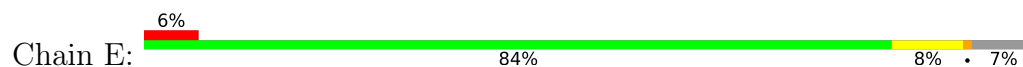


- Molecule 1: Epidermal growth factor receptor

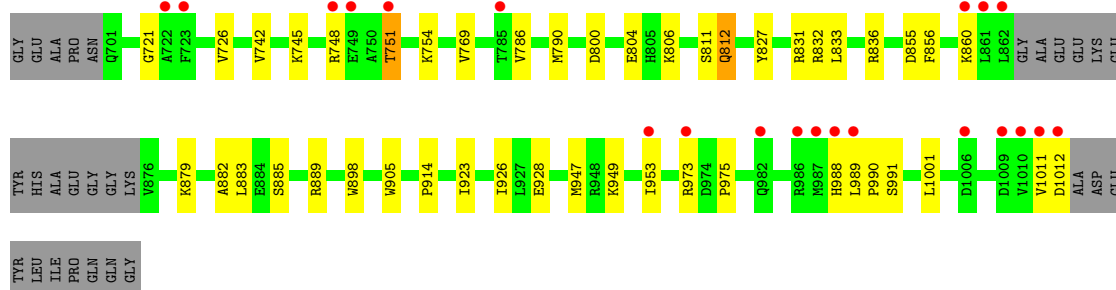
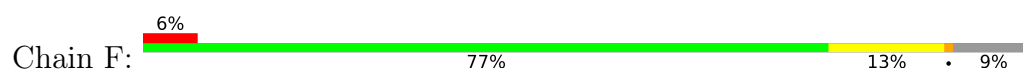




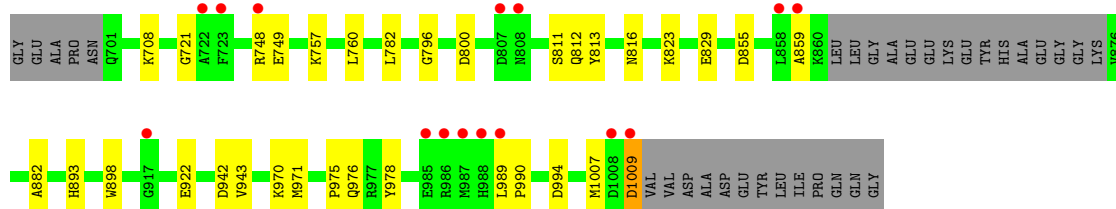
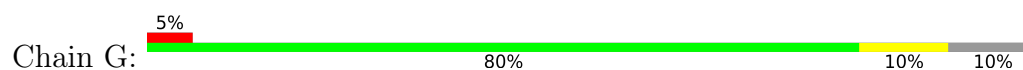
• Molecule 1: Epidermal growth factor receptor



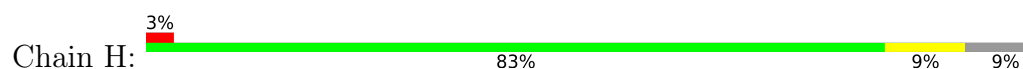
• Molecule 1: Epidermal growth factor receptor

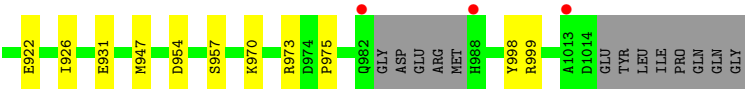


• Molecule 1: Epidermal growth factor receptor



• 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	71.55Å 102.36Å 173.57Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	69.83 – 2.10 69.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (69.83-2.10) 95.3 (69.87-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.221 0.195 , 0.221	Depositor DCC
R_{free} test set	7020 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 54.79 % 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 3.4707e-05. 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: QQM, 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	0.29	0/2525	0.47	0/3412
1	B	0.25	0/2576	0.45	0/3483
1	C	0.25	0/2441	0.46	0/3299
1	D	0.30	0/2585	0.51	0/3495
1	E	0.26	0/2497	0.48	0/3376
1	F	0.31	0/2471	0.51	0/3342
1	G	0.25	0/2430	0.42	0/3285
1	H	0.26	0/2464	0.47	0/3332
All	All	0.27	0/19989	0.47	0/27024

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	2470	0	2511	29	0
1	B	2521	0	2550	17	0
1	C	2390	0	2445	16	0
1	D	2530	0	2555	32	0
1	E	2445	0	2485	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2419	0	2460	34	0
1	G	2378	0	2414	20	0
1	H	2413	0	2455	18	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
2	C	1	0	0	1	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	1	0
2	G	1	0	0	1	0
2	H	1	0	0	0	0
3	A	36	0	0	2	0
3	B	36	0	0	0	0
3	C	36	0	0	0	0
3	D	36	0	0	2	0
3	E	36	0	0	1	0
3	F	36	0	0	2	0
3	G	36	0	0	1	0
3	H	36	0	0	0	0
4	A	172	0	0	2	0
4	B	286	0	0	0	0
4	C	219	0	0	2	0
4	D	196	0	0	6	0
4	E	212	0	0	3	0
4	F	156	0	0	0	0
4	G	188	0	0	2	0
4	H	189	0	0	3	0
All	All	21480	0	19875	178	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 4.

All (178) 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:F:973:ARG:CZ	1:F:1011:VAL:HG13	2.01	0.91
1:D:947:MET:SD	4:D:1478:HOH:O	2.36	0.81
1:D:999:ARG:NH1	1:D:1007:MET:SD	2.56	0.78
1:A:737:LYS:HE3	1:F:804:GLU:HB3	1.71	0.72
1:F:812:GLN:HG2	1:F:975:PRO:HG3	1.71	0.72
1:B:722:ALA:O	1:B:748:ARG:NE	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLN:HG3	1:A:703:LEU:H	1.55	0.70
1:F:721:GLY:O	1:F:748:ARG:NH2	2.22	0.70
1:A:872:GLU:HG2	1:A:920:ALA:H	1.57	0.69
1:G:812:GLN:HG2	1:G:975:PRO:HG3	1.75	0.68
1:B:829:GLU:OE1	1:B:960:LYS:NZ	2.24	0.68
1:F:973:ARG:HG2	1:F:1012:ASP:O	1.95	0.67
1:E:808:ASN:ND2	4:E:1304:HOH:O	2.27	0.66
1:H:836:ARG:NH2	1:H:860:LYS:HD2	2.12	0.65
1:A:962:ARG:NH1	4:A:1304:HOH:O	2.30	0.64
1:F:989:LEU:HD22	1:F:990:PRO:HD2	1.78	0.64
1:H:999:ARG:NH1	4:H:1302:HOH:O	2.23	0.64
1:E:1007:MET:SD	4:E:1324:HOH:O	2.55	0.63
1:E:812:GLN:NE2	1:E:1011:VAL:O	2.32	0.63
1:C:876:VAL:N	4:C:1306:HOH:O	2.33	0.62
1:F:973:ARG:HG3	1:F:1011:VAL:HG12	1.80	0.62
1:H:970:LYS:HA	1:H:973:ARG:NH1	2.15	0.62
1:G:816:ASN:HD21	1:G:989:LEU:HD11	1.65	0.61
1:D:995:SER:O	1:D:999:ARG:HG2	2.01	0.61
1:H:970:LYS:HA	1:H:973:ARG:HH11	1.68	0.58
1:F:973:ARG:CZ	1:F:1011:VAL:CG1	2.80	0.58
1:F:836:ARG:NH1	1:F:860:LYS:HD2	2.20	0.57
1:D:869:TYR:CD2	1:D:876:VAL:HG11	2.39	0.57
1:B:962:ARG:HH22	1:C:913:LYS:HE3	1.70	0.57
1:G:748:ARG:NH2	4:G:1405:HOH:O	2.37	0.57
1:F:751:THR:HG21	1:F:786:VAL:HG23	1.87	0.56
1:F:885:SER:O	1:F:889:ARG:HD3	2.06	0.56
1:E:905:TRP:HD1	1:E:947:MET:HE1	1.69	0.56
1:G:760:LEU:HD11	1:G:782:LEU:HD11	1.89	0.55
1:E:747:LEU:HD13	1:E:862:LEU:HD11	1.88	0.54
1:B:941:ILE:HG13	1:B:945:MET:HE2	1.89	0.54
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.73	0.54
1:C:970:LYS:HA	1:C:973:ARG:NH1	2.22	0.54
1:E:812:GLN:HE21	1:E:816:ASN:ND2	2.06	0.54
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.08	0.54
1:H:926:ILE:HG23	1:H:931:GLU:HB2	1.90	0.53
1:D:1001:LEU:HD11	1:E:742:VAL:HG12	1.90	0.53
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.74	0.53
1:D:730:LEU:HD13	1:D:739:LYS:HB3	1.91	0.52
1:H:905:TRP:HD1	1:H:947:MET:HE1	1.74	0.52
1:H:832:ARG:NH2	4:H:1312:HOH:O	2.42	0.52
1:F:833:LEU:HB3	1:F:856:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:816:ASN:ND2	1:G:989:LEU:HD11	2.25	0.52
1:A:722:ALA:HB1	1:A:875:LYS:HA	1.91	0.51
1:A:756:ASN:HB2	4:A:1338:HOH:O	2.09	0.51
1:B:834:VAL:HG12	1:B:836:ARG:HG3	1.91	0.51
1:F:882:ALA:HA	1:F:898:TRP:CD2	2.45	0.51
1:B:708:LYS:O	1:B:711:GLU:HG3	2.11	0.51
1:F:812:GLN:HB3	1:F:989:LEU:HG	1.92	0.50
1:F:905:TRP:HD1	1:F:947:MET:HE1	1.76	0.50
1:B:723:PHE:HB2	2:B:1201:CL:CL	2.47	0.50
1:F:953:ILE:HD12	1:F:953:ILE:H	1.77	0.49
1:G:882:ALA:HA	1:G:898:TRP:CD2	2.47	0.49
1:E:988:HIS:ND1	1:E:988:HIS:N	2.60	0.49
1:D:790:MET:HG2	3:D:1202:QQM:C07	2.43	0.49
1:F:973:ARG:NH2	1:F:1011:VAL:HG13	2.27	0.49
1:H:766:MET:SD	4:H:1346:HOH:O	2.60	0.49
1:A:999:ARG:NH2	1:A:1005:GLU:O	2.45	0.49
1:A:772:PRO:HB3	1:A:1007:MET:HG2	1.94	0.48
1:G:813:TYR:OH	1:G:990:PRO:HD3	2.13	0.48
1:H:882:ALA:HA	1:H:898:TRP:CD2	2.48	0.48
1:F:836:ARG:CD	1:F:860:LYS:HB2	2.43	0.48
1:A:865:GLU:HG2	1:A:868:GLU:HG3	1.96	0.48
1:A:1001:LEU:HD11	1:F:742:VAL:HG12	1.96	0.48
1:E:802:VAL:HA	1:E:809:ILE:HD11	1.96	0.48
1:A:867:LYS:HD2	1:A:867:LYS:H	1.79	0.47
1:A:790:MET:HG2	3:A:1202:QQM:C07	2.45	0.47
1:D:946:ILE:HD11	1:D:967:GLU:HG2	1.97	0.47
1:A:841:ARG:HH12	1:A:877:PRO:HB3	1.80	0.47
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.49	0.47
1:B:802:VAL:HA	1:B:809:ILE:HD11	1.96	0.47
1:A:742:VAL:HG12	1:F:1001:LEU:HD11	1.97	0.47
1:F:790:MET:HG2	3:F:1202:QQM:C07	2.45	0.46
1:G:990:PRO:HB2	1:G:994:ASP:HB2	1.97	0.46
1:D:754:LYS:HB3	1:D:754:LYS:HE3	1.69	0.46
1:F:973:ARG:NH1	1:F:1011:VAL:HG13	2.29	0.46
1:B:759:ILE:HD13	1:B:786:VAL:HG21	1.98	0.46
1:B:833:LEU:HB3	1:B:856:PHE:CE1	2.51	0.46
1:G:943:VAL:HG22	1:G:971:MET:HE1	1.98	0.46
1:G:971:MET:HE3	1:G:978:TYR:HB3	1.98	0.46
1:D:866:GLU:OE2	1:D:889:ARG:NH2	2.48	0.46
1:D:968:PHE:HA	1:D:971:MET:HE3	1.96	0.46
1:A:833:LEU:HB3	1:A:856:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:GLN:HE21	1:E:816:ASN:HD21	1.62	0.46
1:D:742:VAL:HG12	1:E:1001:LEU:HD11	1.97	0.46
1:C:889:ARG:NH2	1:G:708:LYS:HD2	2.31	0.46
1:D:722:ALA:HB1	1:D:875:LYS:HG2	1.98	0.46
1:D:793:MET:HE1	1:D:846:LYS:HB2	1.98	0.46
1:E:999:ARG:NH1	1:E:1007:MET:SD	2.89	0.46
1:E:813:TYR:OH	1:E:990:PRO:HD3	2.16	0.45
1:F:949:LYS:HB3	1:F:949:LYS:HE2	1.56	0.45
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.52	0.45
1:E:989:LEU:HB3	1:E:990:PRO:HD2	1.98	0.45
1:E:882:ALA:HA	1:E:898:TRP:CD2	2.52	0.45
1:D:748:ARG:NE	1:D:875:LYS:HD3	2.32	0.45
1:A:812:GLN:HG3	1:A:816:ASN:ND2	2.31	0.45
1:D:744:ILE:HG12	1:D:789:ILE:HG13	1.99	0.44
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.51	0.44
1:F:745:LYS:NZ	1:F:855:ASP:OD1	2.50	0.44
1:A:752:SER:O	1:A:754:LYS:N	2.50	0.44
1:A:989:LEU:HB3	1:A:990:PRO:HD2	2.00	0.44
1:G:708:LYS:HA	1:G:708:LYS:HD3	1.71	0.44
1:H:760:LEU:HD13	1:H:782:LEU:HD11	1.98	0.44
1:D:962:ARG:NH1	4:D:1323:HOH:O	2.50	0.44
1:C:723:PHE:HB2	2:C:1201:CL:CL	2.54	0.44
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.82	0.44
1:H:811:SER:OG	1:H:975:PRO:HB2	2.18	0.44
1:A:858:LEU:HD23	1:A:858:LEU:HA	1.87	0.44
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.53	0.44
1:H:754:LYS:HB3	1:H:754:LYS:HE3	1.75	0.44
1:C:1001:LEU:HD23	1:C:1001:LEU:HA	1.84	0.44
1:G:748:ARG:HD3	1:G:748:ARG:HA	1.78	0.44
1:C:982:GLN:OE1	4:C:1301:HOH:O	2.21	0.43
1:D:837:ASP:OD2	1:D:841:ARG:NH1	2.50	0.43
1:E:805:HIS:HB3	1:E:808:ASN:OD1	2.18	0.43
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.19	0.43
1:C:850:HIS:ND1	1:C:1003:ASP:OD2	2.52	0.43
1:F:745:LYS:HE2	2:F:1201:CL:CL	2.55	0.43
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.83	0.43
1:F:883:LEU:HD21	1:F:928:GLU:HG2	2.01	0.43
1:C:858:LEU:HD23	1:C:858:LEU:HA	1.87	0.43
1:H:708:LYS:O	1:H:711:GLU:HG2	2.19	0.43
1:B:812:GLN:HB3	1:B:989:LEU:HG	1.99	0.43
1:B:866:GLU:OE2	1:B:889:ARG:NH2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:986:ARG:NH2	4:D:1328:HOH:O	2.52	0.43
1:A:973:ARG:HH22	1:E:737:LYS:NZ	2.17	0.43
1:C:995:SER:O	1:C:999:ARG:HG3	2.19	0.43
1:A:829:GLU:HA	1:A:893:HIS:CE1	2.54	0.42
1:E:970:LYS:HE3	1:E:970:LYS:HB2	1.81	0.42
1:H:954:ASP:OD2	1:H:957:SER:OG	2.32	0.42
1:D:715:ILE:HD11	1:D:730:LEU:HG	2.00	0.42
1:A:754:LYS:HE3	1:A:861:LEU:O	2.19	0.42
1:E:989:LEU:HD13	1:E:1010:VAL:HG11	2.00	0.42
1:D:717:VAL:HG21	1:A:830:ASP:HB3	2.01	0.42
1:E:962:ARG:NH2	4:E:1310:HOH:O	2.40	0.42
1:F:879:LYS:HD3	1:F:914:PRO:O	2.19	0.42
1:G:721:GLY:HA3	2:G:1302:CL:CL	2.55	0.42
1:D:915:TYR:OH	4:D:1301:HOH:O	2.21	0.42
1:D:946:ILE:CD1	1:D:967:GLU:HG2	2.49	0.42
1:B:867:LYS:HA	1:H:706:ILE:HD12	2.02	0.42
1:C:754:LYS:HE2	1:C:861:LEU:HD12	2.02	0.42
1:G:829:GLU:HA	1:G:893:HIS:CE1	2.55	0.42
1:G:796:GLY:HA2	3:G:1301:QQM:C32	2.49	0.41
1:H:747:LEU:HD12	1:H:786:VAL:HB	2.01	0.41
1:E:790:MET:HG2	3:E:1202:QQM:C07	2.51	0.41
1:A:732:ILE:HG13	1:A:739:LYS:HD2	2.02	0.41
1:H:836:ARG:CZ	1:H:860:LYS:HD2	2.50	0.41
1:A:726:VAL:HG21	3:A:1202:QQM:C17	2.51	0.41
1:F:800:ASP:O	1:F:804:GLU:HG3	2.21	0.41
1:F:827:TYR:OH	1:F:831:ARG:NH1	2.53	0.41
1:D:723:PHE:HB2	2:D:1201:CL:CL	2.58	0.41
1:D:796:GLY:HA2	3:D:1202:QQM:C32	2.50	0.41
1:G:812:GLN:HB3	1:G:989:LEU:HG	2.02	0.41
1:D:869:TYR:CD1	1:D:876:VAL:HG21	2.56	0.41
1:C:709:GLU:HG3	1:C:783:THR:HG21	2.03	0.41
1:D:865:GLU:HG2	4:D:1356:HOH:O	2.20	0.41
1:B:970:LYS:HE3	1:B:970:LYS:HB2	1.81	0.41
1:F:726:VAL:HG21	3:F:1202:QQM:C17	2.51	0.41
1:D:960:LYS:HE3	4:D:1306:HOH:O	2.21	0.41
1:E:748:ARG:HB2	1:F:832:ARG:NH2	2.34	0.41
1:G:800:ASP:OD2	4:G:1401:HOH:O	2.22	0.41
1:G:823:LYS:NZ	1:G:1009:ASP:HB2	2.36	0.41
1:A:723:PHE:HB2	2:A:1201:CL:CL	2.59	0.40
1:E:985:GLU:H	1:E:985:GLU:HG3	1.58	0.40
1:F:811:SER:OG	1:F:975:PRO:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:829:GLU:HA	1:H:893:HIS:CE1	2.56	0.40
1:D:989:LEU:HB3	1:D:990:PRO:HD2	2.02	0.40
1:F:923:ILE:O	1:F:926:ILE:HG13	2.21	0.40
1:G:811:SER:OG	1:G:975:PRO:HB2	2.21	0.40
1:B:945:MET:HE2	1:B:945:MET:HB2	2.03	0.40
1:C:811:SER:OG	1:C:975:PRO:HB2	2.22	0.40
1:F:973:ARG:NH1	1:F:1011:VAL:CG1	2.85	0.40
1:D:850:HIS:ND1	1:D:1003:ASP:OD2	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	305/327 (93%)	299 (98%)	5 (2%)	1 (0%)	41	41
1	B	312/327 (95%)	305 (98%)	6 (2%)	1 (0%)	41	41
1	C	291/327 (89%)	286 (98%)	5 (2%)	0	100	100
1	D	313/327 (96%)	303 (97%)	9 (3%)	1 (0%)	41	41
1	E	300/327 (92%)	293 (98%)	7 (2%)	0	100	100
1	F	296/327 (90%)	286 (97%)	9 (3%)	1 (0%)	41	41
1	G	291/327 (89%)	276 (95%)	13 (4%)	2 (1%)	22	18
1	H	294/327 (90%)	290 (99%)	4 (1%)	0	100	100
All	All	2402/2616 (92%)	2338 (97%)	58 (2%)	6 (0%)	41	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	859	ALA
1	B	874	GLY

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Mol	Chain	Res	Type
1	F	806	LYS
1	G	749	GLU
1	A	753	PRO
1	D	715	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	271/287 (94%)	270 (100%)	1 (0%)	91	94
1	B	277/287 (96%)	276 (100%)	1 (0%)	91	94
1	C	265/287 (92%)	263 (99%)	2 (1%)	81	86
1	D	278/287 (97%)	273 (98%)	5 (2%)	59	65
1	E	271/287 (94%)	268 (99%)	3 (1%)	73	79
1	F	269/287 (94%)	263 (98%)	6 (2%)	52	57
1	G	263/287 (92%)	254 (97%)	9 (3%)	37	39
1	H	268/287 (93%)	265 (99%)	3 (1%)	73	79
All	All	2162/2296 (94%)	2132 (99%)	30 (1%)	69	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	705	ARG
1	D	754	LYS
1	D	757	LYS
1	D	769	VAL
1	D	784	SER
1	A	867	LYS
1	B	711	GLU
1	C	1002	MET
1	C	1007	MET
1	E	749	GLU
1	E	985	GLU

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Mol	Chain	Res	Type
1	E	988	HIS
1	F	751	THR
1	F	754	LYS
1	F	769	VAL
1	F	812	GLN
1	F	988	HIS
1	F	991	SER
1	G	757	LYS
1	G	855	ASP
1	G	922[A]	GLU
1	G	922[B]	GLU
1	G	942	ASP
1	G	970	LYS
1	G	976	GLN
1	G	1007	MET
1	G	1009	ASP
1	H	922[A]	GLU
1	H	922[B]	GLU
1	H	998	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	816	ASN
1	E	812	GLN
1	G	816	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	QQM	C	1202	1	37,39,39	5.98	26 (70%)	46,53,53	2.19	11 (23%)
3	QQM	G	1301	1	37,39,39	5.95	25 (67%)	46,53,53	1.52	10 (21%)
3	QQM	B	1202	1	37,39,39	5.95	26 (70%)	46,53,53	1.51	9 (19%)
3	QQM	A	1202	1	37,39,39	5.94	26 (70%)	46,53,53	1.58	9 (19%)
3	QQM	F	1202	1	37,39,39	5.94	26 (70%)	46,53,53	1.56	10 (21%)
3	QQM	D	1202	1	37,39,39	5.94	25 (67%)	46,53,53	1.52	11 (23%)
3	QQM	E	1202	1	37,39,39	5.96	26 (70%)	46,53,53	1.57	11 (23%)
3	QQM	H	1202	1	37,39,39	5.93	25 (67%)	46,53,53	1.51	9 (19%)

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	QQM	C	1202	1	-	7/24/24/24	0/4/4/4
3	QQM	G	1301	1	-	2/24/24/24	0/4/4/4
3	QQM	B	1202	1	-	5/24/24/24	0/4/4/4
3	QQM	A	1202	1	-	5/24/24/24	0/4/4/4
3	QQM	F	1202	1	-	4/24/24/24	0/4/4/4
3	QQM	D	1202	1	-	5/24/24/24	0/4/4/4
3	QQM	E	1202	1	-	6/24/24/24	0/4/4/4
3	QQM	H	1202	1	-	6/24/24/24	0/4/4/4

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1301	QQM	C32-C30	10.26	1.56	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	QQM	C32-C30	10.25	1.56	1.39
3	H	1202	QQM	C32-C30	10.21	1.56	1.39
3	F	1202	QQM	C32-C30	10.20	1.56	1.39
3	E	1202	QQM	C32-C30	10.19	1.56	1.39
3	A	1202	QQM	C32-C30	10.10	1.55	1.39
3	B	1202	QQM	C32-C30	9.99	1.55	1.39
3	D	1202	QQM	C32-C30	9.79	1.55	1.39
3	E	1202	QQM	C27-C26	9.59	1.56	1.38
3	A	1202	QQM	C27-C26	9.56	1.56	1.38
3	D	1202	QQM	C27-C26	9.55	1.56	1.38
3	F	1202	QQM	C27-C26	9.50	1.56	1.38
3	H	1202	QQM	C27-C26	9.50	1.56	1.38
3	B	1202	QQM	C27-C26	9.44	1.55	1.38
3	G	1301	QQM	C27-C26	9.32	1.55	1.38
3	C	1202	QQM	C27-C26	9.05	1.55	1.38
3	A	1202	QQM	C04-C07	8.84	1.54	1.37
3	D	1202	QQM	C04-C07	8.83	1.54	1.37
3	B	1202	QQM	C04-C07	8.80	1.54	1.37
3	G	1301	QQM	C04-C07	8.78	1.54	1.37
3	C	1202	QQM	C04-C07	8.77	1.54	1.37
3	F	1202	QQM	C04-C07	8.75	1.54	1.37
3	H	1202	QQM	C14-C15	8.71	1.59	1.49
3	H	1202	QQM	C04-C07	8.71	1.54	1.37
3	E	1202	QQM	C04-C07	8.70	1.54	1.37
3	B	1202	QQM	C14-C15	8.65	1.58	1.49
3	E	1202	QQM	C10-C07	8.64	1.54	1.37
3	H	1202	QQM	C10-C07	8.62	1.54	1.37
3	G	1301	QQM	C14-C15	8.62	1.58	1.49
3	G	1301	QQM	C10-C07	8.60	1.54	1.37
3	F	1202	QQM	C10-C07	8.58	1.53	1.37
3	B	1202	QQM	C10-C07	8.55	1.53	1.37
3	C	1202	QQM	C10-C07	8.54	1.53	1.37
3	C	1202	QQM	C14-C15	8.54	1.58	1.49
3	D	1202	QQM	C10-C07	8.52	1.53	1.37
3	A	1202	QQM	C14-C15	8.52	1.58	1.49
3	D	1202	QQM	C21-N11	8.51	1.53	1.38
3	A	1202	QQM	C10-C07	8.49	1.53	1.37
3	D	1202	QQM	C14-C15	8.48	1.58	1.49
3	F	1202	QQM	C14-C15	8.46	1.58	1.49
3	C	1202	QQM	C21-N11	8.45	1.53	1.38
3	B	1202	QQM	C21-N11	8.39	1.53	1.38
3	E	1202	QQM	C21-N08	8.38	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1202	QQM	C21-N08	8.36	1.50	1.34
3	C	1202	QQM	C12-C10	8.36	1.54	1.38
3	G	1301	QQM	C21-N08	8.35	1.50	1.34
3	A	1202	QQM	C21-N11	8.33	1.53	1.38
3	H	1202	QQM	C12-C10	8.33	1.53	1.38
3	B	1202	QQM	C21-N08	8.32	1.50	1.34
3	A	1202	QQM	C21-N08	8.32	1.50	1.34
3	G	1301	QQM	C12-C10	8.31	1.53	1.38
3	E	1202	QQM	C12-C10	8.31	1.53	1.38
3	E	1202	QQM	C21-N11	8.31	1.53	1.38
3	C	1202	QQM	C21-N08	8.31	1.50	1.34
3	D	1202	QQM	C21-N08	8.30	1.50	1.34
3	F	1202	QQM	C21-N11	8.29	1.53	1.38
3	B	1202	QQM	C12-C10	8.27	1.53	1.38
3	F	1202	QQM	C12-C10	8.24	1.53	1.38
3	G	1301	QQM	C21-N11	8.23	1.53	1.38
3	H	1202	QQM	C21-N08	8.18	1.49	1.34
3	A	1202	QQM	C12-C10	8.17	1.53	1.38
3	D	1202	QQM	C12-C10	8.16	1.53	1.38
3	E	1202	QQM	C14-C15	8.08	1.58	1.49
3	H	1202	QQM	C21-N11	8.05	1.52	1.38
3	C	1202	QQM	C32-C29	8.01	1.52	1.39
3	A	1202	QQM	C26-C30	7.94	1.52	1.39
3	H	1202	QQM	C26-C30	7.94	1.52	1.39
3	E	1202	QQM	C26-C30	7.93	1.52	1.39
3	B	1202	QQM	C26-C30	7.89	1.52	1.39
3	A	1202	QQM	C04-C01	7.88	1.53	1.38
3	F	1202	QQM	C26-C30	7.87	1.52	1.39
3	D	1202	QQM	C04-C01	7.85	1.53	1.38
3	B	1202	QQM	C04-C01	7.85	1.53	1.38
3	E	1202	QQM	C32-C29	7.83	1.51	1.39
3	D	1202	QQM	C26-C30	7.81	1.52	1.39
3	G	1301	QQM	C32-C29	7.80	1.51	1.39
3	H	1202	QQM	C32-C29	7.80	1.51	1.39
3	C	1202	QQM	C04-C01	7.79	1.52	1.38
3	G	1301	QQM	C04-C01	7.79	1.52	1.38
3	C	1202	QQM	C29-C28	7.79	1.57	1.40
3	H	1202	QQM	C04-C01	7.78	1.52	1.38
3	A	1202	QQM	C32-C29	7.73	1.51	1.39
3	F	1202	QQM	C04-C01	7.72	1.52	1.38
3	F	1202	QQM	C32-C29	7.70	1.51	1.39
3	G	1301	QQM	C26-C30	7.65	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1202	QQM	C04-C01	7.59	1.52	1.38
3	C	1202	QQM	C26-C30	7.59	1.52	1.39
3	B	1202	QQM	C32-C29	7.50	1.51	1.39
3	D	1202	QQM	C32-C29	7.30	1.50	1.39
3	D	1202	QQM	C27-C28	7.20	1.54	1.39
3	A	1202	QQM	C27-C28	7.15	1.54	1.39
3	C	1202	QQM	C01-C14	7.12	1.54	1.39
3	D	1202	QQM	C01-C14	7.11	1.54	1.39
3	F	1202	QQM	C27-C28	7.10	1.54	1.39
3	G	1301	QQM	C01-C14	7.10	1.54	1.39
3	G	1301	QQM	C29-C28	7.10	1.55	1.40
3	H	1202	QQM	C01-C14	7.10	1.54	1.39
3	A	1202	QQM	C01-C14	7.10	1.54	1.39
3	B	1202	QQM	C01-C14	7.09	1.54	1.39
3	E	1202	QQM	C27-C28	7.07	1.54	1.39
3	F	1202	QQM	C01-C14	7.07	1.54	1.39
3	B	1202	QQM	C27-C28	7.04	1.54	1.39
3	H	1202	QQM	C27-C28	7.03	1.54	1.39
3	E	1202	QQM	C01-C14	7.02	1.54	1.39
3	G	1301	QQM	C27-C28	7.00	1.54	1.39
3	B	1202	QQM	C29-C28	6.98	1.55	1.40
3	A	1202	QQM	C29-C28	6.94	1.55	1.40
3	E	1202	QQM	C23-C16	6.93	1.57	1.49
3	D	1202	QQM	C29-C28	6.93	1.55	1.40
3	F	1202	QQM	C29-C28	6.92	1.55	1.40
3	C	1202	QQM	C27-C28	6.92	1.54	1.39
3	E	1202	QQM	C29-C28	6.92	1.55	1.40
3	B	1202	QQM	C24-C25	6.92	1.52	1.38
3	F	1202	QQM	C24-C25	6.90	1.52	1.38
3	E	1202	QQM	C24-C25	6.89	1.52	1.38
3	G	1301	QQM	C24-C25	6.89	1.52	1.38
3	D	1202	QQM	C23-C16	6.88	1.56	1.49
3	D	1202	QQM	C24-C25	6.88	1.52	1.38
3	A	1202	QQM	C24-C25	6.88	1.52	1.38
3	A	1202	QQM	C25-N08	6.87	1.49	1.34
3	F	1202	QQM	C25-N08	6.83	1.49	1.34
3	H	1202	QQM	C12-C14	6.82	1.53	1.39
3	B	1202	QQM	C25-N08	6.81	1.48	1.34
3	G	1301	QQM	C25-N08	6.81	1.48	1.34
3	C	1202	QQM	C24-C25	6.79	1.52	1.38
3	E	1202	QQM	C25-N08	6.79	1.48	1.34
3	H	1202	QQM	C29-C28	6.79	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	QQM	C12-C14	6.78	1.53	1.39
3	D	1202	QQM	C25-N08	6.78	1.48	1.34
3	D	1202	QQM	C12-C14	6.77	1.53	1.39
3	H	1202	QQM	C24-C25	6.77	1.52	1.38
3	C	1202	QQM	C25-N08	6.77	1.48	1.34
3	F	1202	QQM	C12-C14	6.77	1.53	1.39
3	B	1202	QQM	C23-C16	6.75	1.56	1.49
3	C	1202	QQM	C12-C14	6.75	1.53	1.39
3	E	1202	QQM	C12-C14	6.74	1.53	1.39
3	G	1301	QQM	C12-C14	6.74	1.53	1.39
3	A	1202	QQM	C12-C14	6.72	1.53	1.39
3	H	1202	QQM	C23-C16	6.64	1.56	1.49
3	H	1202	QQM	C25-N08	6.63	1.48	1.34
3	G	1301	QQM	C23-C16	6.60	1.56	1.49
3	C	1202	QQM	C23-C16	6.59	1.56	1.49
3	F	1202	QQM	C23-C16	6.38	1.56	1.49
3	A	1202	QQM	C23-C16	6.15	1.56	1.49
3	G	1301	QQM	C22-C23	5.62	1.49	1.39
3	C	1202	QQM	C22-C23	5.59	1.49	1.39
3	B	1202	QQM	C22-C23	5.50	1.49	1.39
3	D	1202	QQM	C22-C23	5.47	1.49	1.39
3	F	1202	QQM	C22-C23	5.43	1.49	1.39
3	E	1202	QQM	C22-C23	5.42	1.49	1.39
3	A	1202	QQM	C22-C23	5.40	1.49	1.39
3	E	1202	QQM	C24-C23	5.36	1.50	1.39
3	D	1202	QQM	C24-C23	5.34	1.50	1.39
3	H	1202	QQM	C22-C23	5.33	1.49	1.39
3	B	1202	QQM	C24-C23	5.32	1.50	1.39
3	F	1202	QQM	C24-C23	5.29	1.50	1.39
3	G	1301	QQM	C24-C23	5.29	1.50	1.39
3	A	1202	QQM	C24-C23	5.26	1.50	1.39
3	C	1202	QQM	O06-C28	5.24	1.45	1.37
3	C	1202	QQM	C24-C23	5.22	1.50	1.39
3	D	1202	QQM	C22-C21	5.19	1.52	1.39
3	H	1202	QQM	C24-C23	5.15	1.50	1.39
3	C	1202	QQM	C22-C21	5.12	1.52	1.39
3	B	1202	QQM	C22-C21	5.11	1.52	1.39
3	G	1301	QQM	C22-C21	5.10	1.52	1.39
3	E	1202	QQM	C22-C21	5.08	1.52	1.39
3	F	1202	QQM	C22-C21	5.03	1.52	1.39
3	H	1202	QQM	C22-C21	5.00	1.52	1.39
3	D	1202	QQM	C33-N13	4.97	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	QQM	C22-C21	4.94	1.52	1.39
3	E	1202	QQM	O06-C28	4.91	1.45	1.37
3	A	1202	QQM	C33-N13	4.84	1.46	1.35
3	A	1202	QQM	O06-C28	4.81	1.44	1.37
3	E	1202	QQM	C33-N13	4.78	1.46	1.35
3	B	1202	QQM	C33-N13	4.77	1.46	1.35
3	H	1202	QQM	O06-C28	4.76	1.44	1.37
3	F	1202	QQM	O06-C28	4.76	1.44	1.37
3	H	1202	QQM	C33-N13	4.74	1.46	1.35
3	F	1202	QQM	C33-N13	4.74	1.46	1.35
3	C	1202	QQM	C33-N13	4.69	1.46	1.35
3	G	1301	QQM	O06-C28	4.68	1.44	1.37
3	D	1202	QQM	O06-C28	4.67	1.44	1.37
3	B	1202	QQM	O06-C28	4.66	1.44	1.37
3	G	1301	QQM	C33-N13	4.59	1.45	1.35
3	E	1202	QQM	C30-N13	4.52	1.50	1.41
3	A	1202	QQM	C30-N13	4.47	1.50	1.41
3	C	1202	QQM	C30-N13	4.43	1.50	1.41
3	H	1202	QQM	C30-N13	4.41	1.50	1.41
3	F	1202	QQM	C30-N13	4.38	1.50	1.41
3	D	1202	QQM	C30-N13	4.35	1.50	1.41
3	B	1202	QQM	C30-N13	4.33	1.50	1.41
3	G	1301	QQM	C30-N13	4.20	1.50	1.41
3	E	1202	QQM	O06-C31	2.55	1.50	1.42
3	G	1301	QQM	O06-C31	2.54	1.50	1.42
3	B	1202	QQM	O06-C31	2.53	1.50	1.42
3	A	1202	QQM	O06-C31	2.51	1.50	1.42
3	F	1202	QQM	O06-C31	2.49	1.50	1.42
3	D	1202	QQM	O06-C31	2.49	1.50	1.42
3	H	1202	QQM	O06-C31	2.47	1.50	1.42
3	C	1202	QQM	O06-C31	2.26	1.49	1.42
3	C	1202	QQM	C29-N11	2.12	1.45	1.39
3	A	1202	QQM	C29-N11	2.05	1.45	1.39
3	E	1202	QQM	C29-N11	2.03	1.45	1.39
3	B	1202	QQM	C29-N11	2.03	1.45	1.39
3	F	1202	QQM	C29-N11	2.02	1.45	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	QQM	O06-C28-C29	9.31	126.23	114.80
3	C	1202	QQM	O06-C28-C27	-5.59	114.78	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1301	QQM	O06-C28-C29	4.04	119.76	114.80
3	B	1202	QQM	O06-C28-C29	3.72	119.37	114.80
3	F	1202	QQM	O06-C28-C29	3.72	119.36	114.80
3	D	1202	QQM	O06-C28-C29	3.65	119.28	114.80
3	E	1202	QQM	O06-C28-C29	3.63	119.26	114.80
3	H	1202	QQM	C24-C25-N08	-3.60	119.49	123.96
3	A	1202	QQM	O06-C28-C29	3.56	119.17	114.80
3	A	1202	QQM	C22-C21-N08	-3.32	118.12	122.75
3	E	1202	QQM	C24-C25-N08	-3.23	119.94	123.96
3	D	1202	QQM	C22-C21-N08	-3.15	118.36	122.75
3	C	1202	QQM	C22-C21-N08	-3.10	118.43	122.75
3	B	1202	QQM	C24-C25-N08	-3.09	120.12	123.96
3	F	1202	QQM	C22-C21-N08	-3.05	118.50	122.75
3	H	1202	QQM	O06-C28-C29	3.04	118.53	114.80
3	B	1202	QQM	C22-C21-N08	-3.03	118.53	122.75
3	F	1202	QQM	C24-C25-N08	-2.99	120.25	123.96
3	A	1202	QQM	C24-C25-N08	-2.98	120.25	123.96
3	G	1301	QQM	C24-C25-N08	-2.97	120.27	123.96
3	D	1202	QQM	C24-C25-N08	-2.93	120.32	123.96
3	C	1202	QQM	C24-C25-N08	-2.90	120.35	123.96
3	G	1301	QQM	C22-C21-N08	-2.88	118.73	122.75
3	A	1202	QQM	C25-N08-C21	2.85	121.26	117.22
3	H	1202	QQM	N02-C17-N05	-2.80	107.33	115.89
3	B	1202	QQM	N02-C17-N05	-2.79	107.38	115.89
3	E	1202	QQM	N02-C17-N05	-2.74	107.51	115.89
3	D	1202	QQM	N02-C17-N05	-2.71	107.60	115.89
3	A	1202	QQM	N02-C17-N05	-2.71	107.62	115.89
3	E	1202	QQM	C22-C21-N08	-2.69	119.00	122.75
3	F	1202	QQM	N02-C17-N05	-2.68	107.70	115.89
3	C	1202	QQM	N02-C17-N05	-2.67	107.74	115.89
3	H	1202	QQM	C18-C17-N02	2.66	129.99	122.54
3	G	1301	QQM	N02-C17-N05	-2.66	107.77	115.89
3	C	1202	QQM	C30-N13-C33	-2.65	122.86	127.50
3	C	1202	QQM	C34-C33-N13	2.62	121.75	114.75
3	F	1202	QQM	C25-N08-C21	2.59	120.89	117.22
3	C	1202	QQM	C25-N08-C21	2.58	120.88	117.22
3	B	1202	QQM	C25-N08-C21	2.57	120.87	117.22
3	D	1202	QQM	C30-N13-C33	-2.52	123.08	127.50
3	G	1301	QQM	C25-N08-C21	2.51	120.78	117.22
3	C	1202	QQM	C31-O06-C28	2.51	121.31	117.53
3	D	1202	QQM	C25-N08-C21	2.50	120.77	117.22
3	E	1202	QQM	C30-N13-C33	-2.48	123.16	127.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1202	QQM	C25-N08-C21	2.46	120.71	117.22
3	H	1202	QQM	C22-C21-N08	-2.44	119.35	122.75
3	A	1202	QQM	C16-C15-N05	-2.43	107.20	113.76
3	E	1202	QQM	C01-C14-C15	-2.42	116.78	120.61
3	G	1301	QQM	O06-C28-C27	-2.42	120.23	124.37
3	E	1202	QQM	C25-N08-C21	2.36	120.57	117.22
3	H	1202	QQM	C16-C15-N05	-2.36	107.39	113.76
3	E	1202	QQM	C34-C33-N13	2.35	121.04	114.75
3	B	1202	QQM	C31-O06-C28	-2.34	114.00	117.53
3	E	1202	QQM	C15-C16-N02	-2.34	107.44	113.76
3	D	1202	QQM	C31-O06-C28	-2.33	114.01	117.53
3	G	1301	QQM	C31-O06-C28	-2.31	114.04	117.53
3	F	1202	QQM	C16-C15-N05	-2.31	107.54	113.76
3	C	1202	QQM	C16-C15-N05	-2.29	107.57	113.76
3	F	1202	QQM	C30-N13-C33	-2.29	123.49	127.50
3	F	1202	QQM	C34-C33-N13	2.28	120.84	114.75
3	H	1202	QQM	C30-N13-C33	-2.26	123.54	127.50
3	B	1202	QQM	C16-C15-N05	-2.24	107.71	113.76
3	D	1202	QQM	C15-C16-N02	-2.23	107.73	113.76
3	G	1301	QQM	C30-N13-C33	-2.23	123.60	127.50
3	D	1202	QQM	C23-C22-C21	2.23	121.78	118.97
3	B	1202	QQM	C15-C16-N02	-2.22	107.77	113.76
3	G	1301	QQM	C16-C15-N05	-2.22	107.78	113.76
3	B	1202	QQM	O06-C28-C27	-2.19	120.61	124.37
3	G	1301	QQM	C15-C16-N02	-2.18	107.87	113.76
3	E	1202	QQM	C18-C17-N02	2.16	128.59	122.54
3	D	1202	QQM	C16-C15-N05	-2.16	107.93	113.76
3	C	1202	QQM	C15-C16-N02	-2.15	107.96	113.76
3	A	1202	QQM	C22-C23-C16	-2.14	116.04	120.15
3	A	1202	QQM	C34-C33-N13	2.13	120.44	114.75
3	F	1202	QQM	C15-C16-N02	-2.11	108.08	113.76
3	H	1202	QQM	C15-C16-N02	-2.09	108.12	113.76
3	E	1202	QQM	C16-C15-N05	-2.08	108.14	113.76
3	F	1202	QQM	O06-C28-C27	-2.04	120.87	124.37
3	A	1202	QQM	C15-C16-N02	-2.04	108.26	113.76
3	D	1202	QQM	C34-C33-N13	2.03	120.17	114.75

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1202	QQM	C29-C28-O06-C31

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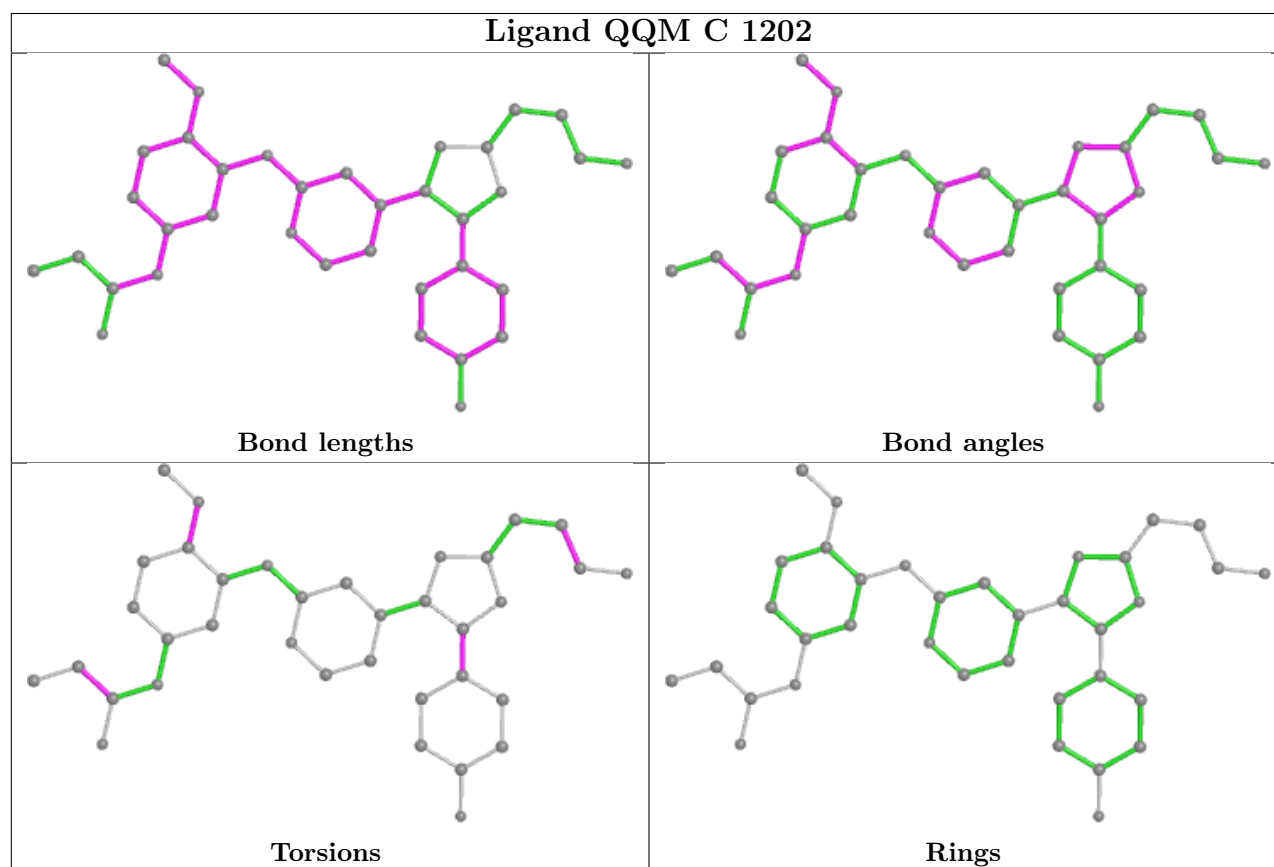
Mol	Chain	Res	Type	Atoms
3	C	1202	QQM	C27-C28-O06-C31
3	D	1202	QQM	C18-C19-C20-O03
3	B	1202	QQM	C18-C19-C20-O03
3	C	1202	QQM	C18-C19-C20-O03
3	E	1202	QQM	C18-C19-C20-O03
3	H	1202	QQM	C18-C19-C20-O03
3	D	1202	QQM	C01-C14-C15-N05
3	D	1202	QQM	C12-C14-C15-N05
3	A	1202	QQM	C12-C14-C15-N05
3	F	1202	QQM	C01-C14-C15-N05
3	F	1202	QQM	C12-C14-C15-N05
3	A	1202	QQM	C18-C19-C20-O03
3	A	1202	QQM	C01-C14-C15-N05
3	B	1202	QQM	C01-C14-C15-N05
3	D	1202	QQM	O09-C33-C34-C35
3	B	1202	QQM	C12-C14-C15-N05
3	C	1202	QQM	C01-C14-C15-N05
3	C	1202	QQM	C12-C14-C15-N05
3	E	1202	QQM	C01-C14-C15-N05
3	D	1202	QQM	N13-C33-C34-C35
3	E	1202	QQM	C12-C14-C15-N05
3	G	1301	QQM	C12-C14-C15-N05
3	H	1202	QQM	C01-C14-C15-N05
3	H	1202	QQM	C12-C14-C15-N05
3	G	1301	QQM	C01-C14-C15-N05
3	A	1202	QQM	N13-C33-C34-C35
3	B	1202	QQM	N13-C33-C34-C35
3	C	1202	QQM	N13-C33-C34-C35
3	F	1202	QQM	N13-C33-C34-C35
3	H	1202	QQM	N13-C33-C34-C35
3	A	1202	QQM	O09-C33-C34-C35
3	B	1202	QQM	O09-C33-C34-C35
3	C	1202	QQM	O09-C33-C34-C35
3	E	1202	QQM	O09-C33-C34-C35
3	F	1202	QQM	O09-C33-C34-C35
3	H	1202	QQM	O09-C33-C34-C35
3	E	1202	QQM	N05-C17-C18-C19
3	H	1202	QQM	N05-C17-C18-C19
3	E	1202	QQM	N13-C33-C34-C35

There are no ring outliers.

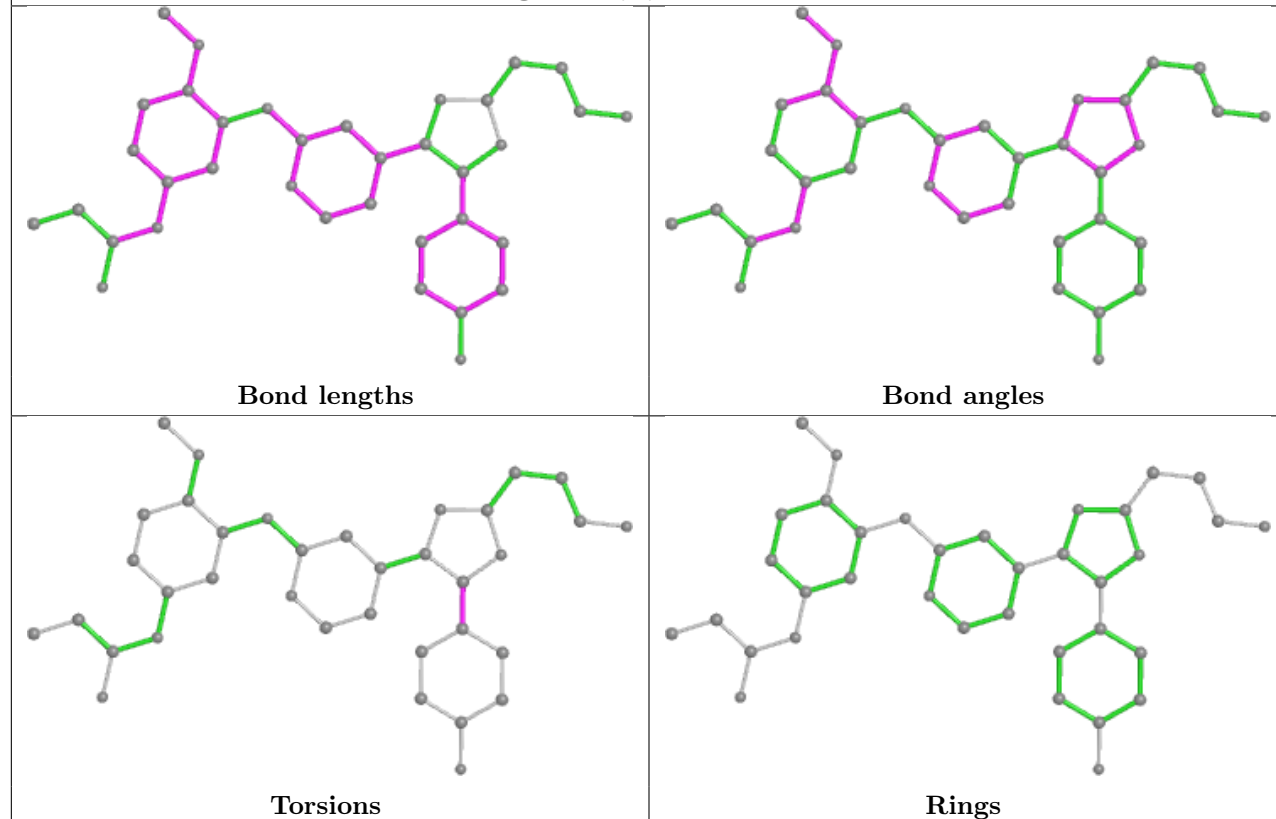
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1301	QQM	1	0
3	A	1202	QQM	2	0
3	F	1202	QQM	2	0
3	D	1202	QQM	2	0
3	E	1202	QQM	1	0

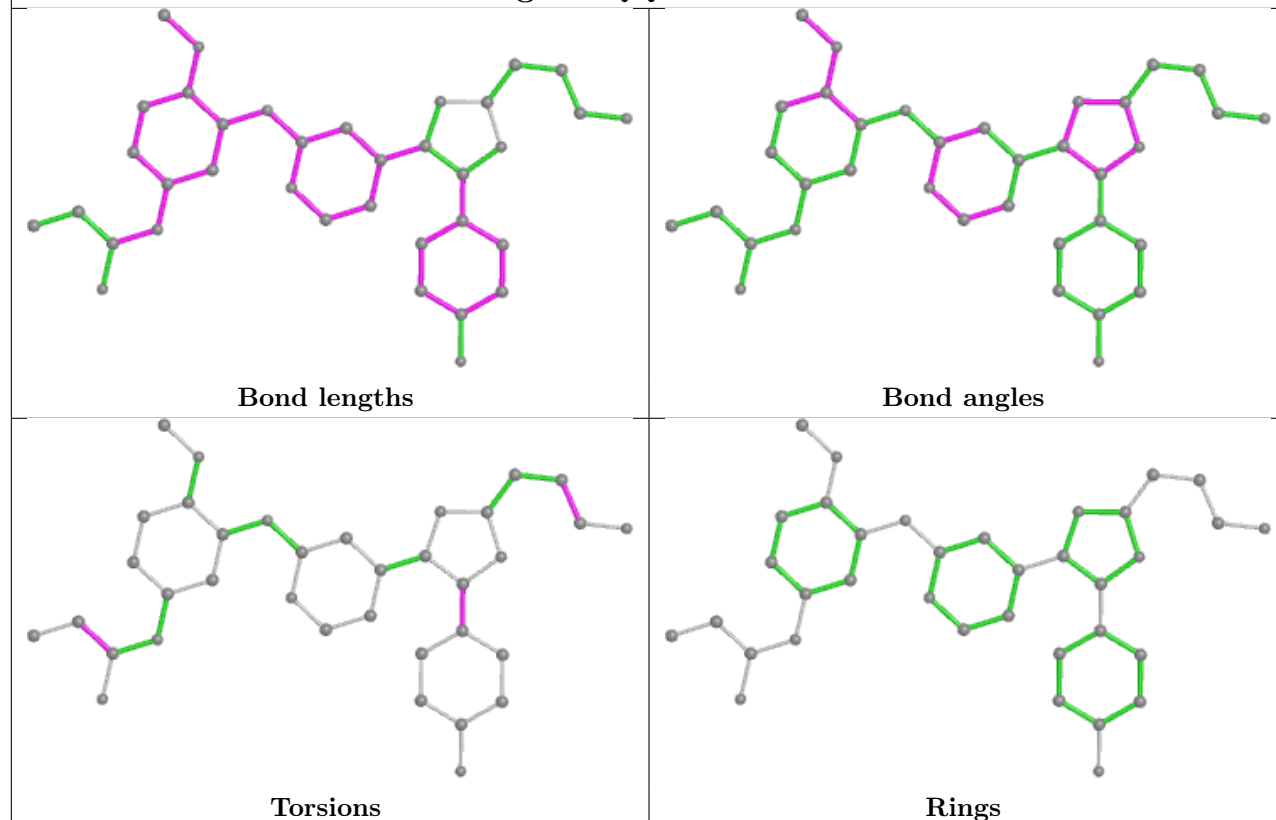
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



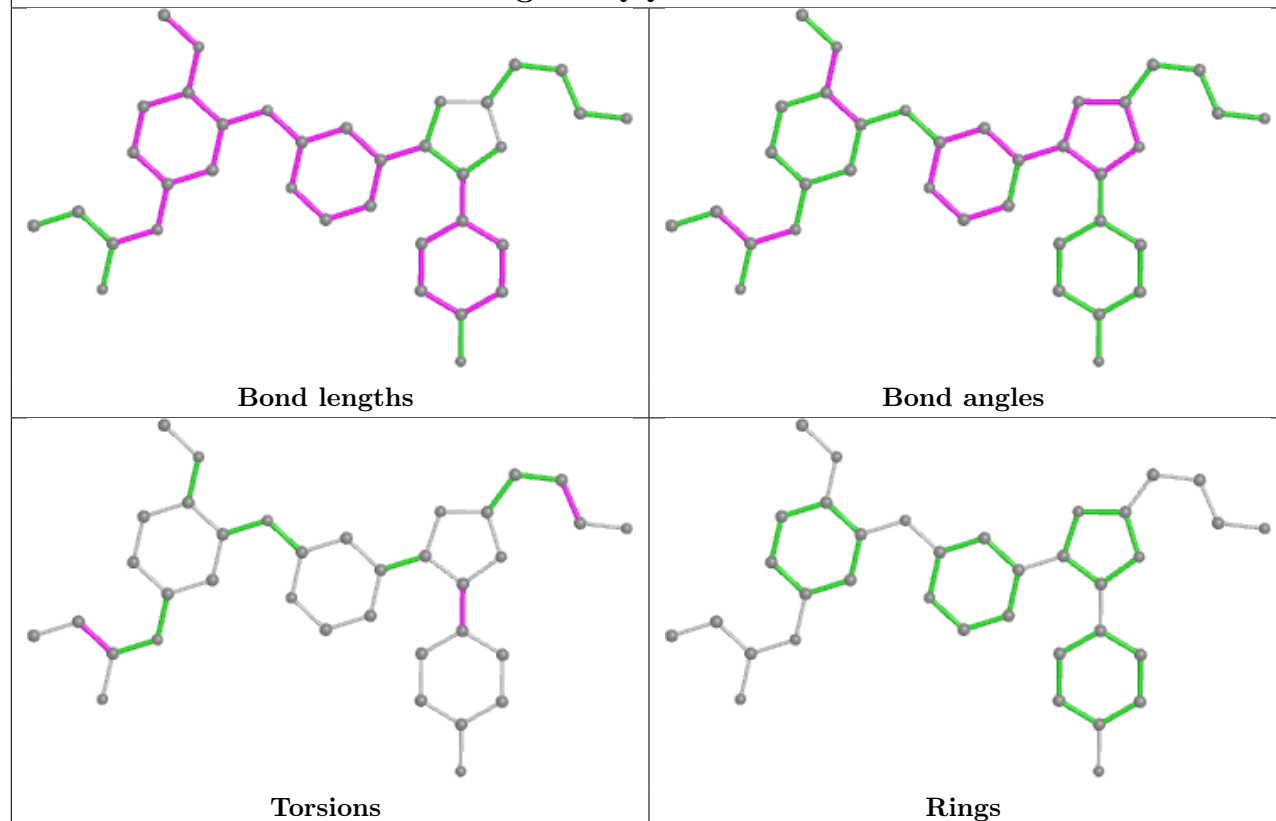
Ligand QQM G 1301



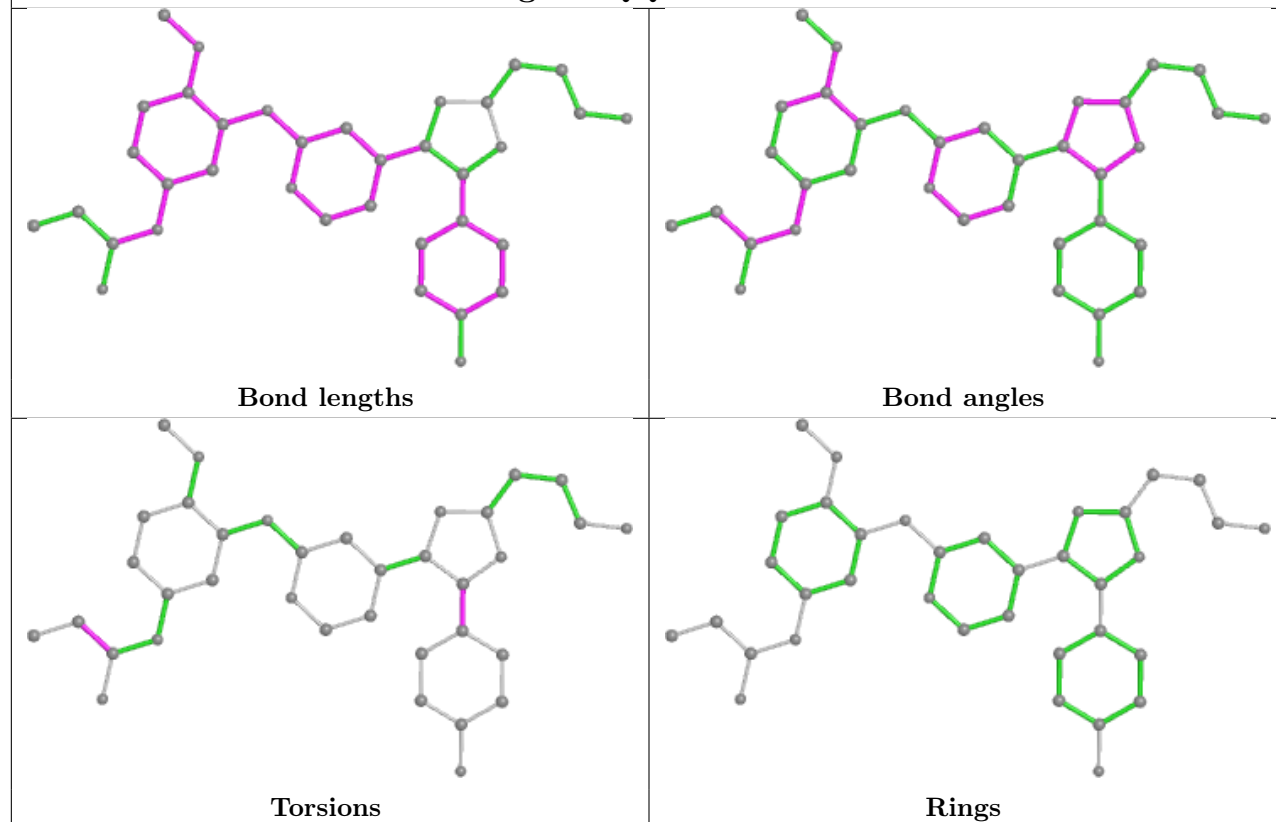
Ligand QQM B 1202



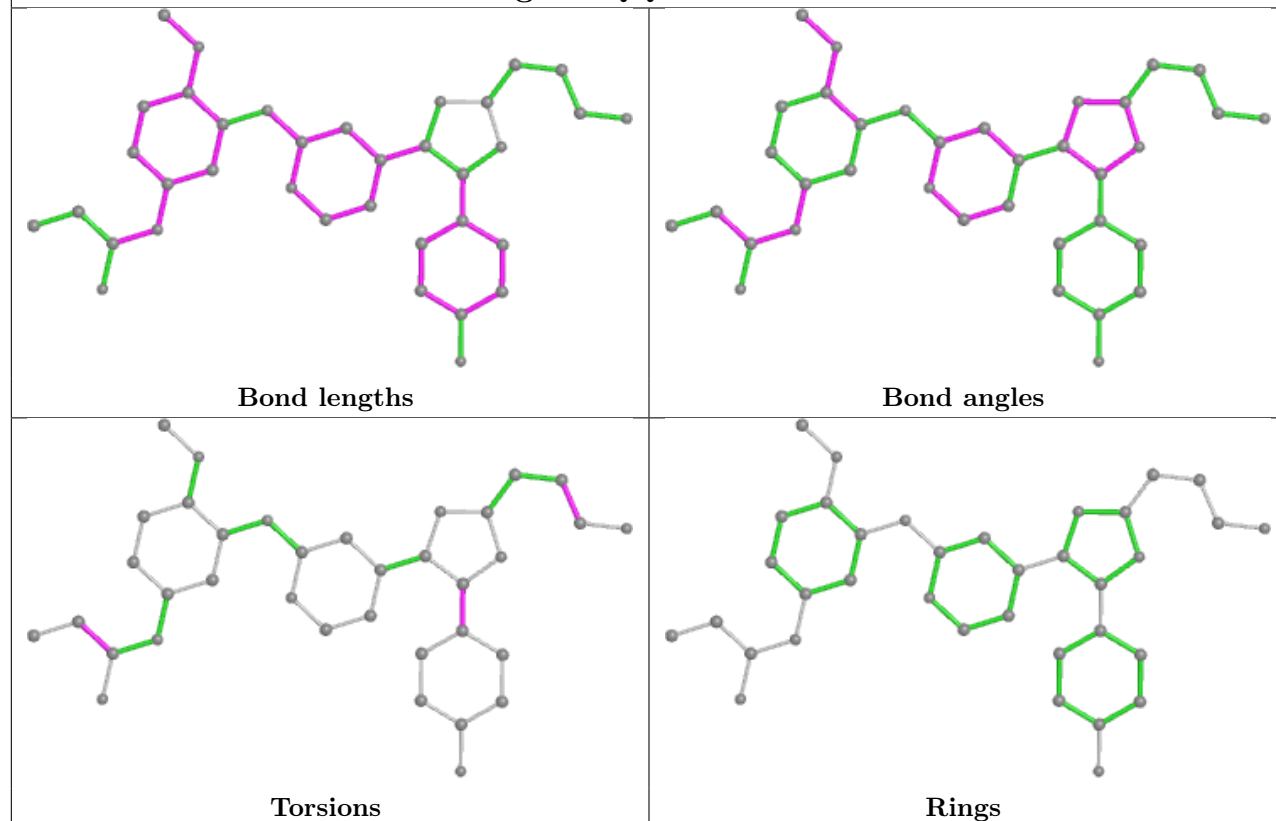
Ligand QQM A 1202



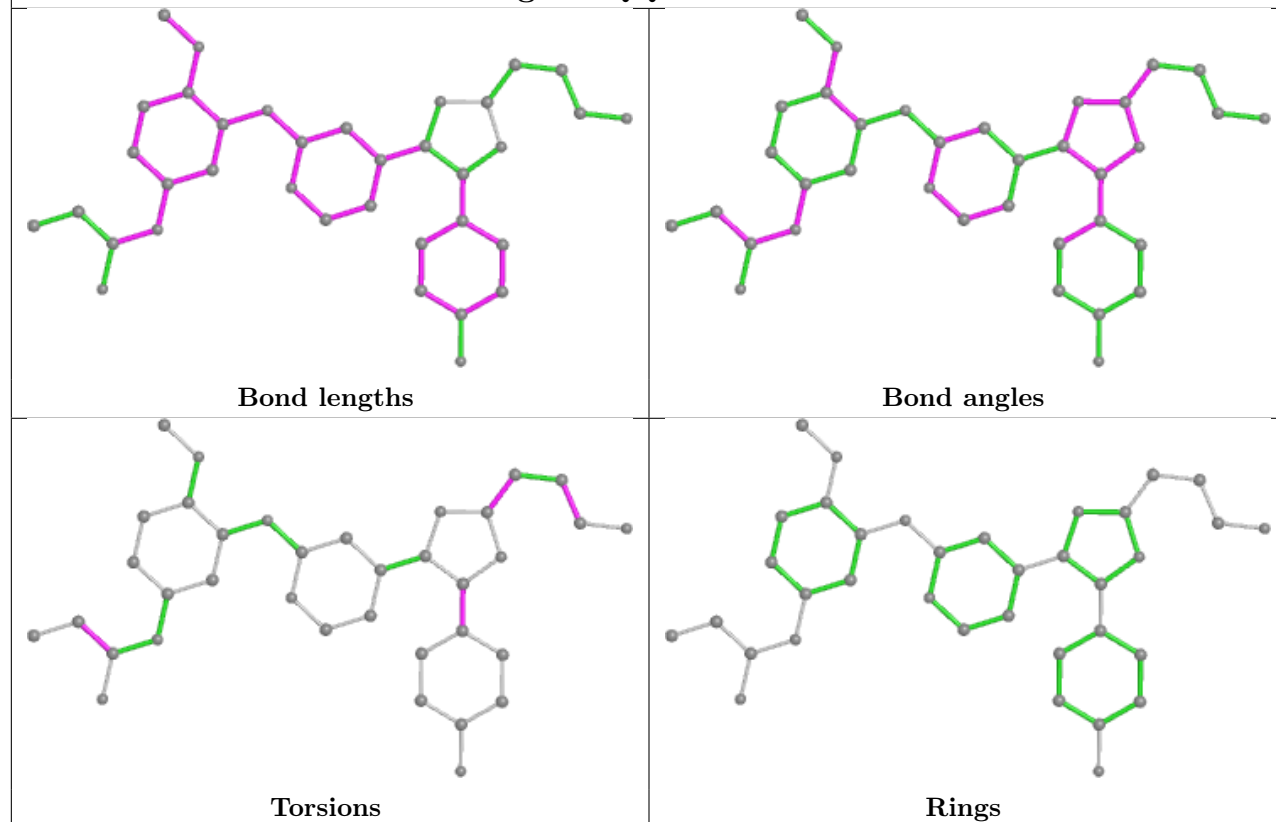
Ligand QQM F 1202

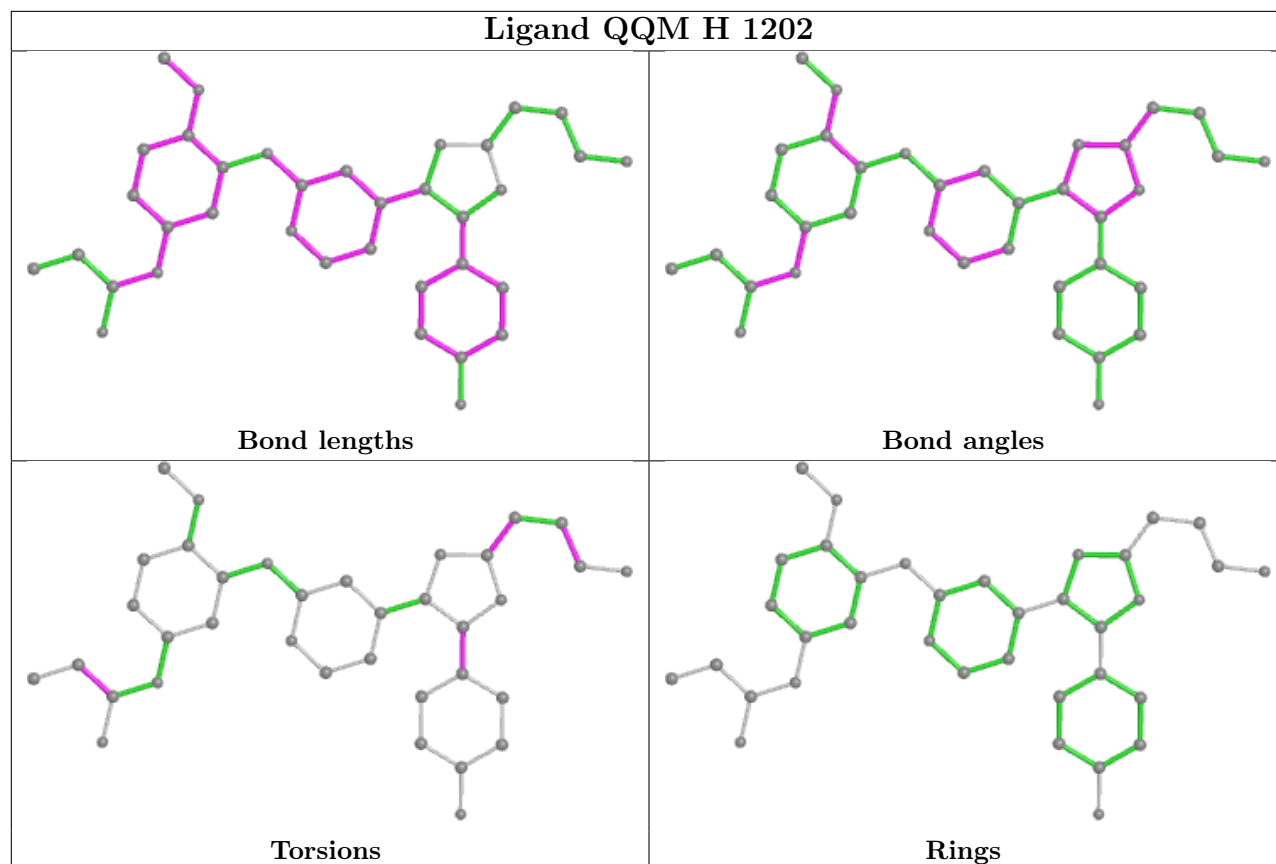


Ligand QQM D 1202



Ligand QQM E 1202





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	307/327 (93%)	0.05	9 (2%) 51 57	14, 30, 58, 75	0
1	B	314/327 (96%)	-0.22	0 100 100	12, 23, 40, 60	0
1	C	297/327 (90%)	-0.06	7 (2%) 59 64	13, 26, 50, 71	0
1	D	314/327 (96%)	-0.02	7 (2%) 62 66	16, 30, 55, 74	0
1	E	303/327 (92%)	-0.01	19 (6%) 20 24	13, 26, 57, 81	0
1	F	299/327 (91%)	0.34	21 (7%) 16 20	17, 34, 64, 89	0
1	G	294/327 (89%)	0.06	15 (5%) 28 33	13, 29, 60, 87	0
1	H	299/327 (91%)	-0.05	9 (3%) 50 56	14, 27, 51, 74	0
All	All	2427/2616 (92%)	0.01	87 (3%) 42 49	12, 28, 56, 89	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	988	HIS	6.3
1	F	723	PHE	5.3
1	E	751	THR	5.3
1	F	986	ARG	5.0
1	C	1010	VAL	4.9
1	G	1009	ASP	4.9
1	H	988	HIS	4.8
1	G	988	HIS	4.7
1	F	722	ALA	4.3
1	E	1010	VAL	4.1
1	E	988	HIS	4.1
1	F	1010	VAL	4.1
1	A	753	PRO	4.0
1	E	1012	ASP	3.9
1	G	723	PHE	3.9
1	F	973	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	987	MET	3.7
1	C	1011	VAL	3.7
1	E	986	ARG	3.7
1	F	1011	VAL	3.7
1	G	722	ALA	3.5
1	G	917	GLY	3.5
1	C	753	PRO	3.5
1	H	982	GLN	3.5
1	G	989	LEU	3.5
1	A	870	HIS	3.4
1	F	749	GLU	3.4
1	G	1008	ASP	3.3
1	G	748	ARG	3.2
1	F	748	ARG	3.2
1	F	785	THR	3.1
1	H	748	ARG	3.1
1	E	1013	ALA	3.1
1	F	1012	ASP	3.1
1	F	861	LEU	3.1
1	D	784	SER	3.0
1	H	863	GLY	3.0
1	D	873	GLY	3.0
1	E	987	MET	3.0
1	F	860	LYS	2.9
1	F	989	LEU	2.9
1	A	871	ALA	2.8
1	H	723	PHE	2.8
1	G	987	MET	2.8
1	G	807	ASP	2.8
1	G	808	ASN	2.8
1	H	1013	ALA	2.7
1	A	988	HIS	2.7
1	C	1006	ASP	2.6
1	F	1006	ASP	2.6
1	F	953	ILE	2.6
1	G	985	GLU	2.6
1	E	862	LEU	2.6
1	E	1014	ASP	2.6
1	F	1009	ASP	2.6
1	G	986	ARG	2.6
1	D	753	PRO	2.6
1	A	872	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	985	GLU	2.6
1	E	860	LYS	2.5
1	D	1007	MET	2.5
1	E	1009	ASP	2.5
1	F	751	THR	2.5
1	E	748	ARG	2.5
1	G	858	LEU	2.4
1	A	889	ARG	2.4
1	E	983	GLY	2.4
1	E	750	ALA	2.4
1	A	1007	MET	2.3
1	C	749	GLU	2.3
1	E	1007	MET	2.3
1	E	875	LYS	2.3
1	C	752	SER	2.2
1	D	764	TYR	2.1
1	F	982	GLN	2.1
1	A	890	ILE	2.1
1	D	869	TYR	2.1
1	G	859	ALA	2.1
1	H	875	LYS	2.1
1	H	749	GLU	2.1
1	F	862	LEU	2.1
1	C	876	VAL	2.1
1	E	808	ASN	2.0
1	H	859	ALA	2.0
1	E	749	GLU	2.0
1	D	875	LYS	2.0
1	A	751	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

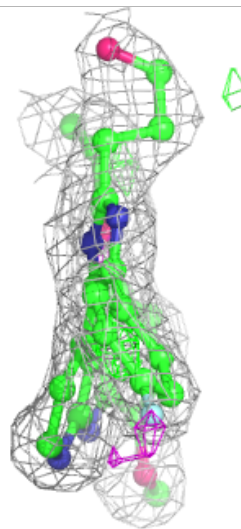
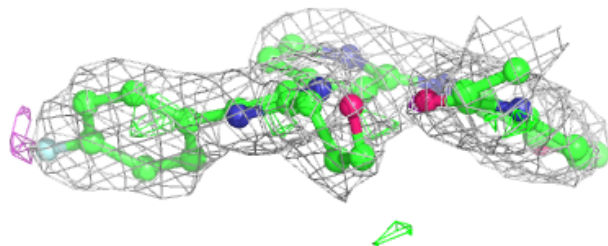
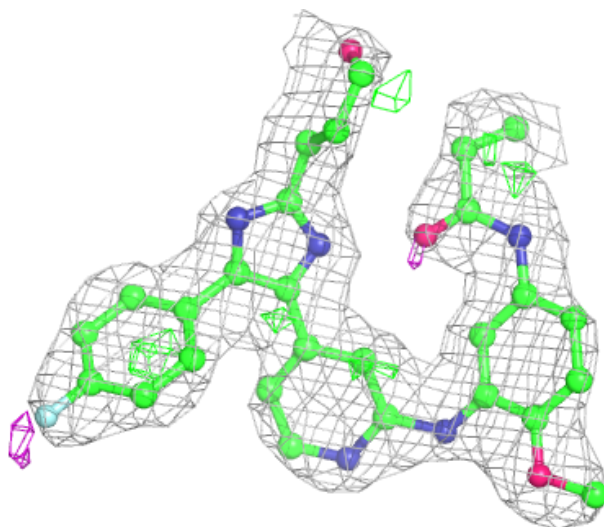
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	G	1302	1/1	0.55	0.15	65,65,65,65	0
2	CL	F	1201	1/1	0.83	0.22	65,65,65,65	0
2	CL	H	1201	1/1	0.87	0.12	56,56,56,56	0
3	QQM	D	1202	36/36	0.89	0.18	18,27,34,40	0
3	QQM	A	1202	36/36	0.91	0.17	17,24,34,42	0
3	QQM	C	1202	36/36	0.91	0.17	13,19,31,34	0
3	QQM	E	1202	36/36	0.91	0.17	16,23,31,34	0
3	QQM	G	1301	36/36	0.91	0.16	17,23,34,38	0
3	QQM	H	1202	36/36	0.91	0.17	15,22,33,38	0
3	QQM	B	1202	36/36	0.92	0.16	15,18,33,33	0
3	QQM	F	1202	36/36	0.92	0.17	16,23,34,43	0
2	CL	D	1201	1/1	0.93	0.09	40,40,40,40	0
2	CL	E	1201	1/1	0.94	0.07	35,35,35,35	0
2	CL	C	1201	1/1	0.95	0.08	28,28,28,28	0
2	CL	A	1201	1/1	0.96	0.06	45,45,45,45	0
2	CL	B	1201	1/1	0.98	0.07	31,31,31,31	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.

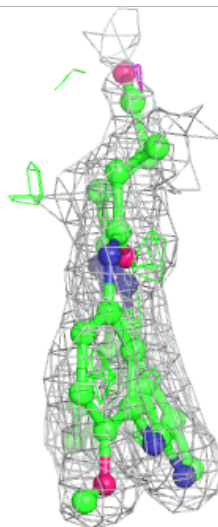
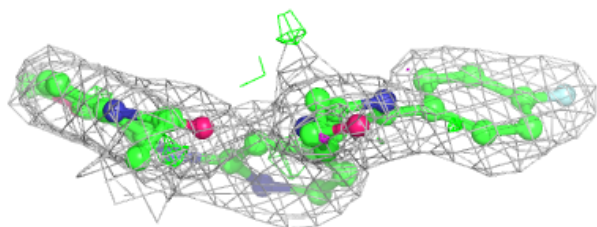
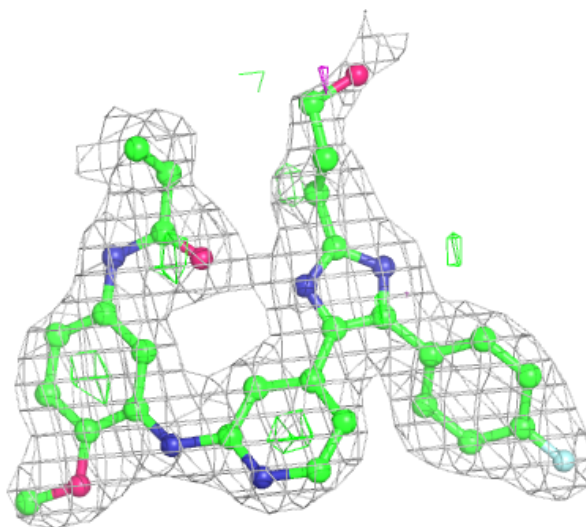
Electron density around QQM D 1202:

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



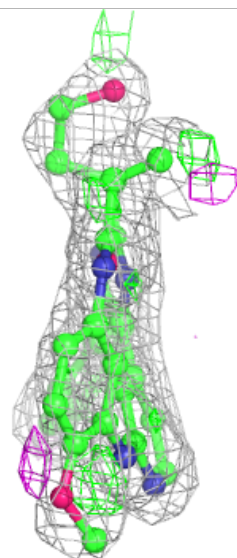
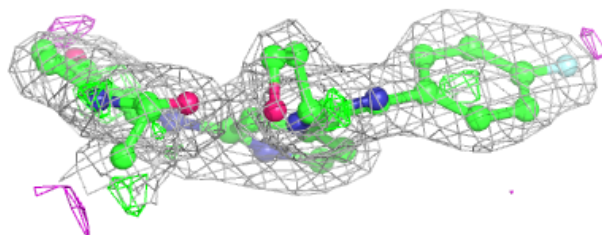
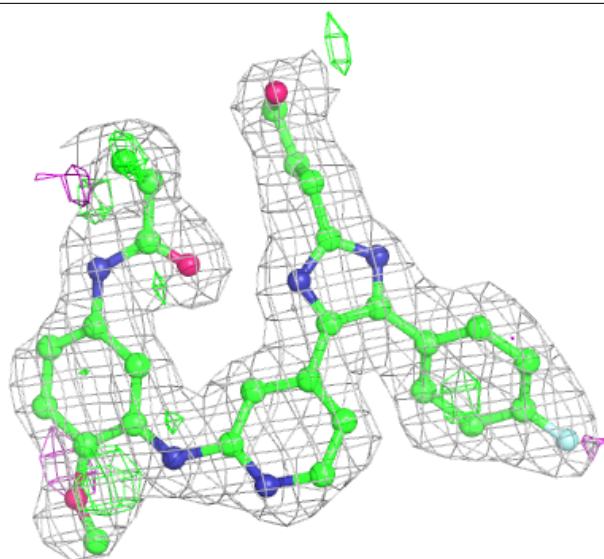
Electron density around QQM A 1202:

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



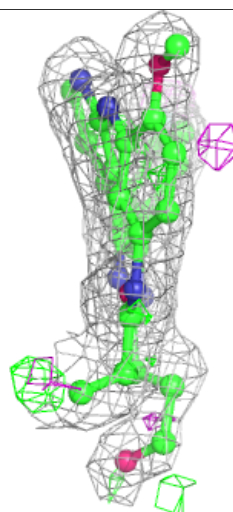
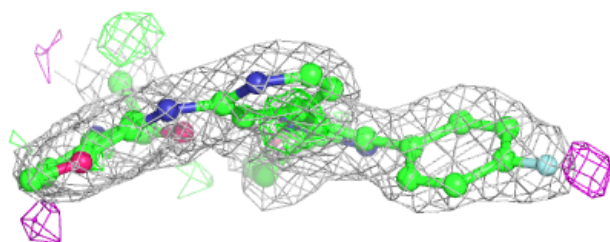
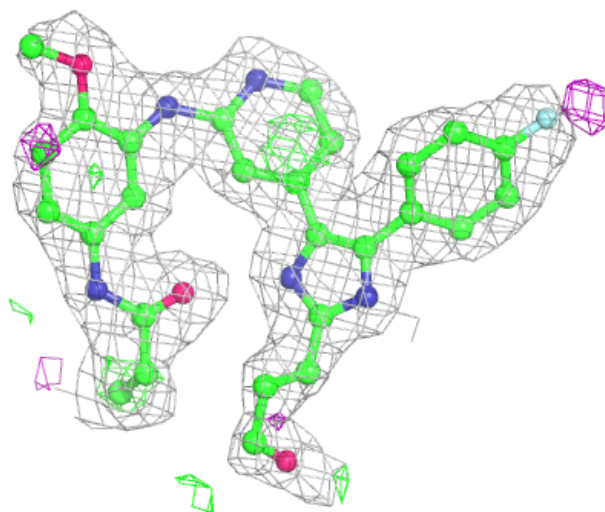
Electron density around QQM C 1202:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



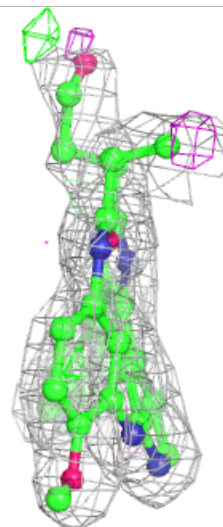
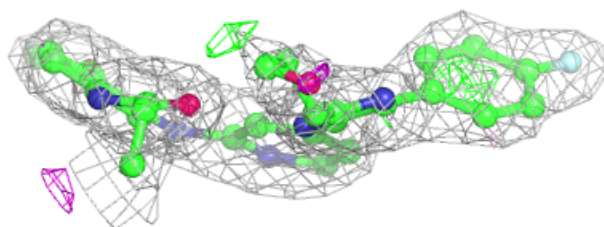
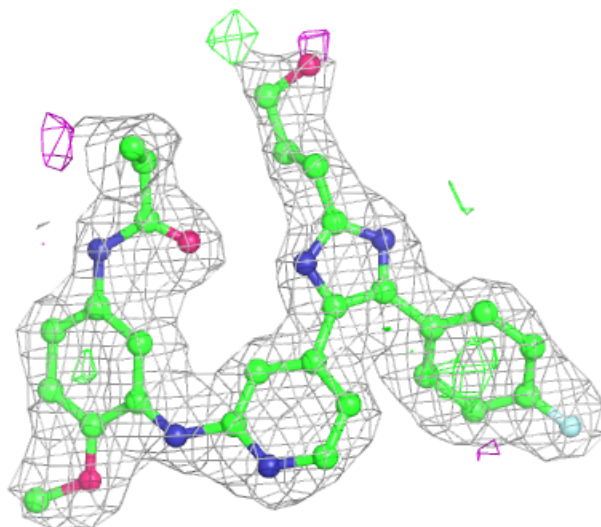
Electron density around QQM E 1202:

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



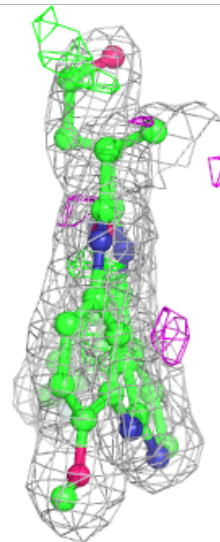
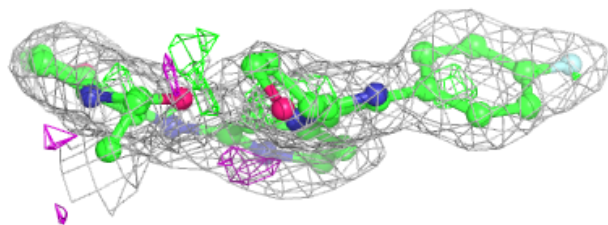
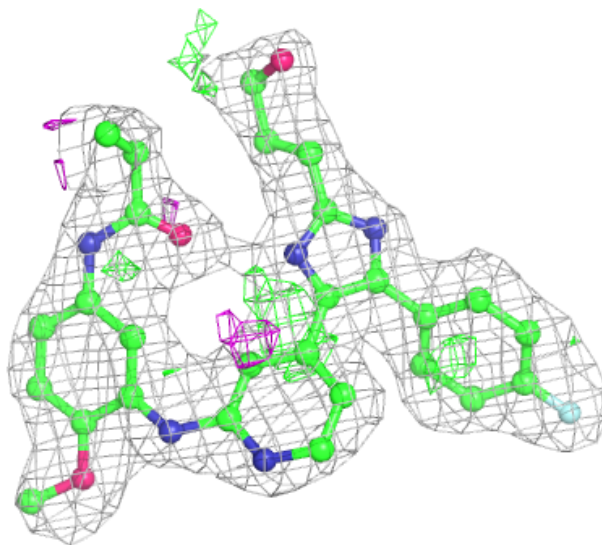
Electron density around QQM G 1301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



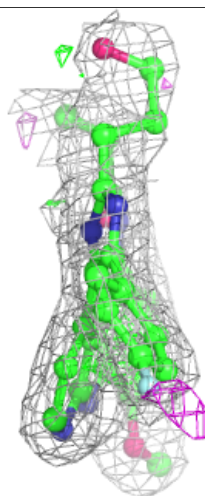
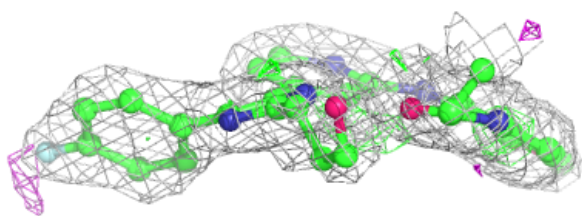
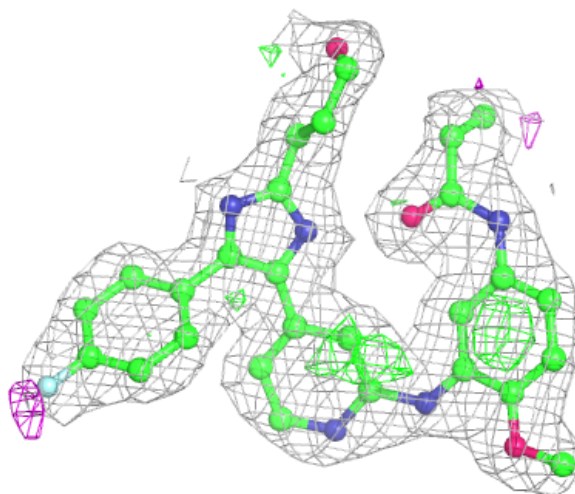
Electron density around QQM H 1202:

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



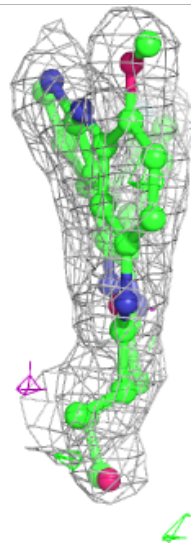
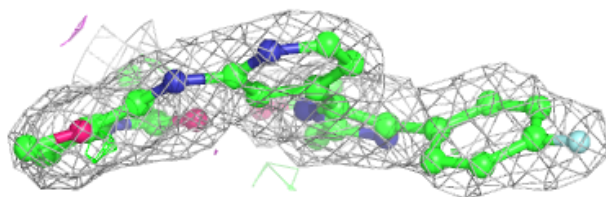
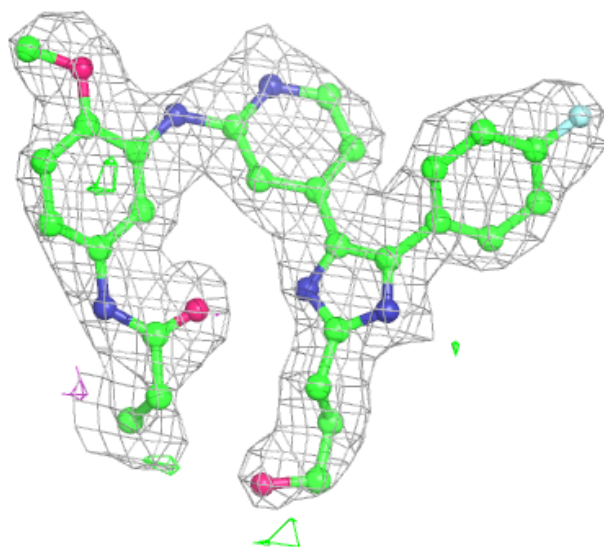
Electron density around QQM B 1202:

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



Electron density around QQM F 1202:

$2mF_o-DF_c$ (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.