



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:56 pm BST

PDB ID : 6V6K  
Title : EGFR(T790M/V948R) in complex with LN2057  
Authors : Heppner, D.E.; Eck, M.J.  
Deposited on : 2019-12-05  
Resolution : 2.20 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](mailto: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.

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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 : 2.11  
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) : 2.11

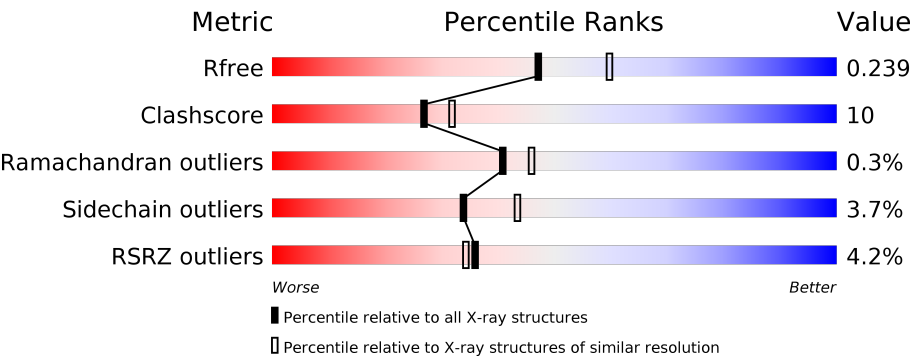
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



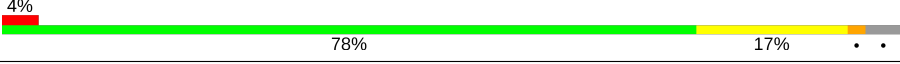

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>73%</div><div>17%</div><div>•</div><div>8%</div></div></div>
1	B	327	<div><div>4%</div><div><div></div><div>73%</div><div>19%</div><div></div><div>8%</div></div></div>
1	C	327	<div><div>3%</div><div><div></div><div>73%</div><div>19%</div><div>•</div><div>8%</div></div></div>
1	D	327	<div><div>5%</div><div><div></div><div>78%</div><div>17%</div><div>• •</div></div></div>
1	E	327	<div><div>6%</div><div><div></div><div>72%</div><div>19%</div><div>•</div><div>7%</div></div></div>
1	F	327	<div><div>4%</div><div><div></div><div>76%</div><div>17%</div><div>•</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	327	
1	H	327	

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	B	1201	-	-	X	-
2	CL	E	1201	-	-	X	-
3	QQJ	F	1202	-	X	-	-
3	QQJ	H	1202	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20750 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	0	0
			2521	1614	427	461	19			
1	A	300	Total	C	N	O	S	0	1	0
			2420	1553	408	440	19			
1	B	301	Total	C	N	O	S	0	0	0
			2424	1554	411	440	19			
1	C	302	Total	C	N	O	S	0	1	0
			2440	1564	413	444	19			
1	E	303	Total	C	N	O	S	0	1	0
			2441	1565	413	444	19			
1	F	306	Total	C	N	O	S	0	0	0
			2453	1572	416	446	19			
1	G	314	Total	C	N	O	S	0	1	0
			2530	1619	428	464	19			
1	H	314	Total	C	N	O	S	0	1	0
			2530	1619	428	464	19			

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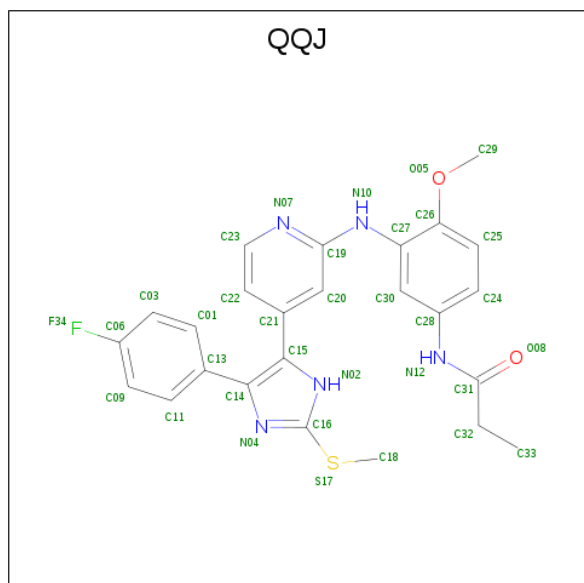
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Chain	Residue	Modelled	Actual	Comment	Reference
G	948	ARG	VAL	engineered mutation	UNP P00533
H	790	MET	THR	engineered mutation	UNP P00533
H	948	ARG	VAL	engineered mutation	UNP P00533

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

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

- Molecule 3 is N-[3-({4-[4-(4-fluorophenyl)-2-(methylsulfanyl)-1H-imidazol-5-yl]pyridin-2-yl}amino)-4-methoxyphenyl]propanamide (three-letter code: QQJ) (formula: C<sub>25</sub>H<sub>24</sub>FN<sub>5</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	A	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	B	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	C	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	E	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	F	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	G	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		
3	H	1	Total	C	F	N	O	S	0	0
			34	25	1	5	2	1		

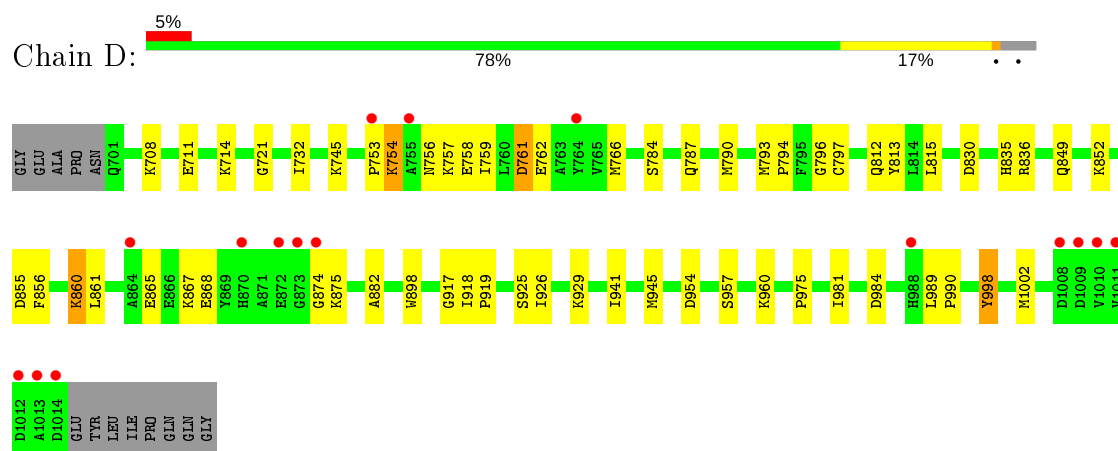
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	87	Total	O	0	0
			87	87		
4	A	81	Total	O	0	0
			81	81		
4	B	80	Total	O	0	0
			80	80		
4	C	103	Total	O	0	0
			103	103		
4	E	78	Total	O	0	0
			78	78		
4	F	85	Total	O	0	0
			85	85		
4	G	86	Total	O	0	0
			86	86		
4	H	111	Total	O	0	0
			111	111		

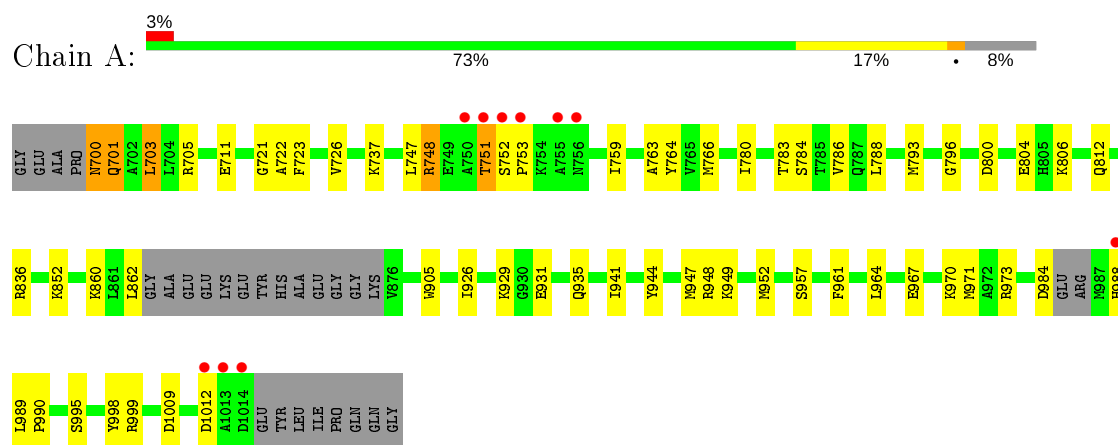
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

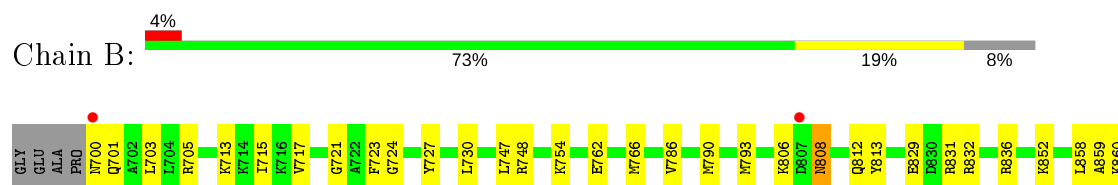
#### • Molecule 1: Epidermal growth factor receptor

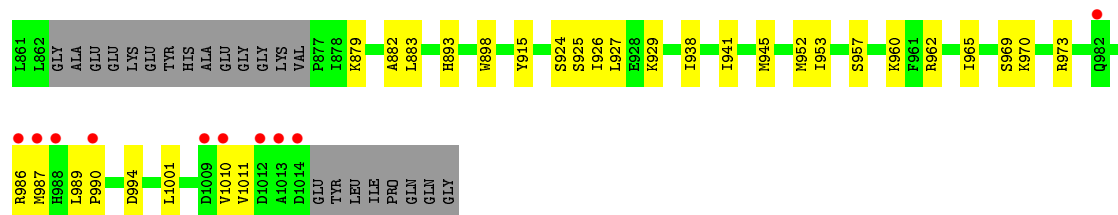


#### • Molecule 1: Epidermal growth factor receptor

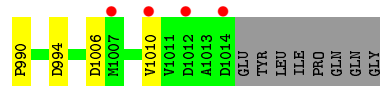
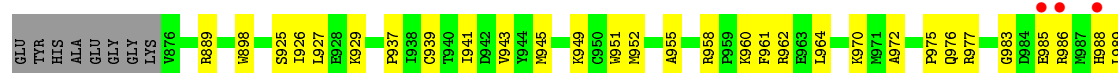


#### • Molecule 1: Epidermal growth factor receptor

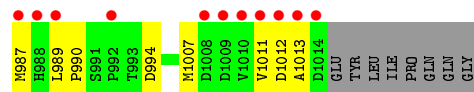
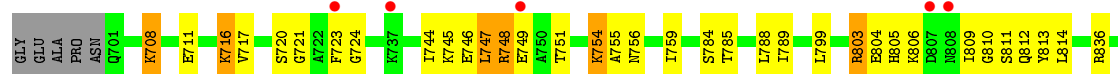




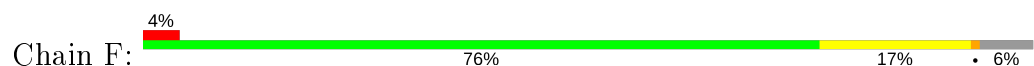
• Molecule 1: Epidermal growth factor receptor



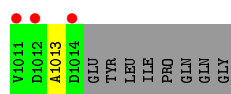
• Molecule 1: Epidermal growth factor receptor



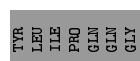
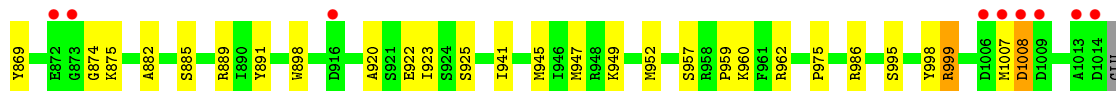
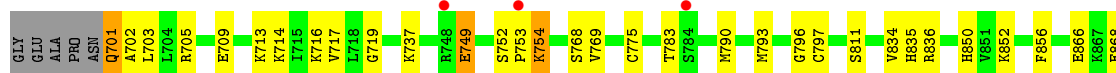
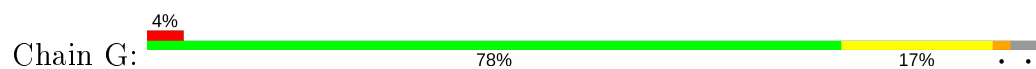
• Molecule 1: Epidermal growth factor receptor



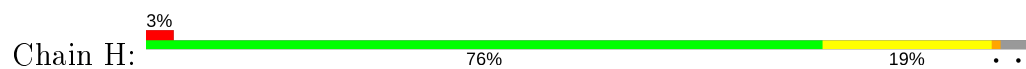




• Molecule 1: Epidermal growth factor receptor



• 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, $\alpha$ , $\beta$ , $\gamma$	71.60Å 102.45Å 174.04Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	85.35 – 2.20 85.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (85.35-2.20) 87.7 (85.35-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.214 , 0.239 0.214 , 0.239	Depositor DCC
$R_{free}$ test set	5816 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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 66.40 % 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 6.0839e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, QQJ

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	0.37	0/2471	0.56	0/3342
1	B	0.37	0/2476	0.56	0/3348
1	C	0.38	0/2492	0.55	0/3371
1	D	0.36	0/2576	0.54	0/3483
1	E	0.41	0/2493	0.60	0/3372
1	F	0.36	0/2505	0.55	0/3386
1	G	0.36	0/2585	0.54	0/3495
1	H	0.38	0/2585	0.55	0/3495
All	All	0.37	0/20183	0.56	0/27292

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	2420	0	2455	45	0
1	B	2424	0	2462	48	0
1	C	2440	0	2475	35	0
1	D	2521	0	2550	54	0
1	E	2441	0	2477	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2453	0	2492	53	0
1	G	2530	0	2555	44	0
1	H	2530	0	2555	57	0
2	A	1	0	0	1	0
2	B	1	0	0	2	0
2	C	1	0	0	1	0
2	D	1	0	0	1	0
2	E	1	0	0	2	0
2	F	1	0	0	1	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	34	0	0	2	0
3	B	34	0	0	2	0
3	C	34	0	0	1	0
3	D	34	0	0	4	0
3	E	34	0	0	2	0
3	F	34	0	0	5	0
3	G	34	0	0	3	0
3	H	34	0	0	5	0
4	A	81	0	0	6	0
4	B	80	0	0	7	0
4	C	103	0	0	2	0
4	D	87	0	0	1	0
4	E	78	0	0	1	0
4	F	85	0	0	4	0
4	G	86	0	0	2	0
4	H	111	0	0	4	0
All	All	20750	0	20021	409	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 10.

All (409) 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:E:813:TYR:CZ	1:E:989:LEU:CD2	2.33	1.12
1:G:952:MET:HE3	1:G:957:SER:HB3	1.31	1.07
1:H:865:GLU:HB3	1:H:867:LYS:HZ3	1.24	1.03
1:E:724:GLY:HA2	1:E:748:ARG:HD3	1.41	1.03
1:E:814:LEU:HB3	1:E:908:MET:HE1	1.40	1.02
1:E:813:TYR:CE2	1:E:989:LEU:HD23	1.95	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:721:GLY:HA3	2:E:1201:CL:CL	2.00	0.97
1:H:760:LEU:HD21	1:H:782:LEU:HD11	1.43	0.97
1:H:712:PHE:O	1:H:713:LYS:HD3	1.64	0.97
1:E:811:SER:OG	1:E:975:PRO:HB2	1.66	0.94
1:H:760:LEU:HD21	1:H:782:LEU:CD1	1.99	0.92
1:H:760:LEU:CD2	1:H:782:LEU:HD11	2.00	0.91
1:F:986:ARG:HG2	1:F:986:ARG:HH21	1.33	0.91
1:E:813:TYR:CE1	1:E:989:LEU:HD21	2.06	0.91
1:E:813:TYR:CE1	1:E:989:LEU:CD2	2.54	0.91
1:H:889:ARG:HG3	1:H:889:ARG:HH21	1.33	0.91
1:F:732:ILE:O	1:F:732:ILE:HD12	1.73	0.89
1:E:716:LYS:HD3	1:E:717:VAL:H	1.38	0.87
1:A:800:ASP:O	1:A:804:GLU:HG3	1.76	0.86
1:E:813:TYR:CD1	1:E:989:LEU:HD21	2.10	0.86
1:A:970:LYS:HG3	4:A:1305:HOH:O	1.75	0.85
1:C:812:GLN:HG2	1:C:989:LEU:HG	1.58	0.84
1:E:813:TYR:CZ	1:E:989:LEU:HD23	2.08	0.84
1:E:810:GLY:HA2	1:E:987:MET:HE3	1.59	0.84
1:B:812:GLN:HB3	1:B:989:LEU:HD11	1.57	0.83
1:E:747:LEU:O	1:E:785:THR:CG2	2.28	0.82
1:B:953:ILE:HD12	1:B:953:ILE:H	1.44	0.82
1:E:814:LEU:HB3	1:E:908:MET:CE	2.10	0.81
1:D:708:LYS:HG2	1:D:711:GLU:OE1	1.81	0.81
1:E:723:PHE:HB3	1:E:862:LEU:HD12	1.61	0.81
1:E:836:ARG:CZ	1:E:860:LYS:HD3	2.11	0.81
1:D:945:MET:CE	1:E:931:GLU:HG2	2.11	0.80
1:D:941:ILE:HB	1:E:922[B]:GLU:HG2	1.63	0.80
1:F:748:ARG:NH1	1:F:875:LYS:HD2	1.97	0.80
1:E:723:PHE:HB3	1:E:862:LEU:CD1	2.12	0.80
1:B:970:LYS:HG2	1:B:973:ARG:HH21	1.47	0.80
1:G:952:MET:CE	1:G:957:SER:HB3	2.10	0.79
1:E:813:TYR:CE2	1:E:989:LEU:CD2	2.59	0.78
1:E:751:THR:OG1	1:E:755:ALA:HB3	1.83	0.77
1:E:814:LEU:CB	1:E:908:MET:HE1	2.14	0.77
1:B:786:VAL:HG23	4:B:1320:HOH:O	1.86	0.76
1:G:811:SER:OG	1:G:975:PRO:HB2	1.86	0.76
1:B:989:LEU:HB3	1:B:990:PRO:HD2	1.68	0.74
1:G:716:LYS:NZ	1:G:716:LYS:HB2	2.01	0.74
1:G:949:LYS:HG2	1:G:959:PRO:HD3	1.69	0.74
1:D:868:GLU:OE2	1:D:874:GLY:HA3	1.86	0.74
1:E:941:ILE:HG21	1:G:922[B]:GLU:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:MET:HA	4:B:1355:HOH:O	1.88	0.74
1:E:716:LYS:HD3	1:E:717:VAL:N	2.03	0.73
1:D:868:GLU:HG3	1:D:875:LYS:HD3	1.69	0.73
1:D:865:GLU:CD	1:D:867:LYS:HG2	2.09	0.73
1:G:749:GLU:OE1	1:G:749:GLU:HA	1.86	0.73
1:A:722:ALA:O	1:A:748:ARG:HD2	1.88	0.73
1:A:793:MET:HE1	1:A:852:LYS:HD3	1.70	0.72
1:G:701:GLN:HG2	1:G:702:ALA:H	1.54	0.72
1:H:756:ASN:O	1:H:760:LEU:HD23	1.90	0.71
1:F:849:GLN:NE2	4:F:1301:HOH:O	2.23	0.71
1:D:754:LYS:HD3	1:D:759:ILE:HD11	1.73	0.71
1:E:813:TYR:CZ	1:E:989:LEU:HD22	2.25	0.71
1:A:701:GLN:HG3	1:A:764:TYR:CE1	2.26	0.70
1:B:970:LYS:HG2	1:B:973:ARG:NH2	2.06	0.70
1:G:995:SER:HB3	1:G:999:ARG:NH1	2.06	0.70
1:G:716:LYS:HZ3	1:G:716:LYS:HB2	1.55	0.70
1:E:812:GLN:HE22	1:E:1013:ALA:H	1.39	0.69
1:D:998:TYR:O	1:D:1002:MET:HG2	1.93	0.69
1:H:794:PRO:HA	3:H:1202:QQJ:C29	2.23	0.69
1:H:831:ARG:HB2	1:H:833:LEU:HD12	1.75	0.69
1:E:812:GLN:HG2	1:E:975:PRO:HG3	1.74	0.69
1:G:719:GLY:HA3	4:G:1303:HOH:O	1.91	0.69
1:D:945:MET:HE1	1:E:931:GLU:HG2	1.73	0.68
1:B:938:ILE:HG23	4:B:1335:HOH:O	1.93	0.68
1:E:747:LEU:O	1:E:785:THR:HG23	1.92	0.68
1:E:814:LEU:HD13	1:E:908:MET:CE	2.22	0.68
1:B:812:GLN:HB3	1:B:989:LEU:CD1	2.23	0.68
1:C:985:GLU:O	1:C:988:HIS:HE1	1.77	0.68
1:E:723:PHE:CB	1:E:862:LEU:HD12	2.23	0.68
1:H:716:LYS:HD2	1:H:717:VAL:N	2.09	0.68
1:A:751:THR:HG21	1:A:786:VAL:HG23	1.75	0.67
1:E:836:ARG:NH2	1:E:860:LYS:HD3	2.10	0.67
1:E:723:PHE:CD1	1:E:862:LEU:HD12	2.30	0.66
1:E:990:PRO:HB2	1:E:994:ASP:HB3	1.77	0.66
1:C:732:ILE:HG23	1:C:732:ILE:O	1.94	0.66
1:C:989:LEU:HD13	1:C:1010:VAL:HG21	1.77	0.66
1:H:971:MET:HE3	1:H:978:TYR:CD1	2.31	0.65
1:H:889:ARG:HG3	1:H:889:ARG:NH2	2.09	0.65
1:F:872:GLU:HB3	1:H:956:ASP:OD2	1.97	0.65
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.62	0.64
1:H:894:GLN:OE1	1:H:960:LYS:HE3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:LYS:CG	4:A:1305:HOH:O	2.39	0.64
1:G:769:VAL:HG11	1:G:856:PHE:CZ	2.33	0.64
1:A:723:PHE:O	1:A:748:ARG:HG3	1.98	0.64
1:D:812:GLN:HG2	1:D:975:PRO:HG3	1.79	0.64
1:B:793:MET:HE3	1:B:852:LYS:HD3	1.78	0.63
1:G:752:SER:OG	1:G:753:PRO:HD2	1.98	0.63
1:H:889:ARG:CG	1:H:889:ARG:HH21	2.11	0.63
1:C:941:ILE:HG13	1:C:945:MET:HG2	1.80	0.63
1:C:925:SER:O	1:C:929:LYS:HG3	1.99	0.63
1:H:865:GLU:HB3	1:H:867:LYS:NZ	2.09	0.62
1:H:747:LEU:HD22	1:H:862:LEU:HD11	1.80	0.62
1:B:808:ASN:ND2	4:B:1303:HOH:O	2.32	0.62
1:E:814:LEU:HD13	1:E:908:MET:HE2	1.82	0.62
1:F:991:SER:HB3	1:F:994:ASP:H	1.65	0.62
1:E:747:LEU:O	1:E:785:THR:HG21	1.97	0.62
1:F:748:ARG:HH11	1:F:875:LYS:HD2	1.65	0.61
1:E:812:GLN:HE22	1:E:1013:ALA:N	1.97	0.61
1:E:805:HIS:HB2	1:E:809:ILE:HD11	1.82	0.61
1:E:925:SER:O	1:E:929:LYS:HE3	1.99	0.61
1:D:830:ASP:HB3	1:G:717:VAL:HG21	1.82	0.61
1:B:990:PRO:HB2	1:B:994:ASP:HB2	1.83	0.60
1:H:717:VAL:HG22	1:H:727:TYR:CE2	2.36	0.60
1:A:973:ARG:NH2	4:A:1305:HOH:O	2.33	0.60
1:D:865:GLU:OE2	1:D:867:LYS:HB3	2.02	0.60
1:A:759:ILE:HD13	1:A:786:VAL:HG21	1.82	0.59
1:E:841:ARG:O	3:E:1202:QQJ:C18	2.50	0.59
1:B:762:GLU:HG3	1:B:766:MET:CE	2.32	0.59
1:G:775:CYS:HB3	1:G:790:MET:HE1	1.84	0.59
1:D:757:LYS:O	1:D:761:ASP:OD1	2.22	0.58
1:B:762:GLU:HG3	1:B:766:MET:HE3	1.86	0.57
1:D:766:MET:HA	1:D:856:PHE:CZ	2.39	0.57
1:E:813:TYR:CG	1:E:989:LEU:HD21	2.38	0.57
1:D:865:GLU:OE2	1:D:867:LYS:HG2	2.04	0.57
1:C:937:PRO:HD2	4:C:1321:HOH:O	2.03	0.57
1:A:783:THR:OG1	1:A:784:SER:N	2.36	0.57
1:B:747:LEU:HD12	1:B:786:VAL:HB	1.87	0.57
1:F:782:LEU:HD22	1:F:786:VAL:HG22	1.85	0.56
1:B:724:GLY:HA2	1:B:748:ARG:HG2	1.87	0.56
1:C:939:CYS:HB3	1:C:943:VAL:HB	1.87	0.56
1:D:790:MET:HG2	3:D:1202:QQJ:C06	2.35	0.56
1:F:723:PHE:HB3	1:F:858:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:960:LYS:HE2	4:H:1314:HOH:O	2.06	0.56
1:E:806:LYS:HG2	1:E:910:PHE:CB	2.36	0.56
1:F:986:ARG:CG	1:F:986:ARG:HH21	2.09	0.56
1:A:836:ARG:NH1	1:A:860:LYS:HG3	2.21	0.55
1:H:943:VAL:HG22	1:H:971:MET:CE	2.36	0.55
1:E:813:TYR:CE1	1:E:989:LEU:HD22	2.40	0.55
1:H:760:LEU:HD21	1:H:782:LEU:HD12	1.88	0.55
1:B:1010:VAL:HB	4:B:1304:HOH:O	2.07	0.55
1:D:836:ARG:NH1	1:D:860:LYS:HD2	2.21	0.55
1:E:751:THR:CG2	1:E:756:ASN:OD1	2.55	0.55
1:H:882:ALA:HA	1:H:898:TRP:CD2	2.42	0.54
1:A:752:SER:HB2	1:A:753:PRO:HD2	1.89	0.54
1:C:715:ILE:HG13	1:C:730:LEU:HG	1.89	0.54
1:E:814:LEU:HD13	1:E:908:MET:HE1	1.89	0.54
1:E:962:ARG:HA	1:E:965:ILE:HD12	1.89	0.54
1:D:759:ILE:CD1	1:D:861:LEU:HD11	2.38	0.54
3:H:1202:QQJ:C20	3:H:1202:QQJ:C30	2.85	0.54
1:H:793:MET:O	3:H:1202:QQJ:C29	2.55	0.54
1:F:715:ILE:HG13	1:F:730:LEU:HG	1.90	0.54
1:G:775:CYS:HB3	1:G:790:MET:CE	2.38	0.54
1:H:831:ARG:HB2	1:H:833:LEU:CD1	2.37	0.54
1:H:937:PRO:HD2	4:H:1375:HOH:O	2.07	0.54
1:C:793:MET:HE1	1:C:852:LYS:HD3	1.90	0.53
1:E:746:GLU:HG3	1:E:785:THR:HG22	1.90	0.53
1:D:925:SER:O	1:D:929:LYS:HG2	2.09	0.53
1:C:762:GLU:O	1:C:766:MET:HG3	2.08	0.53
1:D:960:LYS:NZ	1:D:960:LYS:HB3	2.22	0.53
1:A:944:TYR:CZ	1:A:948:ARG:HD3	2.43	0.53
1:H:973:ARG:HG2	1:H:1014:ASP:OD1	2.08	0.53
1:E:805:HIS:O	1:E:809:ILE:HD12	2.09	0.53
1:B:836:ARG:HE	1:B:860:LYS:HE3	1.73	0.53
1:D:758:GLU:HA	1:D:761:ASP:HB2	1.90	0.52
1:E:879:LYS:HZ1	1:E:923:ILE:HD11	1.74	0.52
1:G:922[B]:GLU:HG3	1:G:925:SER:HB3	1.91	0.52
1:D:793:MET:CE	1:D:852:LYS:HD3	2.38	0.52
1:G:709:GLU:HG3	1:G:783:THR:HG21	1.90	0.52
1:B:721:GLY:HA3	2:B:1201:CL:CL	2.46	0.52
1:D:836:ARG:CZ	1:D:860:LYS:HD2	2.40	0.52
1:H:945:MET:O	1:H:949:LYS:HG3	2.10	0.52
1:C:708:LYS:HE3	1:G:889:ARG:NH1	2.25	0.52
1:E:879:LYS:HE3	1:E:914:PRO:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:LYS:HG2	1:E:910:PHE:HB3	1.92	0.52
3:H:1202:QQJ:C29	3:H:1202:QQJ:N10	2.73	0.52
1:A:747:LEU:HD23	1:A:862:LEU:HD11	1.92	0.52
1:E:723:PHE:CG	1:E:862:LEU:HD12	2.44	0.51
1:H:724:GLY:HA2	1:H:748:ARG:HG2	1.93	0.51
1:D:917:GLY:N	4:D:1310:HOH:O	2.39	0.51
1:H:865:GLU:CB	1:H:867:LYS:HZ3	2.08	0.51
1:F:708:LYS:HE2	1:F:734:GLU:OE1	2.10	0.51
1:F:760:LEU:HD23	1:F:782:LEU:HD11	1.92	0.51
1:G:868:GLU:OE1	1:G:874:GLY:HA3	2.10	0.51
1:C:721:GLY:HA3	2:C:1201:CL:CL	2.48	0.51
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.46	0.51
1:D:998:TYR:HD1	1:D:1002:MET:SD	2.33	0.51
1:A:722:ALA:O	1:A:748:ARG:CD	2.59	0.51
1:F:999:ARG:NH1	1:F:1007:MET:HB2	2.26	0.51
1:E:919:PRO:HD2	1:E:922[A]:GLU:OE1	2.11	0.50
1:G:866:GLU:HA	1:G:869:TYR:CD1	2.46	0.50
1:G:882:ALA:O	1:G:885:SER:HB2	2.10	0.50
1:F:872:GLU:OE1	1:F:872:GLU:HA	2.12	0.50
1:H:990:PRO:HA	4:H:1315:HOH:O	2.11	0.50
1:E:759:ILE:HD12	1:E:861:LEU:HD21	1.94	0.50
3:E:1202:QQJ:C30	3:E:1202:QQJ:C20	2.89	0.50
1:F:999:ARG:HH12	1:F:1007:MET:HG3	1.77	0.50
1:G:836:ARG:NE	4:G:1310:HOH:O	2.43	0.50
1:B:879:LYS:HD3	1:B:915:TYR:HB2	1.94	0.50
1:H:971:MET:HE2	1:H:978:TYR:HB3	1.94	0.50
1:A:812:GLN:HG2	4:A:1312:HOH:O	2.12	0.49
1:H:960:LYS:CE	4:H:1314:HOH:O	2.58	0.49
1:B:973:ARG:HG2	1:B:1011:VAL:HG12	1.94	0.49
1:F:782:LEU:CD2	1:F:786:VAL:HG22	2.42	0.49
1:E:751:THR:HG21	1:E:756:ASN:OD1	2.13	0.49
1:H:905:TRP:HD1	1:H:947:MET:HE1	1.76	0.49
1:A:721:GLY:HA3	2:A:1201:CL:CL	2.50	0.49
1:E:708:LYS:O	1:E:711:GLU:HG2	2.13	0.49
1:F:726:VAL:HG21	3:F:1202:QQJ:C16	2.43	0.49
1:A:700:ASN:CG	1:A:703:LEU:HD22	2.33	0.48
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.13	0.48
1:C:732:ILE:CG2	1:C:732:ILE:O	2.61	0.48
1:F:826:ASN:HD21	1:F:962:ARG:CZ	2.26	0.48
1:D:954:ASP:OD2	1:D:957:SER:OG	2.30	0.48
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:LYS:O	1:C:952:MET:HG3	2.13	0.48
1:D:754:LYS:HD3	1:D:759:ILE:CD1	2.42	0.48
1:B:705:ARG:HG2	1:B:705:ARG:HH11	1.79	0.48
1:F:783:THR:OG1	1:F:784:SER:N	2.46	0.48
1:E:850:HIS:HB2	1:E:1007:MET:HE1	1.96	0.48
1:A:726:VAL:HG21	3:A:1202:QQJ:C16	2.43	0.48
1:D:835:HIS:O	1:D:836:ARG:HB2	2.14	0.48
1:D:989:LEU:HB3	1:D:990:PRO:HD2	1.95	0.48
1:H:905:TRP:CD1	1:H:947:MET:HE1	2.48	0.48
1:B:927:LEU:HD11	4:B:1316:HOH:O	2.12	0.48
1:C:972:ALA:O	1:C:975:PRO:HD3	2.14	0.48
1:D:945:MET:HE2	1:E:931:GLU:HG2	1.89	0.48
1:H:943:VAL:HG22	1:H:971:MET:HE1	1.95	0.48
1:A:752:SER:HB2	1:A:753:PRO:CD	2.43	0.48
1:B:953:ILE:CD1	1:B:953:ILE:H	2.18	0.47
1:F:708:LYS:CE	1:F:734:GLU:OE1	2.62	0.47
1:G:949:LYS:O	1:G:952:MET:HG3	2.14	0.47
1:A:705:ARG:NH2	1:A:711:GLU:OE2	2.47	0.47
1:A:961:PHE:HA	1:A:964:LEU:HD12	1.97	0.47
1:B:836:ARG:HB2	1:B:859:ALA:HB3	1.96	0.47
1:E:754:LYS:HB2	4:E:1325:HOH:O	2.14	0.47
1:F:986:ARG:HG2	1:F:986:ARG:NH2	2.12	0.47
1:E:799:LEU:O	1:E:803:ARG:HG3	2.15	0.47
1:E:805:HIS:O	1:E:809:ILE:CD1	2.63	0.47
1:F:732:ILE:CD1	1:F:732:ILE:O	2.55	0.47
1:F:982:GLN:HA	1:F:982:GLN:OE1	2.14	0.47
1:F:999:ARG:HH12	1:F:1007:MET:HB2	1.80	0.47
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.15	0.47
1:G:797:CYS:HB3	3:G:1202:QQJ:C31	2.45	0.47
1:C:898:TRP:CE3	1:C:951:TRP:HA	2.50	0.47
1:H:943:VAL:CG2	1:H:971:MET:CE	2.93	0.47
1:B:836:ARG:NE	1:B:860:LYS:HE3	2.30	0.46
1:D:793:MET:HE3	1:D:852:LYS:HD3	1.96	0.46
1:E:708:LYS:HG3	1:E:711:GLU:OE1	2.14	0.46
1:G:836:ARG:HG2	1:G:891:TYR:CD1	2.50	0.46
1:H:752:SER:O	1:H:754:LYS:HG2	2.15	0.46
1:C:983:GLY:HA3	1:C:986:ARG:NH2	2.30	0.46
1:B:829:GLU:HG3	1:B:893:HIS:CD2	2.50	0.46
1:C:722:ALA:O	1:C:748:ARG:CD	2.63	0.46
1:D:762:GLU:OE1	1:D:861:LEU:CD1	2.64	0.46
1:C:808:ASN:ND2	4:C:1309:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:723:PHE:CB	1:F:858:LEU:HD13	2.45	0.46
1:G:850:HIS:CG	1:G:1007:MET:SD	3.08	0.46
1:G:703:LEU:HD13	1:G:768:SER:HA	1.98	0.46
1:F:986:ARG:CG	1:F:986:ARG:NH2	2.73	0.46
1:G:920:ALA:HA	1:G:923:ILE:HG12	1.98	0.46
1:A:812:GLN:HB2	4:A:1356:HOH:O	2.15	0.46
3:B:1202:QQJ:C30	3:B:1202:QQJ:C20	2.94	0.46
1:G:941:ILE:O	1:G:945:MET:HG2	2.15	0.46
1:B:723:PHE:HB2	2:B:1201:CL:CL	2.53	0.46
1:B:700:ASN:HB2	1:B:703:LEU:HD12	1.98	0.46
1:F:811:SER:OG	1:F:975:PRO:HB2	2.16	0.46
1:E:751:THR:OG1	1:E:755:ALA:CB	2.58	0.46
1:B:926:ILE:HG13	1:B:927:LEU:N	2.30	0.46
1:F:970:LYS:HG2	1:F:973:ARG:HH22	1.81	0.46
1:A:780:ILE:HG13	1:A:788:LEU:HD23	1.98	0.46
1:G:868:GLU:HG3	1:G:875:LYS:HG2	1.98	0.46
1:A:793:MET:CE	1:A:852:LYS:HD3	2.43	0.45
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.52	0.45
1:F:961:PHE:HA	1:F:964:LEU:HD12	1.99	0.45
1:F:995:SER:O	1:F:999:ARG:HG3	2.17	0.45
1:G:1008:ASP:OD1	1:G:1008:ASP:N	2.49	0.45
1:B:965:ILE:O	1:B:969:SER:OG	2.31	0.45
1:F:945:MET:O	1:F:949:LYS:HG3	2.17	0.45
1:D:732:ILE:N	1:D:732:ILE:HD12	2.32	0.45
1:G:714:LYS:HB2	1:G:714:LYS:HE2	1.78	0.45
1:B:952:MET:CE	1:B:957:SER:OG	2.65	0.45
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.98	0.45
1:D:759:ILE:HD12	1:D:861:LEU:HD11	1.99	0.45
1:F:812:GLN:HG3	1:F:975:PRO:HG3	1.99	0.45
1:F:893:HIS:HD2	4:F:1322:HOH:O	2.00	0.45
1:B:715:ILE:HG13	1:B:730:LEU:HG	1.99	0.44
1:D:794:PRO:HA	3:D:1202:QQJ:C29	2.47	0.44
1:G:790:MET:HG2	3:G:1202:QQJ:C03	2.47	0.44
1:H:759:ILE:HD13	1:H:786:VAL:HG21	1.98	0.44
1:H:920:ALA:HA	1:H:923:ILE:HG12	1.99	0.44
1:E:723:PHE:HB3	1:E:862:LEU:HD11	1.96	0.44
1:G:882:ALA:HA	1:G:898:TRP:CD2	2.52	0.44
1:H:806:LYS:HG3	1:H:910:PHE:CB	2.48	0.44
1:B:941:ILE:O	1:B:945:MET:HG3	2.18	0.44
1:E:882:ALA:HA	1:E:898:TRP:CD2	2.53	0.44
1:F:790:MET:HG2	3:F:1202:QQJ:C03	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:760:LEU:CD2	1:F:782:LEU:HD11	2.48	0.44
1:H:747:LEU:HD11	1:H:788:LEU:HG	1.99	0.44
1:D:797:CYS:HB3	3:D:1202:QQJ:C31	2.47	0.44
1:D:714:LYS:NZ	1:D:787:GLN:OE1	2.35	0.44
1:D:865:GLU:OE2	1:D:867:LYS:CG	2.65	0.44
1:C:716:LYS:HZ2	1:C:716:LYS:HB3	1.83	0.44
1:C:755:ALA:HB3	1:C:758:GLU:OE2	2.17	0.44
1:A:970:LYS:NZ	1:E:803:ARG:HB3	2.33	0.44
1:H:889:ARG:CG	1:H:889:ARG:NH2	2.73	0.44
1:C:926:ILE:HG13	1:C:927:LEU:N	2.33	0.44
3:H:1202:QQJ:N02	3:H:1202:QQJ:O08	2.51	0.44
1:F:987:MET:HA	4:F:1354:HOH:O	2.18	0.44
1:F:721:GLY:HA3	2:F:1201:CL:CL	2.54	0.43
1:A:812:GLN:HB3	1:A:989:LEU:HG	1.99	0.43
1:F:796:GLY:HA2	3:F:1202:QQJ:C30	2.49	0.43
1:A:763:ALA:HA	1:A:766:MET:HE3	2.01	0.43
1:B:858:LEU:HD23	1:B:858:LEU:HA	1.89	0.43
1:C:761:ASP:O	1:C:765:VAL:HG23	2.18	0.43
1:E:751:THR:HG23	1:E:756:ASN:OD1	2.17	0.43
1:F:875:LYS:HB2	1:F:875:LYS:HE2	1.62	0.43
1:A:967:GLU:O	1:A:971:MET:HG3	2.19	0.43
1:B:790:MET:HG2	3:B:1202:QQJ:C03	2.49	0.43
1:C:809:ILE:HD11	1:C:813:TYR:CG	2.53	0.43
1:D:918:ILE:HG21	1:D:926:ILE:HD13	2.00	0.43
1:F:812:GLN:HE21	1:F:1013:ALA:HB2	1.84	0.43
1:E:744:ILE:HG12	1:E:789:ILE:HG13	2.00	0.43
1:E:813:TYR:CD2	1:E:989:LEU:CD2	3.00	0.43
1:G:754:LYS:HB3	1:G:754:LYS:HE2	1.73	0.43
1:D:919:PRO:HG2	1:A:935:GLN:OE1	2.18	0.43
1:E:751:THR:HG1	1:E:755:ALA:HB3	1.81	0.43
1:A:1009:ASP:HA	4:A:1306:HOH:O	2.18	0.43
1:C:989:LEU:HB3	1:C:990:PRO:HD2	2.00	0.43
1:H:772:PRO:O	1:H:852:LYS:HE2	2.19	0.43
1:B:973:ARG:HG2	1:B:1011:VAL:CG1	2.49	0.43
1:D:815:LEU:HD12	1:D:975:PRO:HB3	2.01	0.43
1:F:797:CYS:HB3	3:F:1202:QQJ:C31	2.49	0.43
1:H:883:LEU:HD22	1:H:953:ILE:HD12	2.01	0.43
1:B:989:LEU:HB3	1:B:990:PRO:CD	2.45	0.43
1:C:961:PHE:HA	1:C:964:LEU:HD12	2.01	0.43
1:F:1009:ASP:OD1	1:F:1010:VAL:N	2.52	0.43
1:F:937:PRO:HD2	4:F:1349:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:709:GLU:CG	1:G:783:THR:HG21	2.49	0.43
1:D:849:GLN:HG2	1:D:990:PRO:HG3	2.01	0.43
1:F:858:LEU:HA	1:F:858:LEU:HD23	1.76	0.43
1:A:836:ARG:CZ	1:A:860:LYS:HG3	2.49	0.42
1:E:788:LEU:C	1:E:789:ILE:HD12	2.39	0.42
1:H:971:MET:CE	1:H:978:TYR:CD1	3.00	0.42
1:F:882:ALA:HA	1:F:898:TRP:CD2	2.53	0.42
1:H:879:LYS:HD3	1:H:914:PRO:O	2.20	0.42
1:F:913:LYS:NZ	1:H:963:GLU:OE2	2.50	0.42
1:E:748:ARG:H	1:E:748:ARG:HG2	1.74	0.42
1:H:793:MET:HE1	1:H:846:LYS:HB2	2.01	0.42
1:A:796:GLY:HA2	3:A:1202:QQJ:C30	2.50	0.42
1:A:949:LYS:HA	1:A:952:MET:SD	2.60	0.42
1:C:701:GLN:HA	1:C:764:TYR:CE1	2.54	0.42
1:C:809:ILE:HD12	1:C:809:ILE:HA	1.68	0.42
1:D:759:ILE:HD13	1:D:861:LEU:HD11	2.02	0.42
1:G:793:MET:HE3	1:G:852:LYS:HD3	2.00	0.42
1:A:926:ILE:HA	1:A:929:LYS:CD	2.50	0.42
1:F:706:ILE:CD1	1:F:760:LEU:HD11	2.50	0.42
1:G:752:SER:OG	1:G:753:PRO:CD	2.67	0.42
1:G:834:VAL:HG12	1:G:836:ARG:HG3	2.00	0.42
1:H:798:LEU:HD12	1:H:798:LEU:HA	1.88	0.42
1:A:970:LYS:HG2	1:A:973:ARG:HH22	1.84	0.42
1:A:995:SER:O	1:A:999:ARG:HG3	2.19	0.42
1:C:955:ALA:HA	1:C:958:ARG:CZ	2.50	0.42
1:G:796:GLY:HA2	3:G:1202:QQJ:C30	2.50	0.42
1:G:947:MET:HB2	1:G:947:MET:HE2	1.96	0.42
1:H:747:LEU:CD2	1:H:862:LEU:HD11	2.48	0.42
1:A:700:ASN:HD22	1:A:701:GLN:H	1.67	0.42
1:D:766:MET:HA	1:D:856:PHE:HZ	1.82	0.42
1:F:760:LEU:HD23	1:F:782:LEU:CD1	2.50	0.42
1:H:754:LYS:HD3	1:H:758:GLU:OE1	2.19	0.42
1:E:989:LEU:HA	1:E:989:LEU:HD23	1.74	0.42
1:D:762:GLU:OE1	1:D:861:LEU:HD12	2.20	0.41
1:E:989:LEU:HB3	1:E:990:PRO:HD2	2.02	0.41
1:E:849:GLN:CD	1:E:990:PRO:HG3	2.41	0.41
1:F:790:MET:HG2	3:F:1202:QQJ:C06	2.50	0.41
1:C:793:MET:CE	1:C:852:LYS:HD3	2.49	0.41
1:H:766:MET:O	1:H:769:VAL:HG22	2.20	0.41
1:H:798:LEU:O	1:H:802:VAL:HG22	2.19	0.41
1:A:989:LEU:CD2	1:A:990:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:796:GLY:HA2	3:D:1202:QQJ:C30	2.51	0.41
1:D:998:TYR:CD1	1:D:1002:MET:SD	3.13	0.41
1:B:713:LYS:HG3	1:B:715:ILE:HD11	2.02	0.41
1:H:797:CYS:HA	1:H:844:LEU:HA	2.01	0.41
1:H:943:VAL:CG2	1:H:971:MET:HE1	2.50	0.41
1:B:1001:LEU:HA	1:B:1001:LEU:HD23	1.94	0.41
1:D:745:LYS:NZ	1:D:855:ASP:OD2	2.54	0.41
1:B:883:LEU:HD23	1:B:953:ILE:HG23	2.01	0.41
1:E:745:LYS:NZ	2:E:1201:CL:CL	2.83	0.41
1:E:941:ILE:O	1:E:945:MET:HG3	2.20	0.41
1:A:952:MET:CE	1:A:957:SER:HB3	2.50	0.41
1:E:814:LEU:CD1	1:E:908:MET:HE1	2.51	0.41
1:D:925:SER:HB2	1:A:941:ILE:HG21	2.02	0.41
1:E:987:MET:HB2	1:E:987:MET:HE2	1.85	0.41
1:F:985:GLU:H	1:F:985:GLU:CD	2.24	0.41
1:G:835:HIS:O	1:G:836:ARG:HB2	2.20	0.41
1:D:865:GLU:OE2	1:D:867:LYS:CB	2.66	0.41
1:A:1012:ASP:N	1:A:1012:ASP:OD1	2.47	0.40
1:A:705:ARG:HD2	1:H:994:ASP:OD1	2.20	0.40
1:B:925:SER:O	1:B:929:LYS:HE3	2.21	0.40
1:C:790:MET:HG2	3:C:1202:QQJ:C03	2.51	0.40
1:H:943:VAL:CG2	1:H:971:MET:HE2	2.51	0.40
1:B:829:GLU:HG3	1:B:893:HIS:CG	2.56	0.40
1:D:721:GLY:HA3	2:D:1201:CL:CL	2.58	0.40
1:D:981:ILE:O	1:D:984:ASP:HB2	2.21	0.40
1:E:879:LYS:NZ	1:E:923:ILE:HD11	2.37	0.40
1:E:813:TYR:CD2	1:E:989:LEU:HD21	2.57	0.40
1:F:999:ARG:HH12	1:F:1007:MET:CG	2.34	0.40
1:G:960:LYS:HD3	1:G:962:ARG:NH1	2.36	0.40
1:B:962:ARG:HG3	4:B:1328:HOH:O	2.21	0.40
1:F:708:LYS:HG3	1:F:710:THR:OG1	2.21	0.40
1:B:705:ARG:HG2	1:B:705:ARG:NH1	2.36	0.40
1:C:716:LYS:NZ	1:C:716:LYS:HB3	2.36	0.40
1:C:707:LEU:HD12	1:C:789:ILE:HD13	2.03	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	295/327 (90%)	288 (98%)	6 (2%)	1 (0%)	41	46
1	B	297/327 (91%)	285 (96%)	11 (4%)	1 (0%)	41	46
1	C	299/327 (91%)	290 (97%)	9 (3%)	0	100	100
1	D	312/327 (95%)	302 (97%)	9 (3%)	1 (0%)	41	46
1	E	300/327 (92%)	286 (95%)	11 (4%)	3 (1%)	15	14
1	F	302/327 (92%)	293 (97%)	7 (2%)	2 (1%)	22	22
1	G	313/327 (96%)	302 (96%)	11 (4%)	0	100	100
1	H	313/327 (96%)	304 (97%)	9 (3%)	0	100	100
All	All	2431/2616 (93%)	2350 (97%)	73 (3%)	8 (0%)	41	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	863	GLY
1	F	806	LYS
1	A	701	GLN
1	E	749	GLU
1	F	753	PRO
1	E	986	ARG
1	B	806	LYS
1	D	753	PRO

### 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	269/287 (94%)	259 (96%)	10 (4%)	34	43
1	B	269/287 (94%)	261 (97%)	8 (3%)	41	53
1	C	271/287 (94%)	258 (95%)	13 (5%)	25	32
1	D	277/287 (96%)	271 (98%)	6 (2%)	52	65
1	E	270/287 (94%)	256 (95%)	14 (5%)	23	28
1	F	271/287 (94%)	262 (97%)	9 (3%)	38	49
1	G	278/287 (97%)	268 (96%)	10 (4%)	35	45
1	H	278/287 (97%)	267 (96%)	11 (4%)	31	40
All	All	2183/2296 (95%)	2102 (96%)	81 (4%)	34	43

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	754	LYS
1	D	756	ASN
1	D	761	ASP
1	D	784	SER
1	D	860	LYS
1	D	998	TYR
1	A	700	ASN
1	A	703	LEU
1	A	737	LYS
1	A	748	ARG
1	A	751	THR
1	A	806	LYS
1	A	931	GLU
1	A	984	ASP
1	A	988	HIS
1	A	998	TYR
1	B	701	GLN
1	B	754	LYS
1	B	808	ASN
1	B	831	ARG
1	B	832	ARG
1	B	924	SER
1	B	960	LYS
1	B	986	ARG
1	C	705	ARG
1	C	748	ARG
1	C	749	GLU

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Mol	Chain	Res	Type
1	C	752	SER
1	C	806	LYS
1	C	812	GLN
1	C	889	ARG
1	C	960	LYS
1	C	962	ARG
1	C	970	LYS
1	C	976	GLN
1	C	977	ARG
1	C	1006	ASP
1	E	708	LYS
1	E	716	LYS
1	E	720	SER
1	E	747	LEU
1	E	748	ARG
1	E	754	LYS
1	E	784	SER
1	E	803	ARG
1	E	804	GLU
1	E	856	PHE
1	E	931	GLU
1	E	986	ARG
1	E	1011	VAL
1	E	1012	ASP
1	F	705	ARG
1	F	708	LYS
1	F	754	LYS
1	F	922	GLU
1	F	929	LYS
1	F	942	ASP
1	F	962	ARG
1	F	986	ARG
1	F	998	TYR
1	G	701	GLN
1	G	705	ARG
1	G	713	LYS
1	G	737	LYS
1	G	749	GLU
1	G	754	LYS
1	G	986	ARG
1	G	998	TYR
1	G	999	ARG

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Mol	Chain	Res	Type
1	G	1008	ASP
1	H	705	ARG
1	H	739	LYS
1	H	748	ARG
1	H	752	SER
1	H	768	SER
1	H	784	SER
1	H	860	LYS
1	H	867	LYS
1	H	960	LYS
1	H	967	GLU
1	H	998	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	756	ASN
1	D	805	HIS
1	D	893	HIS
1	A	700	ASN
1	A	808	ASN
1	B	700	ASN
1	B	701	GLN
1	B	849	GLN
1	C	988	HIS
1	E	808	ASN
1	E	812	GLN
1	E	849	GLN
1	F	791	GLN
1	F	812	GLN
1	F	826	ASN
1	F	893	HIS
1	G	756	ASN
1	H	826	ASN
1	H	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 carbohydrates 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	QQJ	E	1202	1	35,37,37	4.75	27 (77%)	42,51,51	2.65	12 (28%)
3	QQJ	G	1202	1	35,37,37	5.92	28 (80%)	42,51,51	1.62	9 (21%)
3	QQJ	A	1202	1	35,37,37	5.71	29 (82%)	42,51,51	1.73	8 (19%)
3	QQJ	C	1202	1	35,37,37	5.80	30 (85%)	42,51,51	1.60	11 (26%)
3	QQJ	H	1202	1	35,37,37	5.97	30 (85%)	42,51,51	2.07	10 (23%)
3	QQJ	D	1202	1	35,37,37	5.82	30 (85%)	42,51,51	1.61	10 (23%)
3	QQJ	F	1202	1	35,37,37	5.74	28 (80%)	42,51,51	1.71	12 (28%)
3	QQJ	B	1202	1	35,37,37	4.79	29 (82%)	42,51,51	2.00	9 (21%)

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	QQJ	E	1202	1	-	4/20/22/22	0/4/4/4
3	QQJ	G	1202	1	-	4/20/22/22	0/4/4/4
3	QQJ	A	1202	1	-	2/20/22/22	0/4/4/4
3	QQJ	C	1202	1	-	2/20/22/22	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QQJ	H	1202	1	-	6/20/22/22	0/4/4/4
3	QQJ	D	1202	1	-	4/20/22/22	0/4/4/4
3	QQJ	F	1202	1	-	6/20/22/22	0/4/4/4
3	QQJ	B	1202	1	-	1/20/22/22	0/4/4/4

All (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	QQJ	C30-C28	9.96	1.55	1.39
3	C	1202	QQJ	C30-C28	9.91	1.55	1.39
3	A	1202	QQJ	C30-C28	9.61	1.55	1.39
3	G	1202	QQJ	C30-C28	9.54	1.55	1.39
3	C	1202	QQJ	C30-C27	9.51	1.54	1.39
3	F	1202	QQJ	C30-C27	9.45	1.54	1.39
3	H	1202	QQJ	C30-C28	9.41	1.54	1.39
3	G	1202	QQJ	C24-C28	9.37	1.55	1.39
3	G	1202	QQJ	C30-C27	9.35	1.54	1.39
3	A	1202	QQJ	C24-C28	9.27	1.54	1.39
3	F	1202	QQJ	C30-C28	9.27	1.54	1.39
3	D	1202	QQJ	C30-C27	9.20	1.53	1.39
3	F	1202	QQJ	C25-C24	9.16	1.55	1.38
3	D	1202	QQJ	C24-C28	9.09	1.54	1.39
3	A	1202	QQJ	C30-C27	9.08	1.53	1.39
3	F	1202	QQJ	C24-C28	9.03	1.54	1.39
3	H	1202	QQJ	C30-C27	9.02	1.53	1.39
3	A	1202	QQJ	C25-C24	9.00	1.55	1.38
3	H	1202	QQJ	C24-C28	8.99	1.54	1.39
3	G	1202	QQJ	C25-C24	8.94	1.55	1.38
3	E	1202	QQJ	C30-C28	8.91	1.54	1.39
3	C	1202	QQJ	C25-C24	8.85	1.54	1.38
3	H	1202	QQJ	C25-C24	8.84	1.54	1.38
3	C	1202	QQJ	C24-C28	8.77	1.54	1.39
3	B	1202	QQJ	C25-C24	8.49	1.54	1.38
3	D	1202	QQJ	C25-C24	8.48	1.54	1.38
3	G	1202	QQJ	C16-S17	8.46	1.82	1.75
3	H	1202	QQJ	C22-C23	8.19	1.55	1.38
3	H	1202	QQJ	C16-S17	8.11	1.82	1.75
3	H	1202	QQJ	C03-C06	8.04	1.52	1.37
3	G	1202	QQJ	C03-C06	8.01	1.52	1.37
3	C	1202	QQJ	C03-C06	7.99	1.52	1.37
3	H	1202	QQJ	C03-C01	7.99	1.53	1.38
3	F	1202	QQJ	C03-C06	7.98	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1202	QQJ	C25-C24	7.92	1.53	1.38
3	D	1202	QQJ	C03-C06	7.90	1.52	1.37
3	A	1202	QQJ	C03-C06	7.88	1.52	1.37
3	C	1202	QQJ	C03-C01	7.87	1.53	1.38
3	A	1202	QQJ	C03-C01	7.84	1.53	1.38
3	G	1202	QQJ	C09-C06	7.83	1.52	1.37
3	A	1202	QQJ	C22-C23	7.79	1.54	1.38
3	G	1202	QQJ	C22-C23	7.76	1.54	1.38
3	D	1202	QQJ	C22-C23	7.75	1.54	1.38
3	G	1202	QQJ	C09-C11	7.73	1.52	1.38
3	H	1202	QQJ	C09-C11	7.71	1.52	1.38
3	G	1202	QQJ	C03-C01	7.70	1.52	1.38
3	D	1202	QQJ	C09-C11	7.68	1.52	1.38
3	F	1202	QQJ	C09-C11	7.68	1.52	1.38
3	C	1202	QQJ	C09-C11	7.67	1.52	1.38
3	B	1202	QQJ	C30-C28	7.67	1.52	1.39
3	D	1202	QQJ	C03-C01	7.63	1.52	1.38
3	E	1202	QQJ	C30-C27	7.63	1.51	1.39
3	F	1202	QQJ	C03-C01	7.62	1.52	1.38
3	B	1202	QQJ	C30-C27	7.58	1.51	1.39
3	H	1202	QQJ	C23-N07	7.58	1.50	1.34
3	D	1202	QQJ	C09-C06	7.58	1.52	1.37
3	C	1202	QQJ	C22-C23	7.58	1.53	1.38
3	F	1202	QQJ	C22-C23	7.58	1.53	1.38
3	D	1202	QQJ	C16-S17	7.50	1.82	1.75
3	H	1202	QQJ	C19-N07	7.50	1.48	1.34
3	H	1202	QQJ	C09-C06	7.48	1.51	1.37
3	F	1202	QQJ	C09-C06	7.46	1.51	1.37
3	C	1202	QQJ	C09-C06	7.43	1.51	1.37
3	D	1202	QQJ	C23-N07	7.40	1.50	1.34
3	A	1202	QQJ	C09-C11	7.40	1.52	1.38
3	C	1202	QQJ	C23-N07	7.37	1.50	1.34
3	E	1202	QQJ	C24-C28	7.35	1.51	1.39
3	A	1202	QQJ	C16-S17	7.29	1.81	1.75
3	F	1202	QQJ	C25-C26	7.26	1.54	1.39
3	A	1202	QQJ	C09-C06	7.26	1.51	1.37
3	G	1202	QQJ	C23-N07	7.23	1.49	1.34
3	F	1202	QQJ	C23-N07	7.21	1.49	1.34
3	F	1202	QQJ	C16-S17	7.21	1.81	1.75
3	A	1202	QQJ	C23-N07	7.21	1.49	1.34
3	H	1202	QQJ	C25-C26	7.17	1.54	1.39
3	B	1202	QQJ	C24-C28	7.16	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1202	QQJ	C19-N07	7.16	1.47	1.34
3	G	1202	QQJ	C25-C26	7.08	1.54	1.39
3	A	1202	QQJ	C25-C26	7.06	1.54	1.39
3	C	1202	QQJ	C25-C26	7.03	1.54	1.39
3	D	1202	QQJ	C25-C26	7.02	1.54	1.39
3	A	1202	QQJ	C19-N07	7.00	1.47	1.34
3	C	1202	QQJ	C19-N07	6.97	1.47	1.34
3	F	1202	QQJ	C19-N07	6.93	1.47	1.34
3	D	1202	QQJ	C19-N07	6.91	1.47	1.34
3	B	1202	QQJ	C22-C23	6.69	1.52	1.38
3	G	1202	QQJ	C11-C13	6.51	1.53	1.39
3	B	1202	QQJ	C33-C32	-6.49	1.22	1.51
3	H	1202	QQJ	C11-C13	6.48	1.53	1.39
3	D	1202	QQJ	C11-C13	6.47	1.53	1.39
3	H	1202	QQJ	C20-C19	6.41	1.55	1.39
3	H	1202	QQJ	C20-C21	6.30	1.50	1.39
3	G	1202	QQJ	C20-C19	6.28	1.55	1.39
3	C	1202	QQJ	C16-S17	6.28	1.81	1.75
3	A	1202	QQJ	C11-C13	6.22	1.52	1.39
3	C	1202	QQJ	C11-C13	6.19	1.52	1.39
3	C	1202	QQJ	C33-C32	-6.18	1.23	1.51
3	D	1202	QQJ	C20-C19	6.15	1.55	1.39
3	B	1202	QQJ	O08-C31	-6.14	1.10	1.23
3	G	1202	QQJ	C20-C21	6.06	1.50	1.39
3	E	1202	QQJ	C22-C23	6.06	1.50	1.38
3	D	1202	QQJ	C20-C21	6.04	1.50	1.39
3	E	1202	QQJ	C09-C11	6.04	1.49	1.38
3	G	1202	QQJ	C01-C13	6.00	1.52	1.39
3	E	1202	QQJ	C16-S17	5.99	1.80	1.75
3	F	1202	QQJ	C11-C13	5.95	1.52	1.39
3	E	1202	QQJ	C03-C01	5.92	1.49	1.38
3	H	1202	QQJ	C27-C26	5.90	1.53	1.40
3	A	1202	QQJ	C20-C19	5.88	1.54	1.39
3	D	1202	QQJ	C01-C13	5.84	1.51	1.39
3	F	1202	QQJ	C01-C13	5.82	1.51	1.39
3	B	1202	QQJ	C03-C01	5.79	1.49	1.38
3	C	1202	QQJ	C20-C19	5.79	1.54	1.39
3	C	1202	QQJ	C01-C13	5.79	1.51	1.39
3	H	1202	QQJ	C01-C13	5.79	1.51	1.39
3	H	1202	QQJ	C21-C15	5.79	1.55	1.49
3	F	1202	QQJ	C20-C21	5.78	1.49	1.39
3	F	1202	QQJ	C20-C19	5.78	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1202	QQJ	C03-C06	5.74	1.48	1.37
3	B	1202	QQJ	C25-C26	5.68	1.51	1.39
3	A	1202	QQJ	C01-C13	5.67	1.51	1.39
3	E	1202	QQJ	C25-C26	5.66	1.51	1.39
3	G	1202	QQJ	C31-N12	5.65	1.48	1.35
3	B	1202	QQJ	C03-C06	5.64	1.48	1.37
3	B	1202	QQJ	C15-N02	-5.64	1.23	1.37
3	F	1202	QQJ	C31-N12	5.63	1.48	1.35
3	E	1202	QQJ	C23-N07	5.53	1.46	1.34
3	C	1202	QQJ	C20-C21	5.52	1.49	1.39
3	E	1202	QQJ	C20-C19	5.52	1.53	1.39
3	B	1202	QQJ	C09-C06	5.51	1.47	1.37
3	A	1202	QQJ	C27-C26	5.50	1.52	1.40
3	D	1202	QQJ	C27-C26	5.50	1.52	1.40
3	H	1202	QQJ	C31-N12	5.50	1.47	1.35
3	F	1202	QQJ	C27-C26	5.41	1.52	1.40
3	A	1202	QQJ	C20-C21	5.41	1.49	1.39
3	C	1202	QQJ	C27-C26	5.38	1.51	1.40
3	D	1202	QQJ	C31-N12	5.37	1.47	1.35
3	G	1202	QQJ	C27-C26	5.36	1.51	1.40
3	B	1202	QQJ	C19-N07	5.27	1.44	1.34
3	C	1202	QQJ	C31-N12	5.23	1.47	1.35
3	A	1202	QQJ	C31-N12	5.22	1.47	1.35
3	E	1202	QQJ	C09-C06	5.22	1.47	1.37
3	B	1202	QQJ	C20-C19	5.21	1.52	1.39
3	B	1202	QQJ	C09-C11	5.19	1.48	1.38
3	H	1202	QQJ	C19-N10	5.13	1.47	1.38
3	E	1202	QQJ	C19-N07	5.13	1.44	1.34
3	E	1202	QQJ	O08-C31	-5.09	1.12	1.23
3	D	1202	QQJ	C19-N10	5.08	1.47	1.38
3	G	1202	QQJ	C19-N10	4.90	1.47	1.38
3	B	1202	QQJ	C11-C13	4.89	1.49	1.39
3	C	1202	QQJ	C19-N10	4.88	1.47	1.38
3	H	1202	QQJ	C22-C21	4.79	1.49	1.39
3	G	1202	QQJ	C21-C15	4.71	1.54	1.49
3	E	1202	QQJ	C20-C21	4.68	1.47	1.39
3	E	1202	QQJ	C15-N02	-4.67	1.26	1.37
3	B	1202	QQJ	C23-N07	4.60	1.44	1.34
3	F	1202	QQJ	C19-N10	4.59	1.46	1.38
3	G	1202	QQJ	C22-C21	4.56	1.49	1.39
3	F	1202	QQJ	C22-C21	4.55	1.49	1.39
3	D	1202	QQJ	C22-C21	4.53	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	QQJ	C13-C14	4.48	1.54	1.49
3	G	1202	QQJ	C13-C14	4.47	1.54	1.49
3	B	1202	QQJ	C14-N04	-4.41	1.26	1.37
3	B	1202	QQJ	C16-S17	4.39	1.79	1.75
3	E	1202	QQJ	C27-C26	4.38	1.49	1.40
3	B	1202	QQJ	C15-C14	-4.38	1.32	1.44
3	A	1202	QQJ	C19-N10	4.36	1.46	1.38
3	A	1202	QQJ	C22-C21	4.34	1.48	1.39
3	B	1202	QQJ	C01-C13	4.33	1.48	1.39
3	D	1202	QQJ	C21-C15	4.29	1.54	1.49
3	C	1202	QQJ	C22-C21	4.28	1.48	1.39
3	H	1202	QQJ	C13-C14	4.27	1.54	1.49
3	E	1202	QQJ	C11-C13	4.17	1.48	1.39
3	E	1202	QQJ	C01-C13	4.15	1.48	1.39
3	B	1202	QQJ	C27-C26	4.04	1.49	1.40
3	E	1202	QQJ	C15-C14	-4.00	1.33	1.44
3	C	1202	QQJ	C21-C15	4.00	1.53	1.49
3	E	1202	QQJ	C14-N04	-3.98	1.27	1.37
3	A	1202	QQJ	C13-C14	3.98	1.53	1.49
3	F	1202	QQJ	C21-C15	3.79	1.53	1.49
3	B	1202	QQJ	C22-C21	3.74	1.47	1.39
3	A	1202	QQJ	C21-C15	3.65	1.53	1.49
3	F	1202	QQJ	C28-N12	3.63	1.49	1.41
3	E	1202	QQJ	C13-C14	3.60	1.53	1.49
3	D	1202	QQJ	C27-N10	3.27	1.49	1.39
3	F	1202	QQJ	C13-C14	3.23	1.52	1.49
3	G	1202	QQJ	C28-N12	3.13	1.48	1.41
3	C	1202	QQJ	C28-N12	3.08	1.47	1.41
3	B	1202	QQJ	C31-N12	3.06	1.42	1.35
3	H	1202	QQJ	C27-N10	3.04	1.48	1.39
3	C	1202	QQJ	C13-C14	2.97	1.52	1.49
3	A	1202	QQJ	C28-N12	2.94	1.47	1.41
3	C	1202	QQJ	C15-C14	-2.94	1.36	1.44
3	A	1202	QQJ	C15-C14	-2.94	1.36	1.44
3	C	1202	QQJ	C27-N10	2.94	1.48	1.39
3	E	1202	QQJ	C22-C21	2.92	1.45	1.39
3	G	1202	QQJ	C27-N10	2.91	1.48	1.39
3	E	1202	QQJ	C31-N12	2.88	1.42	1.35
3	D	1202	QQJ	C28-N12	2.87	1.47	1.41
3	F	1202	QQJ	C15-C14	-2.86	1.36	1.44
3	G	1202	QQJ	O05-C26	2.86	1.41	1.37
3	H	1202	QQJ	C28-N12	2.84	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	QQJ	C27-N10	2.83	1.47	1.39
3	F	1202	QQJ	C27-N10	2.82	1.47	1.39
3	H	1202	QQJ	C33-C32	-2.76	1.39	1.51
3	G	1202	QQJ	C15-C14	-2.74	1.37	1.44
3	H	1202	QQJ	C15-C14	-2.72	1.37	1.44
3	E	1202	QQJ	C21-C15	2.69	1.52	1.49
3	D	1202	QQJ	C15-C14	-2.59	1.37	1.44
3	B	1202	QQJ	C20-C21	2.56	1.44	1.39
3	D	1202	QQJ	C15-N02	-2.54	1.31	1.37
3	C	1202	QQJ	O05-C26	2.52	1.41	1.37
3	B	1202	QQJ	C13-C14	2.47	1.51	1.49
3	G	1202	QQJ	C15-N02	-2.45	1.31	1.37
3	B	1202	QQJ	F34-C06	-2.39	1.30	1.36
3	F	1202	QQJ	O05-C26	2.35	1.40	1.37
3	F	1202	QQJ	C15-N02	-2.33	1.31	1.37
3	B	1202	QQJ	C32-C31	2.32	1.58	1.51
3	H	1202	QQJ	O08-C31	-2.29	1.18	1.23
3	A	1202	QQJ	O05-C26	2.29	1.40	1.37
3	C	1202	QQJ	C15-N02	-2.26	1.31	1.37
3	H	1202	QQJ	C15-N02	-2.26	1.31	1.37
3	H	1202	QQJ	O05-C26	2.23	1.40	1.37
3	A	1202	QQJ	C15-N02	-2.21	1.31	1.37
3	B	1202	QQJ	O05-C29	-2.19	1.36	1.42
3	A	1202	QQJ	C14-N04	-2.18	1.32	1.37
3	E	1202	QQJ	F34-C06	-2.18	1.31	1.36
3	D	1202	QQJ	C14-N04	-2.06	1.32	1.37
3	D	1202	QQJ	O05-C26	2.03	1.40	1.37
3	D	1202	QQJ	O08-C31	-2.01	1.19	1.23
3	C	1202	QQJ	C14-N04	-2.00	1.32	1.37

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1202	QQJ	C18-S17-C16	12.83	111.85	102.27
3	H	1202	QQJ	C18-S17-C16	8.17	108.36	102.27
3	B	1202	QQJ	C18-S17-C16	7.59	107.93	102.27
3	A	1202	QQJ	C18-S17-C16	6.16	106.86	102.27
3	H	1202	QQJ	C28-N12-C31	-5.11	118.56	127.50
3	E	1202	QQJ	C28-N12-C31	-5.01	118.73	127.50
3	F	1202	QQJ	C18-S17-C16	5.00	106.00	102.27
3	B	1202	QQJ	O05-C26-C27	4.38	120.18	114.80
3	H	1202	QQJ	O05-C26-C27	4.05	119.77	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	QQJ	O08-C31-N12	-3.97	116.38	123.63
3	B	1202	QQJ	C33-C32-C31	3.87	125.58	113.30
3	E	1202	QQJ	O05-C26-C27	3.80	119.46	114.80
3	G	1202	QQJ	C18-S17-C16	3.76	105.08	102.27
3	A	1202	QQJ	C22-C23-N07	-3.55	119.55	123.96
3	D	1202	QQJ	C20-C19-N07	-3.49	117.89	122.75
3	D	1202	QQJ	C23-N07-C19	3.30	121.90	117.22
3	E	1202	QQJ	C15-C14-N04	-3.28	104.92	113.76
3	B	1202	QQJ	C22-C23-N07	-3.23	119.94	123.96
3	G	1202	QQJ	C22-C23-N07	-3.22	119.96	123.96
3	C	1202	QQJ	O05-C26-C27	3.21	118.74	114.80
3	C	1202	QQJ	C22-C23-N07	-3.10	120.10	123.96
3	F	1202	QQJ	C28-N12-C31	-3.07	122.13	127.50
3	G	1202	QQJ	C23-N07-C19	3.04	121.53	117.22
3	G	1202	QQJ	O05-C26-C27	3.01	118.49	114.80
3	H	1202	QQJ	C22-C23-N07	-2.99	120.25	123.96
3	G	1202	QQJ	C28-N12-C31	-2.97	122.30	127.50
3	E	1202	QQJ	C22-C23-N07	-2.95	120.29	123.96
3	F	1202	QQJ	C29-O05-C26	-2.84	113.25	117.53
3	C	1202	QQJ	C29-O05-C26	-2.83	113.26	117.53
3	D	1202	QQJ	C20-C21-C15	-2.83	114.71	120.15
3	G	1202	QQJ	C20-C19-N07	-2.78	118.88	122.75
3	F	1202	QQJ	C20-C19-N07	-2.78	118.88	122.75
3	C	1202	QQJ	C23-N07-C19	2.76	121.14	117.22
3	E	1202	QQJ	C22-C21-C15	-2.76	116.24	120.61
3	D	1202	QQJ	C22-C21-C20	2.75	122.05	118.16
3	H	1202	QQJ	C29-O05-C26	-2.70	113.46	117.53
3	D	1202	QQJ	C15-C14-N04	-2.65	106.62	113.76
3	H	1202	QQJ	O05-C26-C25	-2.63	119.86	124.37
3	F	1202	QQJ	C23-N07-C19	2.63	120.95	117.22
3	A	1202	QQJ	C23-N07-C19	2.62	120.94	117.22
3	C	1202	QQJ	C20-C19-N07	-2.62	119.10	122.75
3	A	1202	QQJ	O05-C26-C27	2.61	118.00	114.80
3	F	1202	QQJ	C22-C21-C20	2.59	121.82	118.16
3	C	1202	QQJ	C22-C21-C20	2.57	121.80	118.16
3	A	1202	QQJ	C22-C21-C20	2.56	121.79	118.16
3	F	1202	QQJ	O05-C26-C27	2.55	117.93	114.80
3	E	1202	QQJ	C23-N07-C19	2.53	120.81	117.22
3	D	1202	QQJ	C22-C23-N07	-2.52	120.82	123.96
3	H	1202	QQJ	C20-C19-N07	-2.52	119.23	122.75
3	E	1202	QQJ	C09-C06-C03	-2.47	119.55	122.83
3	H	1202	QQJ	C23-N07-C19	2.47	120.72	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	QQJ	C33-C32-C31	-2.46	105.49	113.30
3	G	1202	QQJ	C15-C14-N04	-2.44	107.16	113.76
3	G	1202	QQJ	C33-C32-C31	-2.42	105.60	113.30
3	A	1202	QQJ	C15-C14-N04	-2.42	107.24	113.76
3	D	1202	QQJ	O05-C26-C25	-2.38	120.29	124.37
3	E	1202	QQJ	F34-C06-C03	2.37	122.57	118.54
3	B	1202	QQJ	C15-C14-N04	-2.35	107.42	113.76
3	F	1202	QQJ	C22-C23-N07	-2.31	121.09	123.96
3	D	1202	QQJ	C18-S17-C16	2.27	103.96	102.27
3	C	1202	QQJ	C11-C13-C01	2.24	122.06	117.59
3	F	1202	QQJ	C15-C14-N04	-2.24	107.71	113.76
3	D	1202	QQJ	O05-C26-C27	2.24	117.54	114.80
3	B	1202	QQJ	C11-C09-C06	2.24	120.67	118.36
3	D	1202	QQJ	C28-N12-C31	-2.23	123.59	127.50
3	A	1202	QQJ	C11-C13-C01	2.21	121.99	117.59
3	H	1202	QQJ	C14-C15-N02	-2.17	107.90	113.76
3	H	1202	QQJ	C15-C14-N04	-2.17	107.91	113.76
3	A	1202	QQJ	C29-O05-C26	-2.16	114.27	117.53
3	F	1202	QQJ	C32-C31-N12	2.15	120.51	114.75
3	G	1202	QQJ	C22-C21-C20	2.13	121.18	118.16
3	F	1202	QQJ	C11-C13-C01	2.13	121.84	117.59
3	F	1202	QQJ	C20-C21-C15	-2.11	116.09	120.15
3	B	1202	QQJ	O05-C26-C25	-2.10	120.76	124.37
3	E	1202	QQJ	C22-C21-C20	2.10	121.13	118.16
3	E	1202	QQJ	C01-C13-C14	2.09	123.92	120.61
3	C	1202	QQJ	C15-C14-N04	-2.09	108.13	113.76
3	B	1202	QQJ	C14-C15-N02	-2.08	108.14	113.76
3	E	1202	QQJ	O05-C26-C25	-2.08	120.81	124.37
3	C	1202	QQJ	O05-C26-C25	-2.08	120.81	124.37
3	C	1202	QQJ	C20-C21-C15	-2.04	116.23	120.15

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	QQJ	C01-C13-C14-N04
3	H	1202	QQJ	C27-C26-O05-C29
3	F	1202	QQJ	C27-C26-O05-C29
3	H	1202	QQJ	C25-C26-O05-C29
3	D	1202	QQJ	C25-C26-O05-C29
3	F	1202	QQJ	C25-C26-O05-C29
3	D	1202	QQJ	C27-C26-O05-C29

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Mol	Chain	Res	Type	Atoms
3	G	1202	QQJ	C01-C13-C14-N04
3	E	1202	QQJ	N12-C31-C32-C33
3	H	1202	QQJ	C01-C13-C14-N04
3	H	1202	QQJ	C11-C13-C14-N04
3	A	1202	QQJ	C11-C13-C14-N04
3	G	1202	QQJ	C11-C13-C14-N04
3	F	1202	QQJ	N12-C31-C32-C33
3	C	1202	QQJ	C01-C13-C14-N04
3	C	1202	QQJ	C11-C13-C14-N04
3	F	1202	QQJ	C01-C13-C14-N04
3	F	1202	QQJ	C11-C13-C14-N04
3	F	1202	QQJ	O08-C31-C32-C33
3	H	1202	QQJ	O08-C31-C32-C33
3	E	1202	QQJ	O08-C31-C32-C33
3	D	1202	QQJ	C11-C13-C14-N04
3	G	1202	QQJ	N12-C31-C32-C33
3	G	1202	QQJ	O08-C31-C32-C33
3	B	1202	QQJ	C01-C13-C14-N04
3	D	1202	QQJ	C01-C13-C14-N04
3	E	1202	QQJ	C01-C13-C14-N04
3	E	1202	QQJ	C11-C13-C14-N04
3	H	1202	QQJ	N12-C31-C32-C33

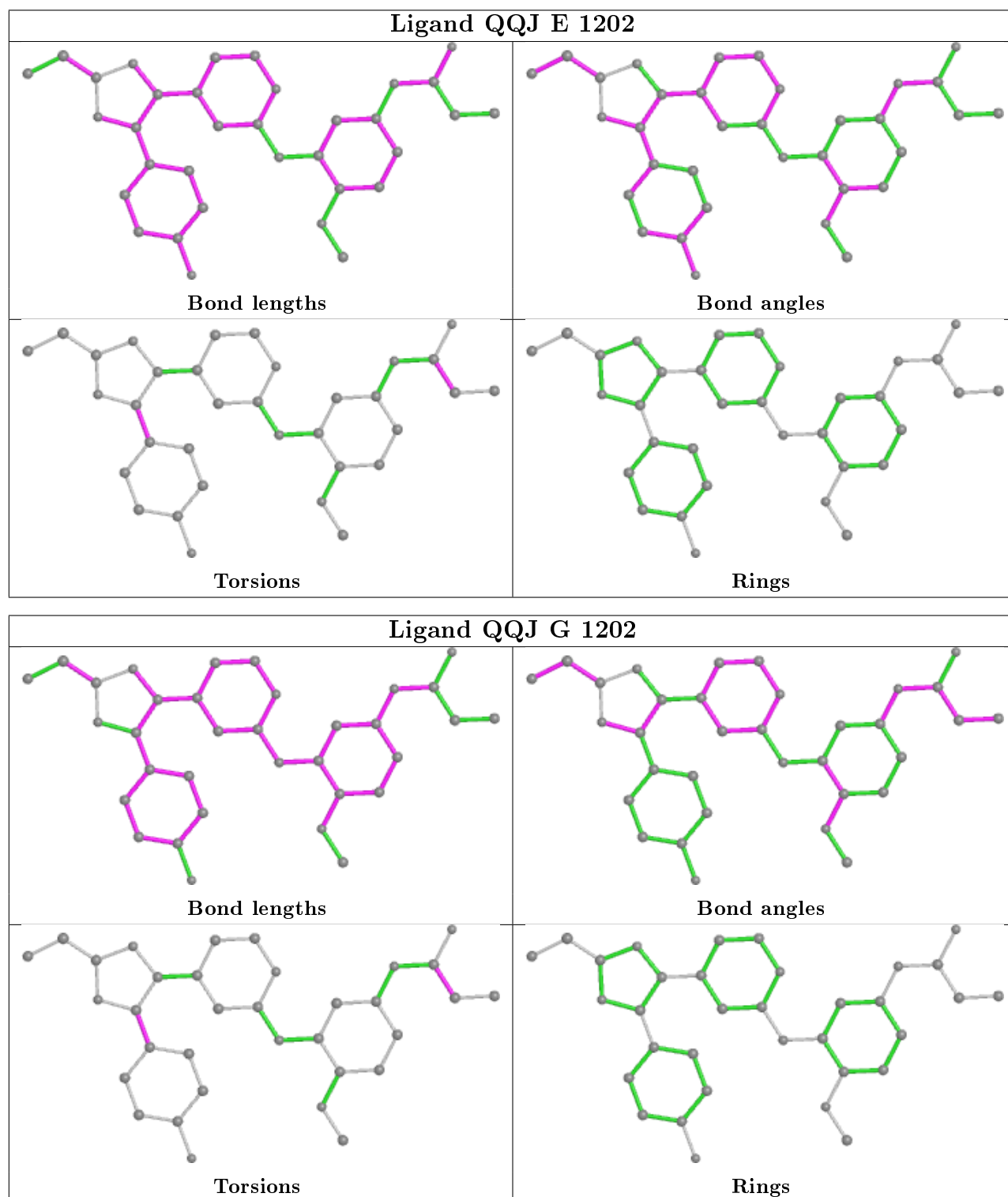
There are no ring outliers.

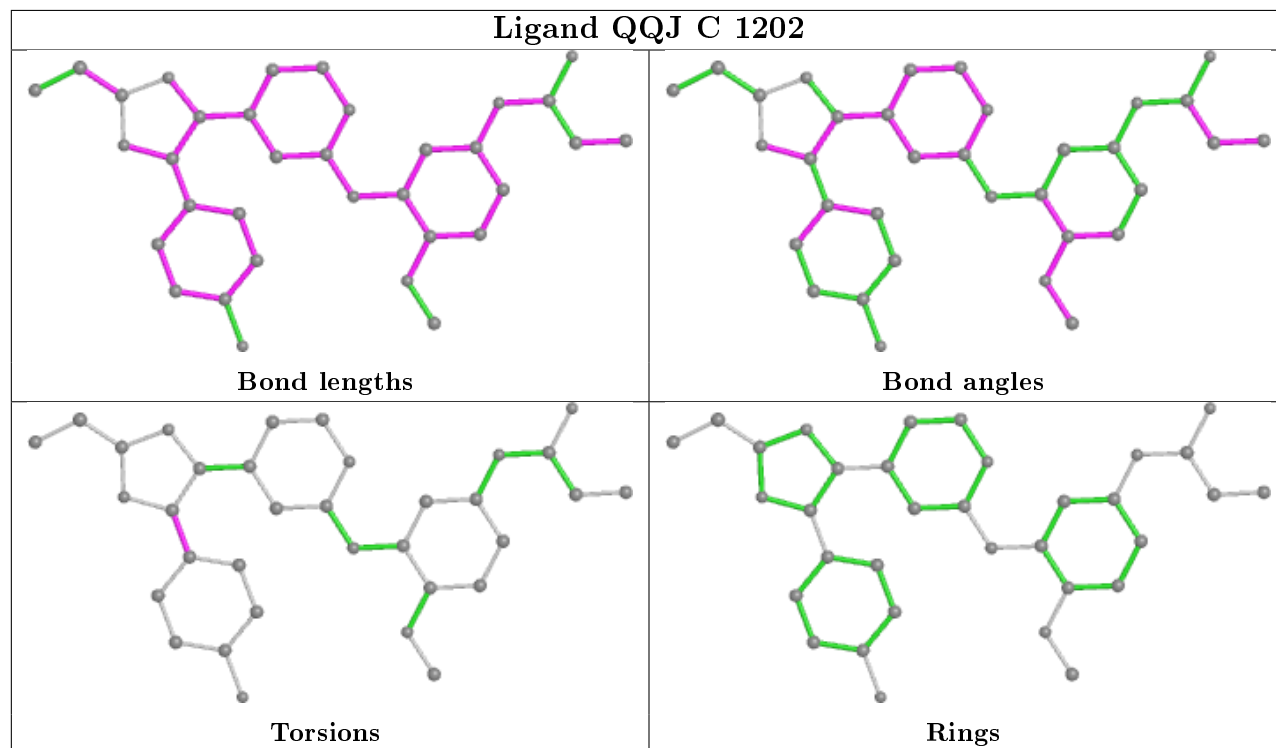
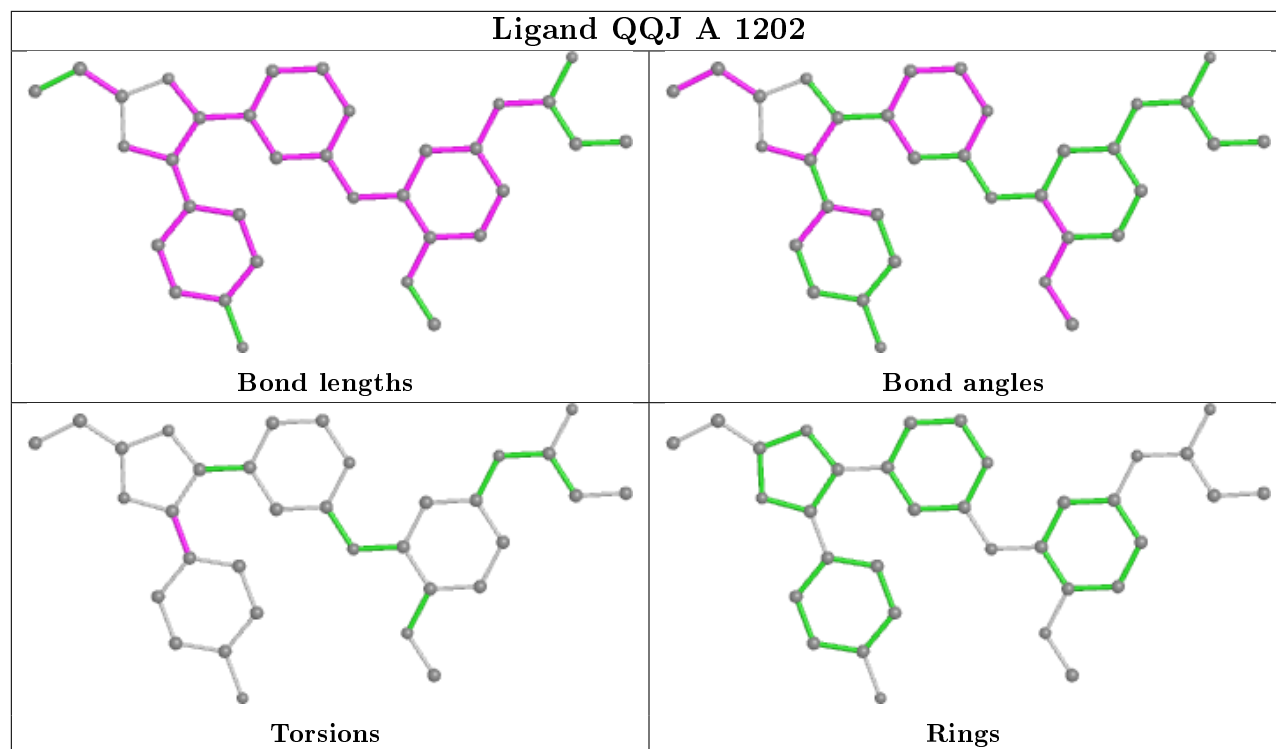
8 monomers are involved in 24 short contacts:

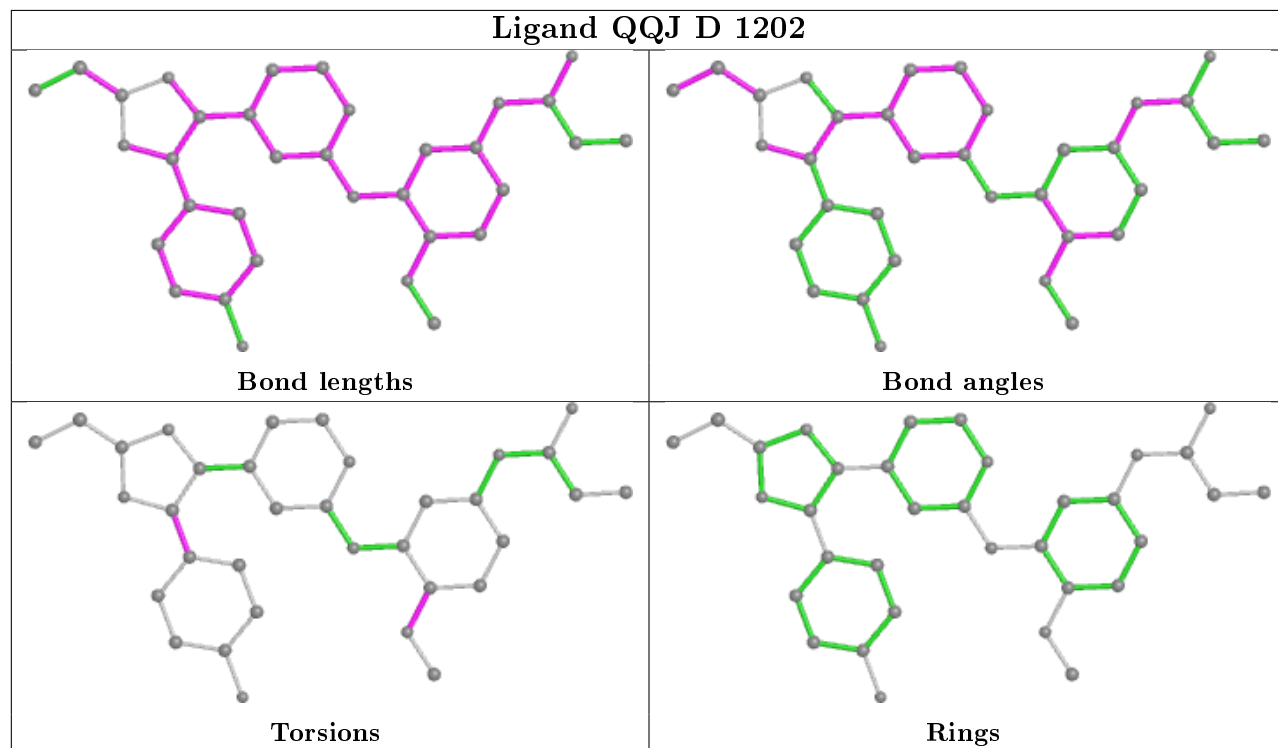
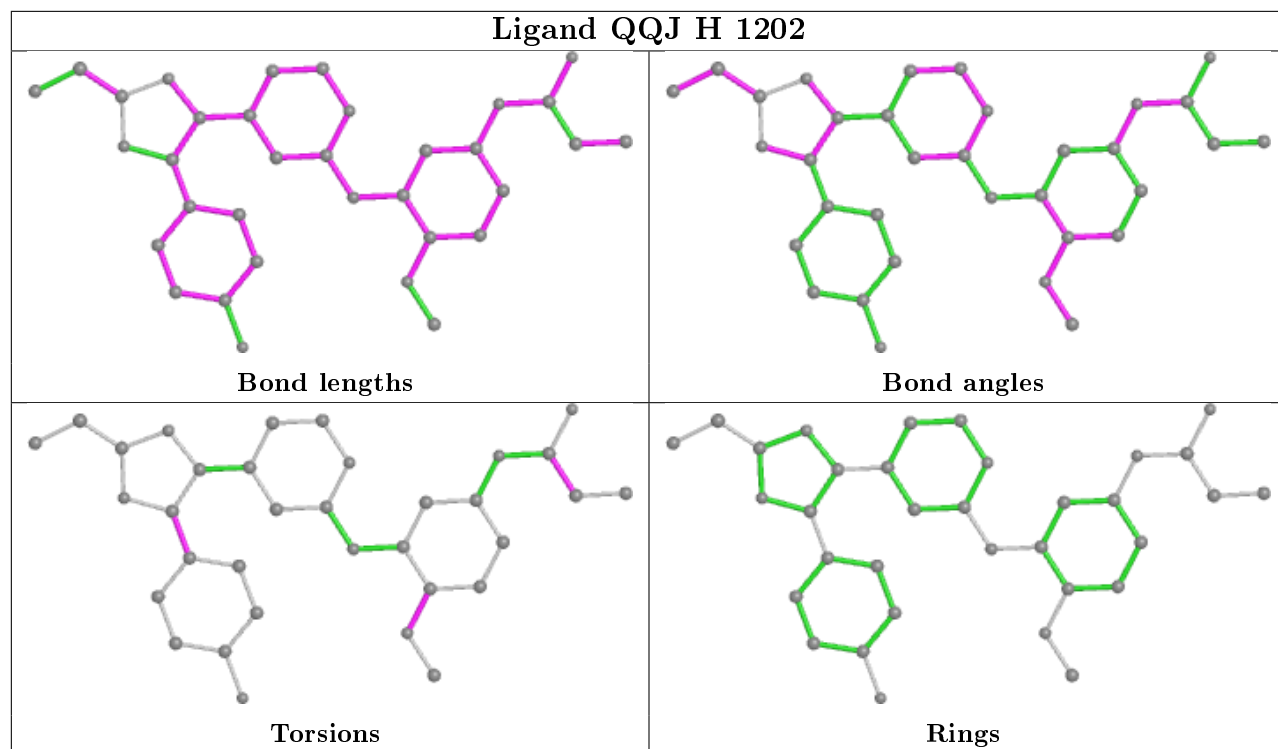
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1202	QQJ	2	0
3	G	1202	QQJ	3	0
3	A	1202	QQJ	2	0
3	C	1202	QQJ	1	0
3	H	1202	QQJ	5	0
3	D	1202	QQJ	4	0
3	F	1202	QQJ	5	0
3	B	1202	QQJ	2	0

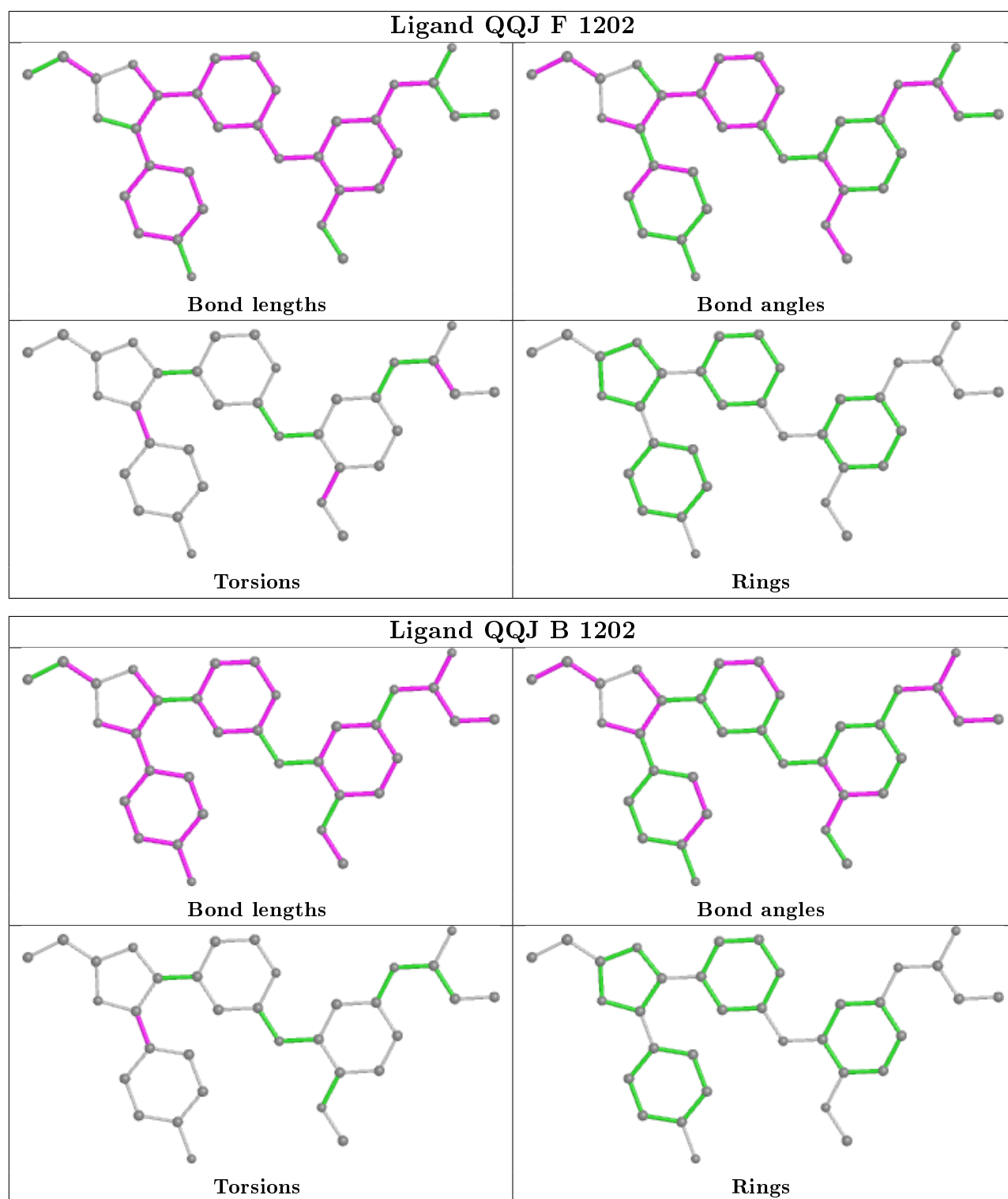
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	300/327 (91%)	-0.01	10 (3%)	46	44	18, 32, 57, 75	0
1	B	301/327 (92%)	0.07	12 (3%)	38	36	18, 35, 61, 98	0
1	C	302/327 (92%)	-0.04	11 (3%)	42	41	16, 30, 60, 87	0
1	D	314/327 (96%)	0.06	16 (5%)	28	26	16, 33, 71, 92	0
1	E	303/327 (92%)	0.26	21 (6%)	16	15	16, 37, 76, 96	0
1	F	306/327 (93%)	-0.02	12 (3%)	39	37	16, 33, 64, 104	0
1	G	314/327 (96%)	0.07	12 (3%)	40	38	19, 35, 66, 84	0
1	H	314/327 (96%)	0.10	9 (2%)	51	49	20, 35, 55, 70	0
All	All	2454/2616 (93%)	0.06	103 (4%)	36	34	16, 34, 63, 104	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1012	ASP	6.2
1	E	864	ALA	5.4
1	G	753	PRO	5.4
1	E	807	ASP	4.8
1	H	874	GLY	4.7
1	B	1013	ALA	4.5
1	D	1009	ASP	4.5
1	F	873	GLY	4.5
1	E	1013	ALA	4.3
1	B	1009	ASP	4.3
1	F	1009	ASP	4.2
1	C	751	THR	4.1
1	H	873	GLY	4.1
1	C	750	ALA	4.1
1	D	1014	ASP	4.1
1	E	723	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	864	ALA	3.9
1	D	1013	ALA	3.9
1	D	870	HIS	3.8
1	F	1008	ASP	3.8
1	F	753	PRO	3.7
1	E	1009	ASP	3.7
1	F	872	GLU	3.7
1	B	1012	ASP	3.6
1	D	873	GLY	3.6
1	B	990	PRO	3.6
1	E	1011	VAL	3.5
1	F	1010	VAL	3.5
1	B	807	ASP	3.5
1	C	985	GLU	3.4
1	G	872	GLU	3.3
1	B	1014	ASP	3.3
1	B	986	ARG	3.3
1	E	863	GLY	3.3
1	D	764	TYR	3.3
1	A	751	THR	3.3
1	E	1010	VAL	3.1
1	B	1010	VAL	3.1
1	D	753	PRO	3.1
1	G	1008	ASP	3.0
1	H	753	PRO	3.0
1	B	700	ASN	3.0
1	G	1007	MET	2.9
1	F	1007	MET	2.9
1	E	986	ARG	2.9
1	E	987	MET	2.9
1	B	987	MET	2.8
1	D	1011	VAL	2.8
1	G	873	GLY	2.8
1	G	1006	ASP	2.7
1	H	1013	ALA	2.7
1	E	1014	ASP	2.7
1	D	874	GLY	2.7
1	G	916	ASP	2.7
1	A	750	ALA	2.7
1	A	755	ALA	2.7
1	A	1014	ASP	2.7
1	B	988	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	1008	ASP	2.6
1	D	872	GLU	2.6
1	A	1013	ALA	2.6
1	H	941	ILE	2.6
1	E	749	GLU	2.6
1	C	1012	ASP	2.6
1	C	749	GLU	2.6
1	D	1012	ASP	2.6
1	F	1014	ASP	2.6
1	G	784	SER	2.6
1	B	982	GLN	2.6
1	E	989	LEU	2.5
1	F	1012	ASP	2.5
1	C	986	ARG	2.5
1	A	752	SER	2.5
1	E	808	ASN	2.5
1	D	988	HIS	2.5
1	C	988	HIS	2.4
1	C	1014	ASP	2.4
1	A	756	ASN	2.4
1	E	988	HIS	2.4
1	A	1012	ASP	2.3
1	A	988	HIS	2.3
1	F	1011	VAL	2.3
1	C	1010	VAL	2.3
1	D	1008	ASP	2.3
1	G	1009	ASP	2.3
1	C	807	ASP	2.2
1	H	1014	ASP	2.2
1	H	762	GLU	2.2
1	E	860	LYS	2.1
1	G	1014	ASP	2.1
1	A	753	PRO	2.1
1	F	875	LYS	2.1
1	H	1006	ASP	2.1
1	D	755	ALA	2.1
1	D	1010	VAL	2.1
1	E	985	GLU	2.1
1	F	748	ARG	2.1
1	C	1007	MET	2.0
1	E	992	PRO	2.0
1	G	748	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	737	LYS	2.0
1	H	751	THR	2.0
1	G	1013	ALA	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

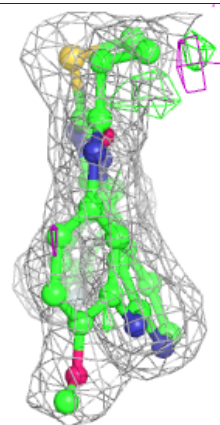
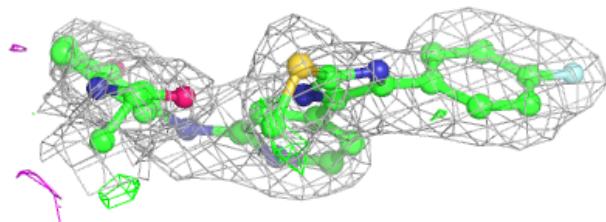
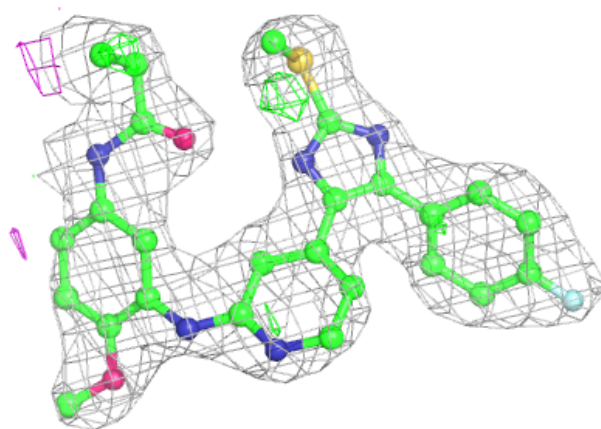
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	E	1201	1/1	0.82	0.21	70,70,70,70	0
2	CL	B	1201	1/1	0.84	0.15	60,60,60,60	0
3	QQJ	G	1202	34/34	0.90	0.15	22,34,39,43	0
3	QQJ	H	1202	34/34	0.92	0.14	25,31,39,56	0
3	QQJ	F	1202	34/34	0.93	0.15	20,25,34,39	0
3	QQJ	E	1202	34/34	0.93	0.13	24,30,44,46	0
3	QQJ	D	1202	34/34	0.94	0.15	18,27,34,41	0
3	QQJ	C	1202	34/34	0.94	0.14	19,26,30,33	0
2	CL	G	1201	1/1	0.94	0.07	44,44,44,44	0
2	CL	F	1201	1/1	0.95	0.11	41,41,41,41	0
3	QQJ	B	1202	34/34	0.95	0.12	20,27,31,43	0
3	QQJ	A	1202	34/34	0.95	0.14	20,23,28,29	0
2	CL	D	1201	1/1	0.96	0.07	43,43,43,43	0
2	CL	H	1201	1/1	0.97	0.07	38,38,38,38	0
2	CL	A	1201	1/1	0.97	0.10	41,41,41,41	0
2	CL	C	1201	1/1	0.97	0.09	39,39,39,39	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.

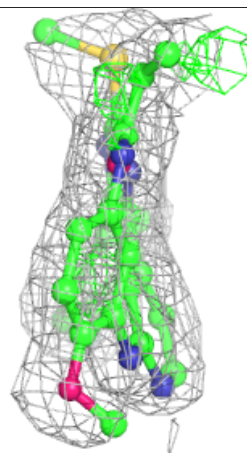
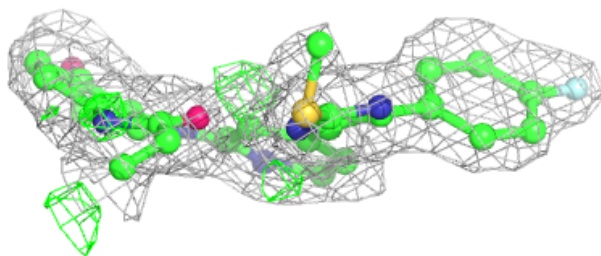
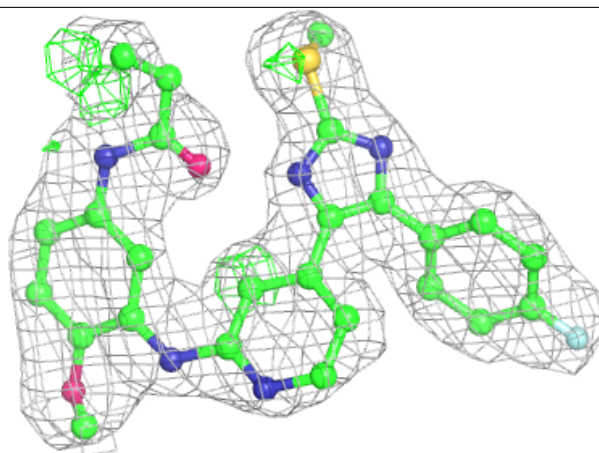
**Electron density around QQJ G 1202:**

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



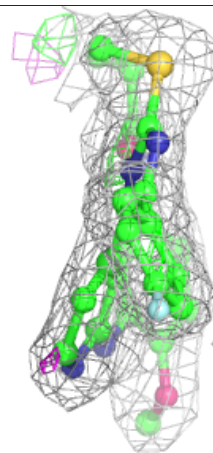
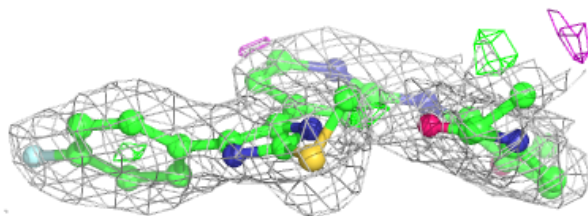
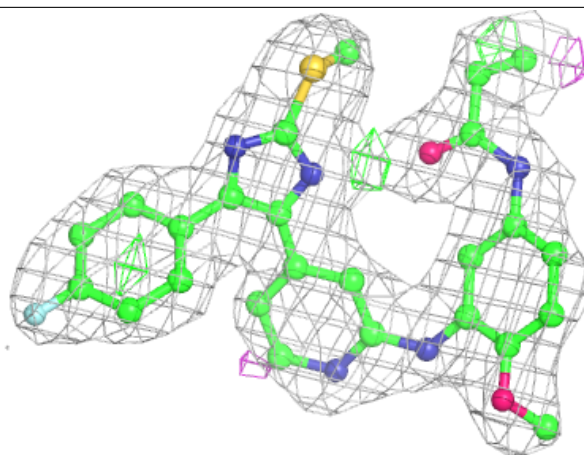
**Electron density around QQJ H 1202:**

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



**Electron density around QQJ F 1202:**

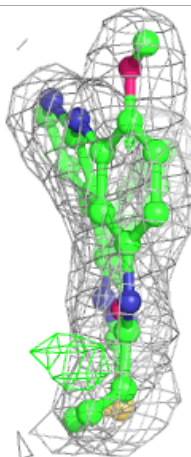
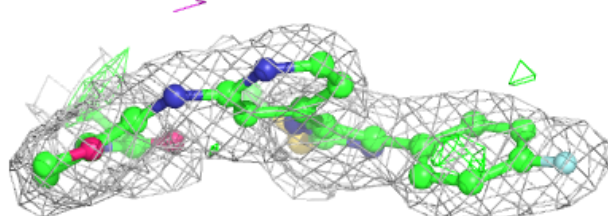
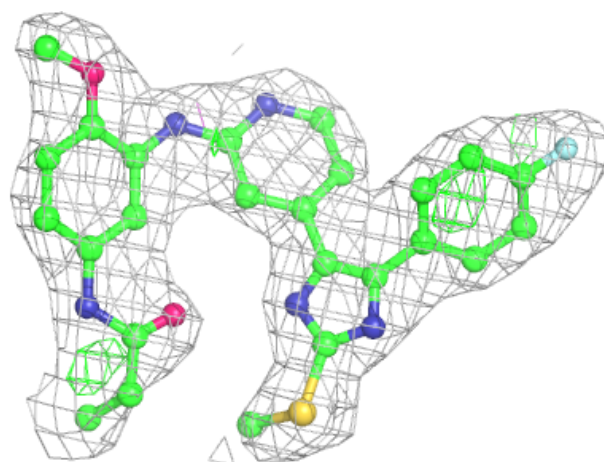
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





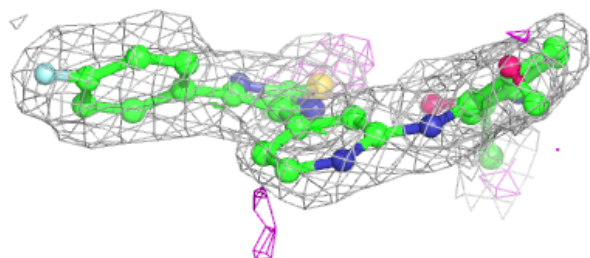
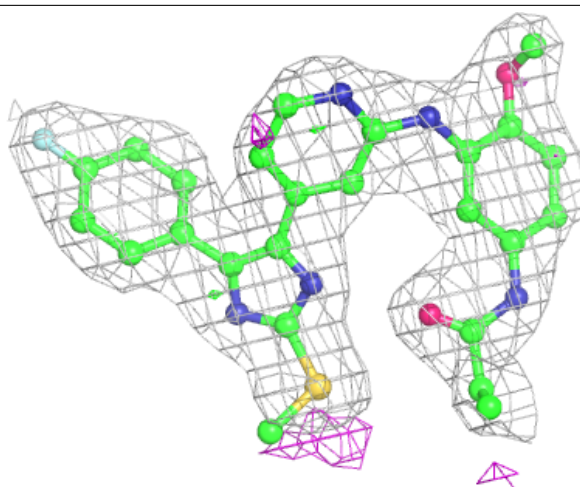
**Electron density around QQJ E 1202:**

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



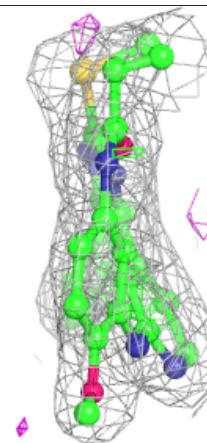
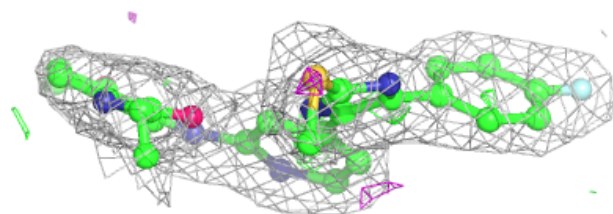
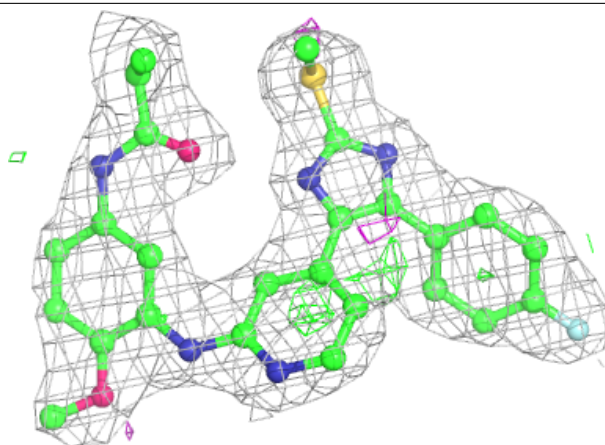
**Electron density around QQJ D 1202:**

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



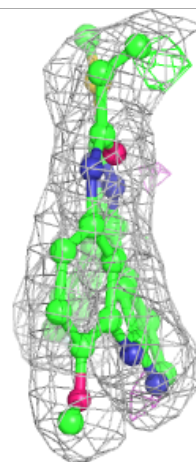
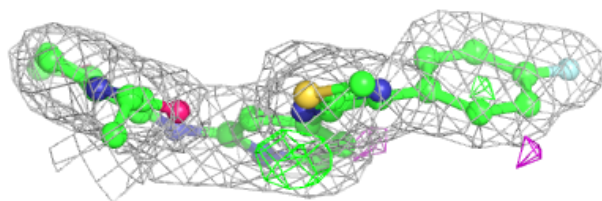
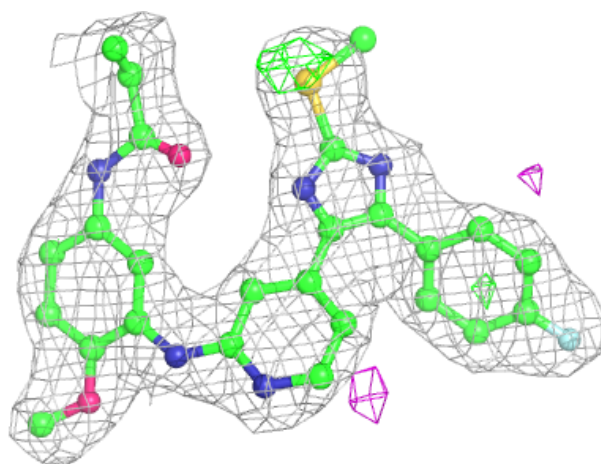
**Electron density around QQJ C 1202:**

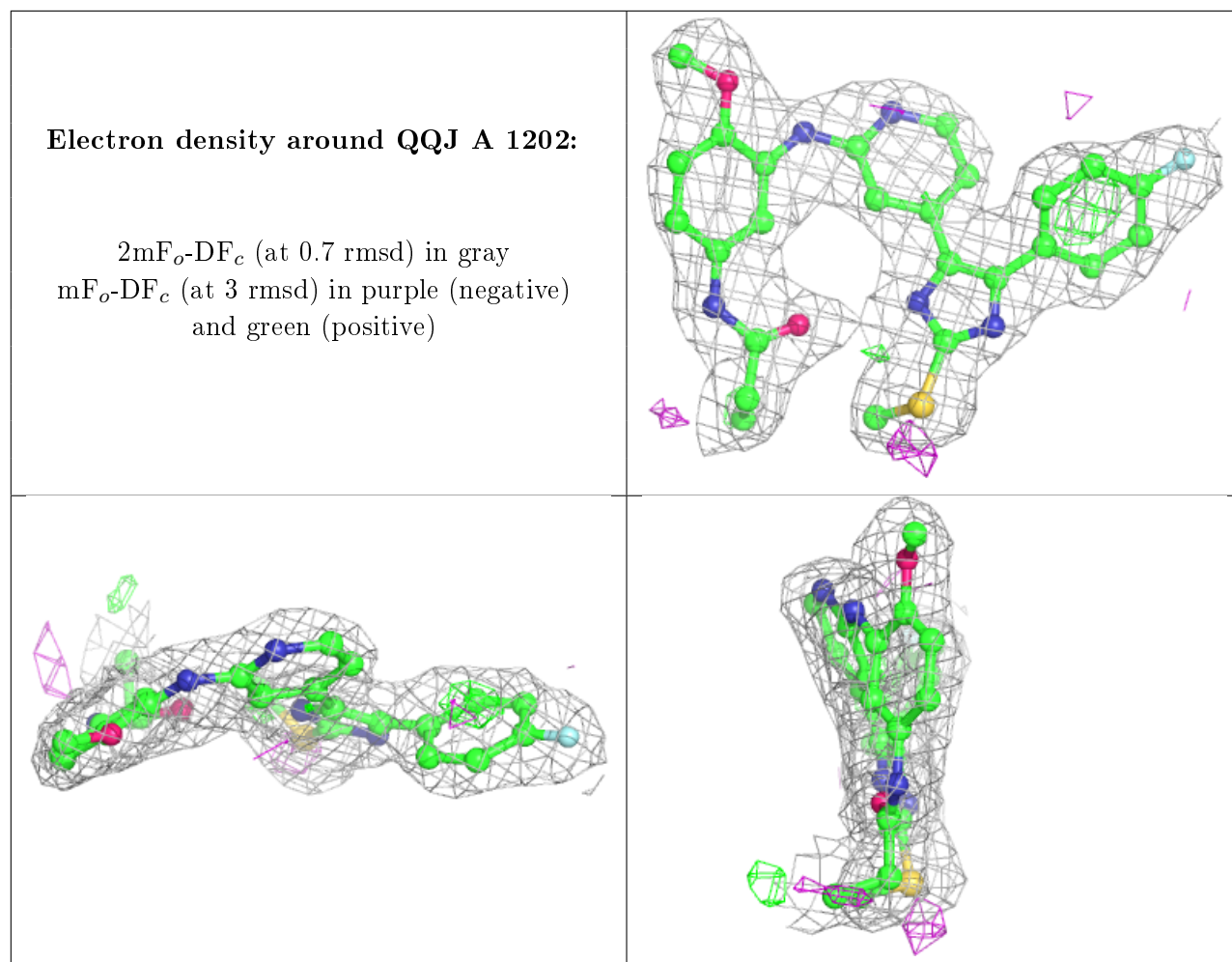
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around QQJ 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.