



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:49 AM EDT

PDB ID : 5FWR
Title : Breaking down the wall: mutation of the tyrosine gate of the universal Escherichia coli fimbrial adhesin FimH
Authors : Bouckaert, J.
Deposited on : 2016-02-21
Resolution : 2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

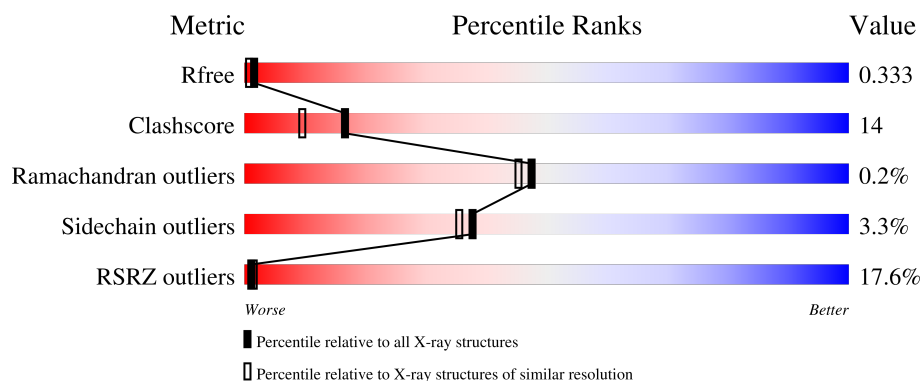
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	158	<div> <div>3%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
1	B	158	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	C	158	<div> <div>%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	D	158	<div> <div>%</div> <div>80%</div> <div>20%</div> <div>.</div> </div>
1	E	158	<div> <div>17%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	158	<div><div></div><div>34%</div><div></div><div>82%</div><div></div><div>17%</div><div></div></div>
1	G	158	<div><div></div><div>34%</div><div></div><div>66%</div><div></div><div>31%</div><div></div></div>
1	H	158	<div><div></div><div>51%</div><div></div><div>69%</div><div></div><div>28%</div><div></div></div>

2 Entry composition

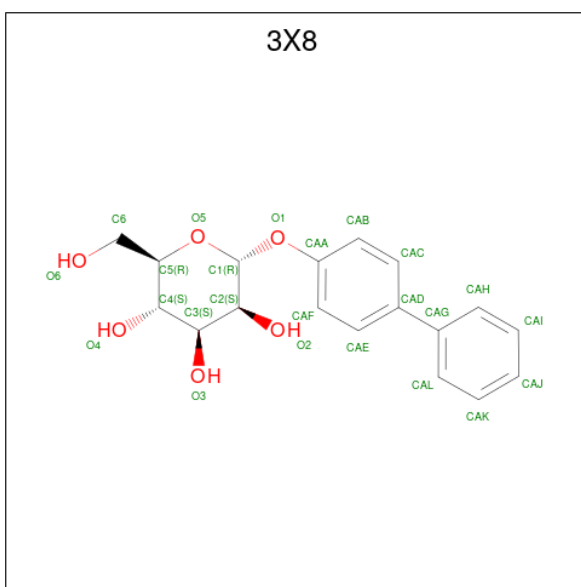
There are 3 unique types of molecules in this entry. The entry contains 21092 atoms, of which 9515 are hydrogens and 0 are deuteriums.

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 FimH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	H	N	O	S	0	3	0
			2381	770	1174	198	235	4			
1	B	158	Total	C	H	N	O	S	0	0	0
			2361	763	1165	197	234	2			
1	C	158	Total	C	H	N	O	S	0	0	0
			2362	763	1166	197	234	2			
1	D	158	Total	C	H	N	O	S	0	0	0
			2361	763	1166	197	233	2			
1	E	158	Total	C	H	N	O	S	0	2	0
			2387	769	1180	201	235	2			
1	F	158	Total	C	H	N	O	S	0	0	0
			2361	763	1166	197	233	2			
1	G	158	Total	C	H	N	O	S	0	2	0
			2380	768	1175	199	236	2			
1	H	158	Total	C	H	N	O	S	0	1	0
			2375	771	1171	197	234	2			

- Molecule 2 is biphenyl-4-yl alpha-D-mannopyranoside (three-letter code: 3X8) (formula: C₁₈H₂₀O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			43	18	19	6		
2	B	1	Total	C	H	O	0	0
			43	18	19	6		
2	C	1	Total	C	H	O	0	0
			43	18	19	6		
2	D	1	Total	C	H	O	0	0
			43	18	19	6		
2	E	1	Total	C	H	O	0	0
			43	18	19	6		
2	F	1	Total	C	H	O	0	0
			43	18	19	6		
2	G	1	Total	C	H	O	0	0
			43	18	19	6		
2	H	1	Total	C	H	O	0	0
			43	18	19	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	190	Total	O	0	0
			190	190		
3	B	229	Total	O	0	0
			229	229		
3	C	212	Total	O	0	0
			212	212		
3	D	227	Total	O	0	0
			227	227		

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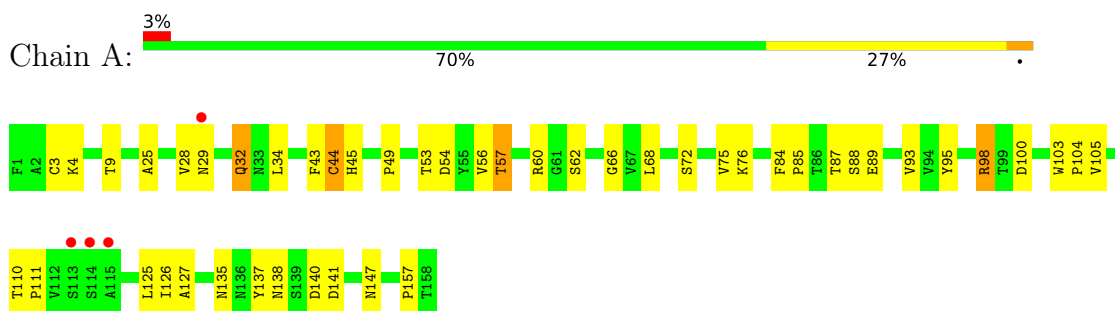
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	197	Total 197	O 197	0	0
3	F	244	Total 244	O 244	0	0
3	G	233	Total 233	O 233	0	0
3	H	248	Total 248	O 248	0	0

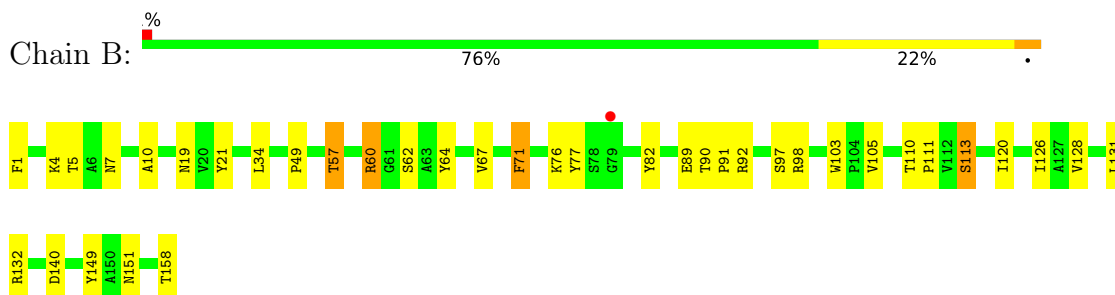
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

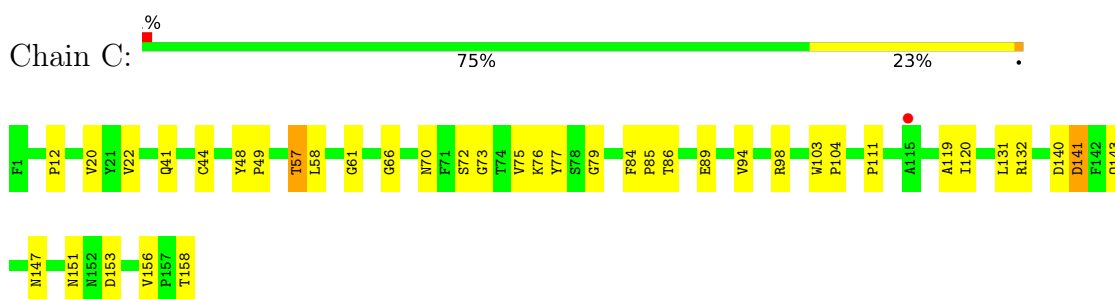
- Molecule 1: FimH



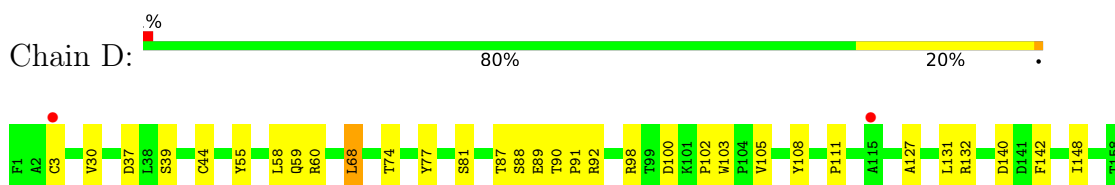
- Molecule 1: FimH



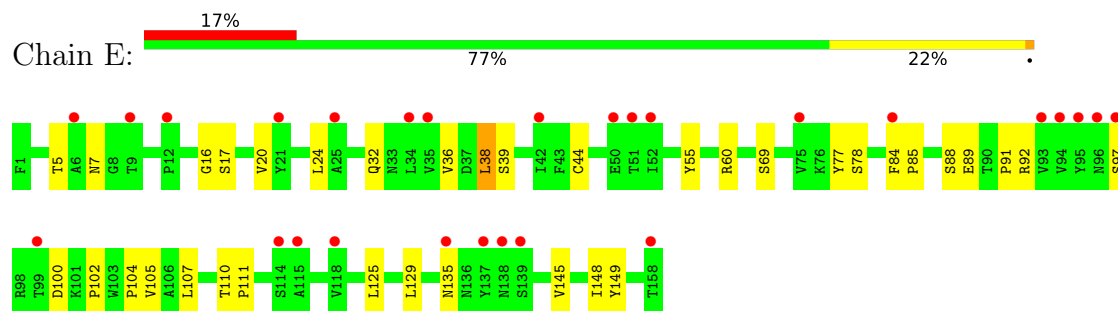
- Molecule 1: FimH



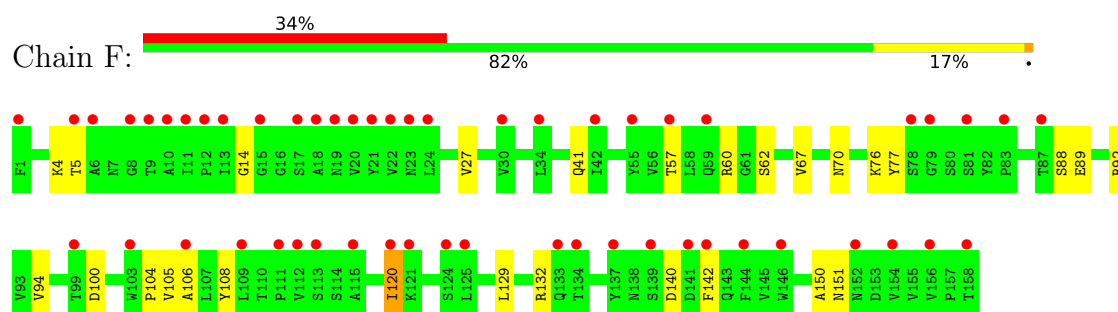
- Molecule 1: FimH



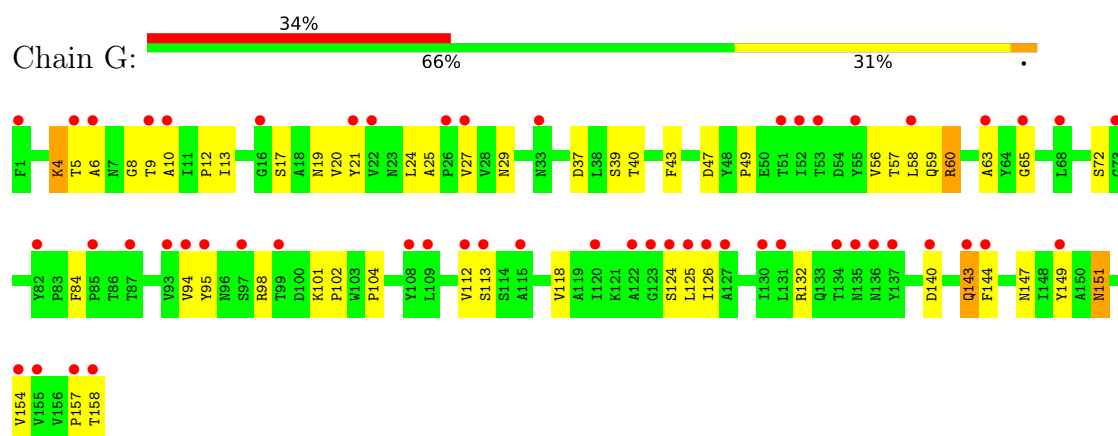
- Molecule 1: FimH



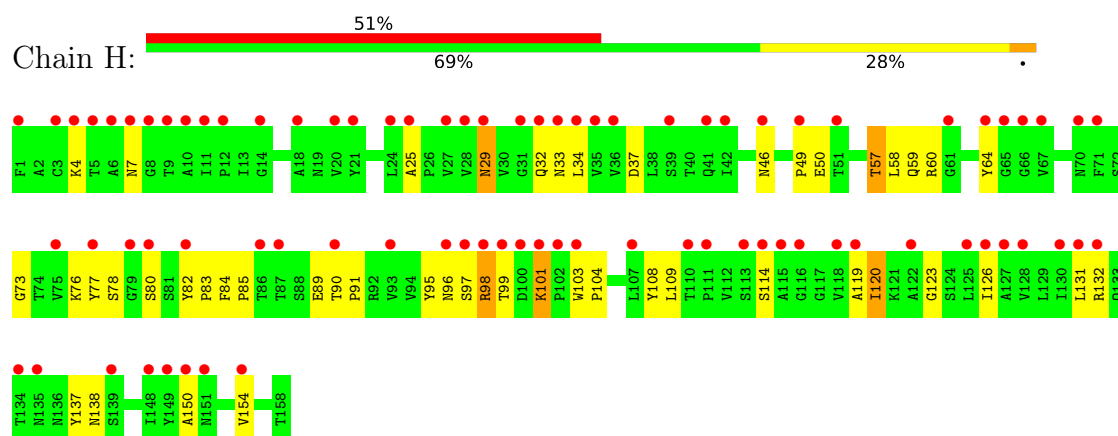
- Molecule 1: FimH



- Molecule 1: FimH



- Molecule 1: FimH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.02Å 74.00Å 111.77Å 99.32° 102.97° 97.83°	Depositor
Resolution (Å)	47.63 – 2.13 47.63 – 2.13	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.63-2.13) 94.6 (47.63-2.13)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.225 , 0.332 0.234 , 0.333	Depositor DCC
R_{free} test set	4253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.854	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 99.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21092	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 27.17 % 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 2.3085e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3X8

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	0.81	1/1246 (0.1%)	0.85	3/1711 (0.2%)
1	B	0.89	2/1226 (0.2%)	0.83	3/1684 (0.2%)
1	C	0.90	4/1226 (0.3%)	0.85	2/1684 (0.1%)
1	D	0.83	0/1225	0.85	2/1684 (0.1%)
1	E	0.55	0/1244	0.65	0/1708
1	F	0.56	0/1225	0.64	0/1684
1	G	0.56	0/1247	0.67	0/1712
1	H	0.52	0/1238	0.60	0/1702
All	All	0.72	7/9877 (0.1%)	0.75	10/13569 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	TRP	C-N	10.55	1.54	1.34
1	A	103	TRP	C-N	8.12	1.49	1.34
1	C	156	VAL	CB-CG2	7.49	1.68	1.52
1	C	20	VAL	CB-CG2	7.30	1.68	1.52
1	C	103	TRP	C-N	5.31	1.44	1.34
1	C	94	VAL	CB-CG2	-5.11	1.42	1.52
1	B	71	PHE	CD2-CE2	-5.11	1.29	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	98	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	98	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	D	98	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	140	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	141	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	140	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	140	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	140	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	131	LEU	CB-CG-CD2	5.22	119.88	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	THR	Peptide
1	C	57	THR	Peptide
1	G	10	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1207	1174	1180	38	0
1	B	1196	1165	1164	24	0
1	C	1196	1166	1166	27	0
1	D	1195	1166	1166	28	0
1	E	1207	1180	1170	27	0
1	F	1195	1166	1166	21	0
1	G	1205	1175	1165	62	0
1	H	1204	1171	1173	53	0
2	A	24	19	20	1	0
2	B	24	19	20	1	0
2	C	24	19	20	0	0
2	D	24	19	20	0	0
2	E	24	19	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	24	19	20	0	0
2	G	24	19	20	0	0
2	H	24	19	20	0	0
3	A	190	0	0	24	1
3	B	229	0	0	8	1
3	C	212	0	0	12	1
3	D	227	0	0	14	0
3	E	197	0	0	10	0
3	F	244	0	0	11	1
3	G	233	0	0	39	1
3	H	248	0	0	26	1
All	All	11577	9515	9510	274	3

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 14.

All (274) 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:H:78:SER:O	3:H:401:HOH:O	1.76	1.01
1:G:147:ASN:O	3:G:401:HOH:O	1.82	0.96
1:D:37:ASP:OD2	3:D:401:HOH:O	1.85	0.95
1:C:111:PRO:O	3:C:401:HOH:O	1.83	0.94
1:H:91:PRO:O	3:H:402:HOH:O	1.86	0.94
1:G:124:SER:O	3:G:402:HOH:O	1.84	0.94
1:D:92:ARG:NH1	3:D:405:HOH:O	1.98	0.94
1:G:94:VAL:O	1:G:101:LYS:NZ	2.00	0.94
1:G:25:ALA:O	3:G:403:HOH:O	1.86	0.93
1:A:138[B]:ASN:ND2	3:A:404:HOH:O	2.02	0.90
1:E:32:GLN:OE1	3:E:401:HOH:O	1.89	0.90
1:B:10:ALA:O	3:B:401:HOH:O	1.89	0.89
1:A:76:LYS:O	3:A:401:HOH:O	1.92	0.88
1:C:143:GLN:OE1	3:C:402:HOH:O	1.93	0.86
1:C:61:GLY:N	3:C:403:HOH:O	2.08	0.85
1:D:37:ASP:OD2	3:D:402:HOH:O	1.94	0.85
1:A:100:ASP:OD1	3:A:402:HOH:O	1.96	0.83
1:E:111:PRO:O	3:E:402:HOH:O	1.94	0.83
1:F:89:GLU:OE1	3:F:401:HOH:O	1.96	0.83
1:G:17:SER:O	3:G:404:HOH:O	1.95	0.83
1:D:74:THR:O	3:D:404:HOH:O	1.96	0.83
1:D:30:VAL:O	3:D:403:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:ALA:O	3:G:405:HOH:O	1.97	0.81
1:G:29:ASN:ND2	3:G:413:HOH:O	2.14	0.80
1:A:127:ALA:N	3:A:407:HOH:O	2.14	0.80
1:A:88:SER:O	3:A:403:HOH:O	1.99	0.79
1:H:37:ASP:OD2	3:H:403:HOH:O	2.00	0.78
1:H:99:THR:N	3:H:410:HOH:O	2.16	0.78
1:E:100:ASP:OD2	3:E:403:HOH:O	2.01	0.77
1:H:89:GLU:N	3:H:411:HOH:O	2.17	0.76
1:F:100:ASP:OD1	3:F:402:HOH:O	2.02	0.76
1:G:20:VAL:O	3:G:401:HOH:O	2.03	0.75
1:A:111:PRO:O	3:A:405:HOH:O	2.05	0.75
1:G:27:VAL:O	3:G:406:HOH:O	2.05	0.74
1:G:118:VAL:O	3:G:407:HOH:O	2.07	0.73
1:H:37:ASP:O	3:H:405:HOH:O	2.08	0.72
1:B:60:ARG:NH1	1:C:147:ASN:OD1	2.23	0.71
1:F:67:VAL:O	3:F:403:HOH:O	2.07	0.70
1:G:151:ASN:OD1	3:G:409:HOH:O	2.09	0.70
1:H:90:THR:O	3:H:407:HOH:O	2.10	0.69
1:A:32:GLN:NE2	3:A:410:HOH:O	2.24	0.69
1:C:141:ASP:O	3:C:404:HOH:O	2.10	0.69
1:C:158:THR:O	3:C:405:HOH:O	2.11	0.69
1:H:57:THR:HA	3:H:402:HOH:O	1.94	0.67
1:F:27:VAL:O	3:F:404:HOH:O	2.12	0.67
1:G:140:ASP:O	3:G:412:HOH:O	2.14	0.66
1:H:4:LYS:NZ	3:H:416:HOH:O	2.28	0.65
1:G:40:THR:OG1	3:G:411:HOH:O	2.14	0.65
1:G:58:LEU:O	3:G:414:HOH:O	2.15	0.65
1:C:132:ARG:NH2	3:C:408:HOH:O	2.29	0.64
1:D:108:TYR:N	3:D:404:HOH:O	2.18	0.64
1:F:140:ASP:OD1	3:F:405:HOH:O	2.15	0.64
1:D:111:PRO:O	3:D:406:HOH:O	2.14	0.63
1:H:29:ASN:ND2	1:H:32:GLN:OE1	2.31	0.63
1:G:126:ILE:N	3:G:402:HOH:O	2.32	0.63
1:D:140:ASP:N	3:D:411:HOH:O	2.26	0.63
1:G:58:LEU:N	3:G:414:HOH:O	2.30	0.63
1:G:47:ASP:O	1:G:98:ARG:NH1	2.23	0.62
1:F:60:ARG:HE	1:F:62:SER:HB3	1.65	0.61
1:G:98:ARG:NH1	3:G:416:HOH:O	2.19	0.61
1:A:125:LEU:HG	3:A:407:HOH:O	1.99	0.61
1:C:158:THR:OXT	1:C:158:THR:HG22	2.00	0.60
1:A:137:TYR:N	3:A:406:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:GLN:OE1	1:G:143[B]:GLN:NE2	2.36	0.59
1:C:86:THR:HG21	3:C:403:HOH:O	2.03	0.59
1:H:29:ASN:OD1	1:H:29:ASN:N	2.36	0.59
1:H:49:PRO:HD2	1:H:98:ARG:NH2	2.18	0.59
1:H:82:TYR:OH	3:H:406:HOH:O	2.10	0.58
1:D:100:ASP:OD1	3:D:407:HOH:O	2.17	0.58
1:F:4:LYS:NZ	3:F:413:HOH:O	2.37	0.57
1:D:60:ARG:NH2	1:G:37:ASP:OD2	2.38	0.56
1:H:114:SER:N	3:H:417:HOH:O	2.28	0.56
1:G:158:THR:HG22	1:G:158:THR:OXT	2.04	0.56
1:F:70:ASN:N	3:F:403:HOH:O	2.39	0.55
1:B:57:THR:HG22	1:B:132:ARG:HB3	1.89	0.55
1:H:64:TYR:OH	3:H:408:HOH:O	2.14	0.55
1:E:38:LEU:HD11	1:E:129:LEU:CD1	2.36	0.55
1:H:97:SER:HA	3:H:455:HOH:O	2.05	0.55
1:E:89:GLU:HB3	3:E:428:HOH:O	2.06	0.55
1:H:120:ILE:HG23	1:H:154:VAL:HB	1.89	0.54
1:B:1:PHE:N	2:B:182:3X8:O2	2.32	0.54
1:H:7:ASN:N	3:H:424:HOH:O	2.40	0.54
1:H:57:THR:HG22	1:H:132:ARG:HB3	1.88	0.54
1:A:147:ASN:OD1	3:A:408:HOH:O	2.19	0.54
1:D:60:ARG:NH2	1:G:39:SER:OG	2.41	0.53
1:A:66:GLY:HA2	3:A:412:HOH:O	2.09	0.53
1:H:96:ASN:ND2	3:H:419:HOH:O	2.29	0.53
1:A:53:THR:O	1:A:135:ASN:HA	2.09	0.53
1:G:154:VAL:HG22	3:G:403:HOH:O	2.08	0.53
1:A:56:VAL:N	1:A:93:VAL:O	2.38	0.52
1:A:75:VAL:HG22	3:A:401:HOH:O	2.09	0.52
1:G:17:SER:O	3:G:415:HOH:O	2.18	0.52
1:H:95:TYR:OH	1:H:103:TRP:HA	2.10	0.52
1:G:5:THR:HG22	1:G:6:ALA:N	2.24	0.52
1:G:57:THR:HB	3:G:414:HOH:O	2.09	0.52
1:G:20:VAL:N	3:G:401:HOH:O	2.41	0.52
1:G:19:ASN:OD1	3:G:417:HOH:O	2.19	0.52
1:G:65:GLY:HA3	3:G:487:HOH:O	2.10	0.52
1:H:50:GLU:CD	1:H:98:ARG:HH22	2.14	0.51
1:H:138:ASN:HA	3:H:412:HOH:O	2.10	0.51
1:A:54:ASP:OD2	2:A:182:3X8:O6	2.21	0.51
1:B:5:THR:OG1	1:B:7:ASN:OD1	2.29	0.51
1:H:123:GLY:N	1:H:150:ALA:O	2.41	0.51
1:A:87:THR:HA	3:A:444:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:CZ	1:B:62:SER:HB2	2.41	0.51
1:C:58:LEU:HG	3:C:403:HOH:O	2.10	0.50
1:B:60:ARG:NH2	1:B:62:SER:OG	2.43	0.50
1:G:102:PRO:O	1:G:104:PRO:HD3	2.10	0.50
1:B:49:PRO:HD2	1:B:98:ARG:NH2	2.25	0.50
1:A:57:THR:HG21	1:A:89:GLU:OE2	2.12	0.50
1:B:77:TYR:HD1	1:B:105:VAL:HG22	1.76	0.50
1:B:57:THR:HG21	1:B:89:GLU:OE2	2.11	0.49
1:C:84:PHE:HA	1:C:85:PRO:C	2.33	0.49
1:H:108:TYR:OH	3:H:409:HOH:O	2.15	0.49
1:A:141:ASP:OD2	1:E:69:SER:HB3	2.12	0.49
1:B:19:ASN:OD1	3:B:404:HOH:O	2.19	0.49
1:C:22:VAL:O	1:C:151:ASN:HB2	2.12	0.49
1:A:76:LYS:HD2	3:A:419:HOH:O	2.12	0.49
1:G:72:SER:OG	3:G:408:HOH:O	2.08	0.49
1:G:12:PRO:HD2	3:G:471:HOH:O	2.12	0.49
1:B:158:THR:HG23	3:B:529:HOH:O	2.13	0.49
1:H:37:ASP:N	3:H:405:HOH:O	2.45	0.49
1:B:132:ARG:NE	3:B:414:HOH:O	2.46	0.48
1:G:37:ASP:HB3	3:G:448:HOH:O	2.12	0.48
1:A:3[A]:CYS:SG	1:A:44[A]:CYS:HB3	2.53	0.48
1:G:149:TYR:HA	3:G:402:HOH:O	2.13	0.48
1:E:20:VAL:O	1:E:149:TYR:HB2	2.14	0.48
1:G:65:GLY:HA3	3:G:410:HOH:O	2.14	0.48
1:B:90:THR:HB	1:B:91:PRO:HD2	1.95	0.48
1:E:84:PHE:HA	1:E:85:PRO:C	2.35	0.47
1:H:84:PHE:HA	1:H:85:PRO:C	2.35	0.47
1:A:68:LEU:HD21	1:E:16:GLY:HA2	1.96	0.47
1:E:92[A]:ARG:NH2	3:E:414:HOH:O	2.46	0.47
1:A:29:ASN:OD1	1:A:157:PRO:HG2	2.15	0.47
1:C:76:LYS:HE2	1:C:79:GLY:HA2	1.96	0.47
1:G:143[B]:GLN:OE1	1:G:143[B]:GLN:HA	2.15	0.47
1:H:120:ILE:HD11	1:H:150:ALA:HB2	1.96	0.47
1:A:49:PRO:HD2	1:A:98:ARG:NH2	2.30	0.47
1:D:90:THR:OG1	1:D:91:PRO:HD2	2.15	0.47
1:H:73:GLY:O	3:H:413:HOH:O	2.21	0.47
1:D:59:GLN:HA	1:D:89:GLU:HG3	1.95	0.46
1:D:77:TYR:HD1	1:D:105:VAL:HG22	1.79	0.46
1:G:58:LEU:C	3:G:414:HOH:O	2.53	0.46
1:E:55:TYR:CD1	1:E:92[A]:ARG:HD2	2.49	0.46
1:G:63:ALA:HB2	1:G:84:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:SER:HA	3:E:430:HOH:O	2.16	0.46
1:F:14:GLY:HA2	1:F:142:PHE:CD2	2.51	0.46
1:G:37:ASP:O	3:G:411:HOH:O	2.21	0.46
1:H:126:ILE:HG21	1:H:150:ALA:HB2	1.97	0.46
1:H:137:TYR:O	3:H:412:HOH:O	2.20	0.46
1:A:75:VAL:CG2	3:A:401:HOH:O	2.63	0.46
1:H:4:LYS:HG3	3:H:415:HOH:O	2.16	0.46
1:C:73:GLY:N	3:C:411:HOH:O	2.36	0.46
1:C:77:TYR:HA	1:C:104:PRO:O	2.15	0.46
1:D:39:SER:O	1:D:102:PRO:HB3	2.16	0.46
1:E:88:SER:OG	1:F:94:VAL:HG21	2.15	0.46
1:D:108:TYR:HD1	3:D:404:HOH:O	1.99	0.46
1:F:57:THR:OG1	1:F:132:ARG:HB3	2.16	0.46
1:A:95:TYR:HA	3:A:446:HOH:O	2.15	0.45
1:H:34:LEU:N	1:H:109:LEU:O	2.39	0.45
1:B:34:LEU:HD11	3:B:426:HOH:O	2.16	0.45
1:D:81:SER:HB2	3:D:452:HOH:O	2.17	0.45
1:F:92:ARG:NH1	3:F:422:HOH:O	2.48	0.45
1:G:65:GLY:CA	3:G:487:HOH:O	2.63	0.45
1:B:67:VAL:HG21	1:B:126:ILE:HB	1.97	0.45
1:G:43:PHE:CE2	3:G:433:HOH:O	2.68	0.45
1:G:9:THR:HG23	3:G:461:HOH:O	2.15	0.45
1:H:57:THR:HG23	1:H:59:GLN:N	2.32	0.45
1:H:104:PRO:HG3	3:H:422:HOH:O	2.16	0.45
1:D:58:LEU:H	1:D:90:THR:CG2	2.30	0.45
1:E:78:SER:OG	3:E:405:HOH:O	2.21	0.45
1:A:126:ILE:C	3:A:407:HOH:O	2.51	0.44
1:G:125:LEU:N	3:G:419:HOH:O	2.50	0.44
1:C:151:ASN:HB3	3:C:438:HOH:O	2.15	0.44
1:E:24:LEU:HA	3:E:422:HOH:O	2.17	0.44
1:F:94:VAL:CG1	3:F:470:HOH:O	2.65	0.44
1:A:28:VAL:CG1	1:A:32:GLN:HG2	2.48	0.44
1:F:120:ILE:HD11	1:F:150:ALA:CB	2.47	0.44
1:A:4:LYS:HD2	3:A:436:HOH:O	2.17	0.44
1:A:87:THR:O	1:E:60:ARG:NH2	2.51	0.44
1:B:21:TYR:CD1	1:B:149:TYR:HB2	2.53	0.44
1:B:64:TYR:CE1	1:B:128:VAL:HG23	2.52	0.44
1:D:59:GLN:HB2	1:D:132:ARG:HB2	2.00	0.44
1:E:39:SER:O	1:E:102:PRO:HB3	2.18	0.43
1:E:102:PRO:O	1:E:104:PRO:HD3	2.17	0.43
1:E:5:THR:HG21	3:E:437:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:PRO:HD2	1:G:98:ARG:NH2	2.33	0.43
1:H:49:PRO:HD2	1:H:98:ARG:CZ	2.49	0.43
1:H:83:PRO:HG2	3:H:435:HOH:O	2.18	0.43
1:E:125:LEU:HD12	1:E:148:ILE:O	2.18	0.43
1:A:84:PHE:HA	1:A:85:PRO:C	2.39	0.43
1:H:7:ASN:HB2	3:H:424:HOH:O	2.19	0.43
1:H:95:TYR:CD2	1:H:101:LYS:HE2	2.53	0.43
1:B:60:ARG:NH2	3:B:416:HOH:O	2.47	0.43
1:C:120:ILE:O	1:C:153:ASP:HA	2.19	0.43
1:E:107:LEU:HD12	1:E:107:LEU:N	2.34	0.43
1:G:151:ASN:ND2	1:G:151:ASN:O	2.49	0.43
1:H:76:LYS:HA	1:H:80:SER:O	2.18	0.43
1:A:9:THR:HG21	3:A:437:HOH:O	2.18	0.43
1:D:103:TRP:CZ2	1:D:131:LEU:HB2	2.54	0.43
1:F:105:VAL:HG11	1:F:129:LEU:HD13	2.00	0.43
1:H:131:LEU:C	1:H:131:LEU:HD23	2.38	0.43
1:G:95:TYR:HA	3:G:428:HOH:O	2.19	0.42
1:H:46:ASN:N	1:H:97:SER:O	2.30	0.42
1:A:60:ARG:HE	1:A:62:SER:HB2	1.84	0.42
1:G:102:PRO:HA	3:G:433:HOH:O	2.19	0.42
1:H:120:ILE:CD1	1:H:126:ILE:HG21	2.50	0.42
1:D:88:SER:N	3:D:427:HOH:O	2.53	0.42
1:C:58:LEU:CG	3:C:403:HOH:O	2.66	0.42
1:D:74:THR:C	3:D:404:HOH:O	2.51	0.42
1:A:45:HIS:HB2	1:A:98:ARG:O	2.20	0.42
1:A:76:LYS:C	3:A:401:HOH:O	2.50	0.42
1:F:77:TYR:HA	1:F:104:PRO:O	2.19	0.42
1:G:112:VAL:HG22	1:G:113:SER:N	2.33	0.42
1:A:3[A]:CYS:HB3	1:A:43:PHE:O	2.19	0.42
1:G:49:PRO:O	3:G:418:HOH:O	2.20	0.42
1:G:59:GLN:HB2	1:G:132:ARG:HB2	2.02	0.42
1:A:25:ALA:HB3	1:A:34:LEU:HD13	2.00	0.42
1:E:77:TYR:CD1	1:E:105:VAL:HG22	2.55	0.42
1:F:108:TYR:OH	3:F:406:HOH:O	2.20	0.42
1:H:58:LEU:HB3	1:H:90:THR:CG2	2.49	0.42
1:B:71:PHE:CE1	1:B:120:ILE:HD11	2.55	0.42
1:B:82:TYR:HB3	3:B:504:HOH:O	2.20	0.42
1:C:70:ASN:O	1:C:111:PRO:HA	2.20	0.42
1:G:24:LEU:HB3	3:G:405:HOH:O	2.19	0.42
1:H:120:ILE:HD11	1:H:126:ILE:HG21	2.00	0.42
1:D:77:TYR:CD2	1:D:90:THR:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:N	3:A:425:HOH:O	2.51	0.41
1:C:49:PRO:HD2	1:C:98:ARG:NH2	2.35	0.41
1:C:76:LYS:HD3	3:C:418:HOH:O	2.20	0.41
1:H:50:GLU:OE2	1:H:98:ARG:NH2	2.39	0.41
1:G:5:THR:HG22	1:G:6:ALA:H	1.85	0.41
1:D:68:LEU:HD13	1:G:101:LYS:CE	2.50	0.41
1:F:76:LYS:HB2	1:F:106:ALA:HB3	2.02	0.41
1:F:151:ASN:ND2	3:F:428:HOH:O	2.53	0.41
1:H:60:ARG:NH2	3:H:423:HOH:O	2.38	0.41
1:F:120:ILE:HD11	1:F:150:ALA:HB2	2.02	0.41
1:H:120:ILE:HD11	1:H:150:ALA:CB	2.50	0.41
1:C:66:GLY:HA3	1:C:119:ALA:O	2.21	0.41
1:H:25:ALA:O	1:H:154:VAL:HG13	2.19	0.41
1:D:55:TYR:HB3	1:D:92:ARG:HD2	2.01	0.41
1:D:127:ALA:HB3	1:D:148:ILE:HB	2.02	0.41
1:E:17:SER:HA	1:E:145:VAL:O	2.21	0.41
1:B:113:SER:HB3	3:B:512:HOH:O	2.20	0.41
1:C:131:LEU:HD23	1:C:131:LEU:C	2.40	0.41
1:A:104:PRO:C	3:A:425:HOH:O	2.58	0.41
1:C:57:THR:HG21	1:C:89:GLU:OE2	2.21	0.41
1:C:75:VAL:HG13	1:C:75:VAL:O	2.21	0.41
1:C:119:ALA:O	1:C:120:ILE:HD13	2.21	0.41
1:G:4:LYS:HD2	1:G:8:GLY:O	2.21	0.41
1:H:119:ALA:C	1:H:120:ILE:HG22	2.41	0.41
1:B:110:THR:HA	1:B:111:PRO:HD3	1.98	0.41
1:D:142:PHE:HZ	3:D:501:HOH:O	2.03	0.41
1:E:135:ASN:OD1	1:E:135:ASN:C	2.59	0.41
1:F:5:THR:HA	1:F:41:GLN:O	2.20	0.41
1:G:21:TYR:HB2	3:G:503:HOH:O	2.20	0.41
1:G:56:VAL:HA	1:G:132:ARG:O	2.20	0.41
1:G:60:ARG:CZ	3:G:442:HOH:O	2.69	0.41
1:C:158:THR:OXT	1:C:158:THR:CG2	2.67	0.40
1:G:29:ASN:OD1	1:G:157:PRO:HG2	2.21	0.40
1:B:90:THR:HB	1:B:91:PRO:CD	2.50	0.40
1:G:158:THR:OXT	1:G:158:THR:CG2	2.70	0.40
1:E:38:LEU:HD12	1:E:105:VAL:HB	2.02	0.40
1:H:138:ASN:CB	3:H:412:HOH:O	2.69	0.40
1:D:3:CYS:HG	1:D:44:CYS:CB	2.35	0.40
1:E:7:ASN:OD1	1:E:7:ASN:C	2.59	0.40
1:E:36:VAL:HA	3:E:410:HOH:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:482:HOH:O	3:G:494:HOH:O[1_666]	1.99	0.21
3:C:564:HOH:O	3:H:527:HOH:O[1_565]	2.06	0.14
3:A:523:HOH:O	3:B:514:HOH:O[1_455]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/158 (101%)	150 (94%)	9 (6%)	0	100	100
1	B	156/158 (99%)	146 (94%)	10 (6%)	0	100	100
1	C	156/158 (99%)	147 (94%)	9 (6%)	0	100	100
1	D	156/158 (99%)	148 (95%)	8 (5%)	0	100	100
1	E	158/158 (100%)	148 (94%)	10 (6%)	0	100	100
1	F	156/158 (99%)	146 (94%)	10 (6%)	0	100	100
1	G	158/158 (100%)	140 (89%)	13 (8%)	5 (3%)	4	0
1	H	157/158 (99%)	147 (94%)	10 (6%)	0	100	100
All	All	1256/1264 (99%)	1172 (93%)	79 (6%)	5 (0%)	47	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	144[A]	PHE
1	G	144[B]	PHE
1	G	13	ILE
1	G	143[A]	GLN
1	G	143[B]	GLN

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	136/133 (102%)	131 (96%)	5 (4%)	34	31
1	B	133/133 (100%)	125 (94%)	8 (6%)	19	14
1	C	133/133 (100%)	128 (96%)	5 (4%)	33	30
1	D	133/133 (100%)	131 (98%)	2 (2%)	65	68
1	E	135/133 (102%)	130 (96%)	5 (4%)	34	31
1	F	133/133 (100%)	131 (98%)	2 (2%)	65	68
1	G	135/133 (102%)	132 (98%)	3 (2%)	52	53
1	H	134/133 (101%)	128 (96%)	6 (4%)	27	23
All	All	1072/1064 (101%)	1036 (97%)	36 (3%)	38	34

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	44[A]	CYS
1	A	44[B]	CYS
1	A	72	SER
1	A	110	THR
1	B	4	LYS
1	B	57	THR
1	B	60	ARG
1	B	76	LYS
1	B	92	ARG
1	B	97	SER
1	B	113	SER
1	B	151	ASN
1	C	12	PRO
1	C	41	GLN
1	C	44	CYS
1	C	48	TYR
1	C	72	SER
1	D	68	LEU

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Mol	Chain	Res	Type
1	D	87	THR
1	E	38	LEU
1	E	44	CYS
1	E	91	PRO
1	E	97	SER
1	E	110	THR
1	F	88	SER
1	F	120	ILE
1	G	4	LYS
1	G	60	ARG
1	G	151	ASN
1	H	29	ASN
1	H	33	ASN
1	H	57	THR
1	H	98	ARG
1	H	101	LYS
1	H	120	ILE

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

Mol	Chain	Res	Type
1	C	143	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	3X8	F	182	-	26,26,26	0.68	0	36,36,36	1.68	5 (13%)
2	3X8	B	182	-	26,26,26	0.93	1 (3%)	36,36,36	1.64	3 (8%)
2	3X8	E	182	-	26,26,26	0.39	0	36,36,36	1.26	3 (8%)
2	3X8	C	182	-	26,26,26	0.84	1 (3%)	36,36,36	1.60	5 (13%)
2	3X8	D	182	-	26,26,26	0.78	0	36,36,36	1.38	3 (8%)
2	3X8	G	182	-	26,26,26	0.45	0	36,36,36	1.28	2 (5%)
2	3X8	A	182	-	26,26,26	0.89	0	36,36,36	1.56	7 (19%)
2	3X8	H	182	-	26,26,26	0.60	1 (3%)	36,36,36	1.61	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3X8	F	182	-	-	1/10/30/30	0/3/3/3
2	3X8	B	182	-	-	2/10/30/30	0/3/3/3
2	3X8	E	182	-	-	1/10/30/30	0/3/3/3
2	3X8	C	182	-	-	1/10/30/30	0/3/3/3
2	3X8	D	182	-	-	0/10/30/30	0/3/3/3
2	3X8	G	182	-	-	0/10/30/30	0/3/3/3
2	3X8	A	182	-	-	1/10/30/30	0/3/3/3
2	3X8	H	182	-	-	1/10/30/30	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	182	3X8	O1-C1	2.67	1.45	1.41
2	H	182	3X8	O1-C1	2.51	1.45	1.41
2	B	182	3X8	O1-C1	2.27	1.44	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	182	3X8	CAA-O1-C1	7.82	129.26	117.79
2	F	182	3X8	CAA-O1-C1	6.70	127.61	117.79
2	B	182	3X8	CAA-O1-C1	6.62	127.50	117.79
2	A	182	3X8	CAA-O1-C1	5.47	125.81	117.79
2	G	182	3X8	CAA-O1-C1	5.46	125.80	117.79
2	D	182	3X8	CAA-O1-C1	5.25	125.48	117.79
2	E	182	3X8	CAA-O1-C1	5.09	125.25	117.79
2	C	182	3X8	CAA-O1-C1	4.77	124.78	117.79
2	B	182	3X8	C1-O5-C5	-4.00	105.84	113.69
2	C	182	3X8	C6-C5-C4	-3.87	103.94	113.00
2	F	182	3X8	O2-C2-C3	-3.58	102.07	110.35
2	B	182	3X8	C3-C4-C5	-3.41	104.16	110.24
2	A	182	3X8	C6-C5-C4	-3.32	105.22	113.00
2	F	182	3X8	C6-C5-C4	-3.17	105.59	113.00
2	A	182	3X8	O5-C5-C6	3.04	113.99	106.44
2	C	182	3X8	O3-C3-C2	2.95	117.16	110.35
2	C	182	3X8	O1-C1-C2	2.85	111.27	107.14
2	H	182	3X8	O5-C1-O1	2.84	115.50	108.29
2	C	182	3X8	O5-C5-C6	2.41	112.43	106.44
2	G	182	3X8	C2-C3-C4	-2.40	106.64	110.82
2	A	182	3X8	O5-C1-C2	2.36	115.35	110.35
2	A	182	3X8	O1-C1-C2	-2.36	103.72	107.14
2	D	182	3X8	C1-C2-C3	-2.35	105.10	110.00
2	F	182	3X8	O5-C5-C6	2.29	112.12	106.44
2	F	182	3X8	O4-C4-C5	-2.17	103.92	109.30
2	H	182	3X8	C6-C5-C4	-2.16	107.95	113.00
2	D	182	3X8	CAC-CAD-CAG	-2.11	117.71	121.36
2	E	182	3X8	C6-C5-C4	-2.07	108.15	113.00
2	A	182	3X8	O4-C4-C3	-2.05	105.62	110.35
2	E	182	3X8	C3-C4-C5	2.01	113.83	110.24
2	A	182	3X8	O3-C3-C2	2.00	114.98	110.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

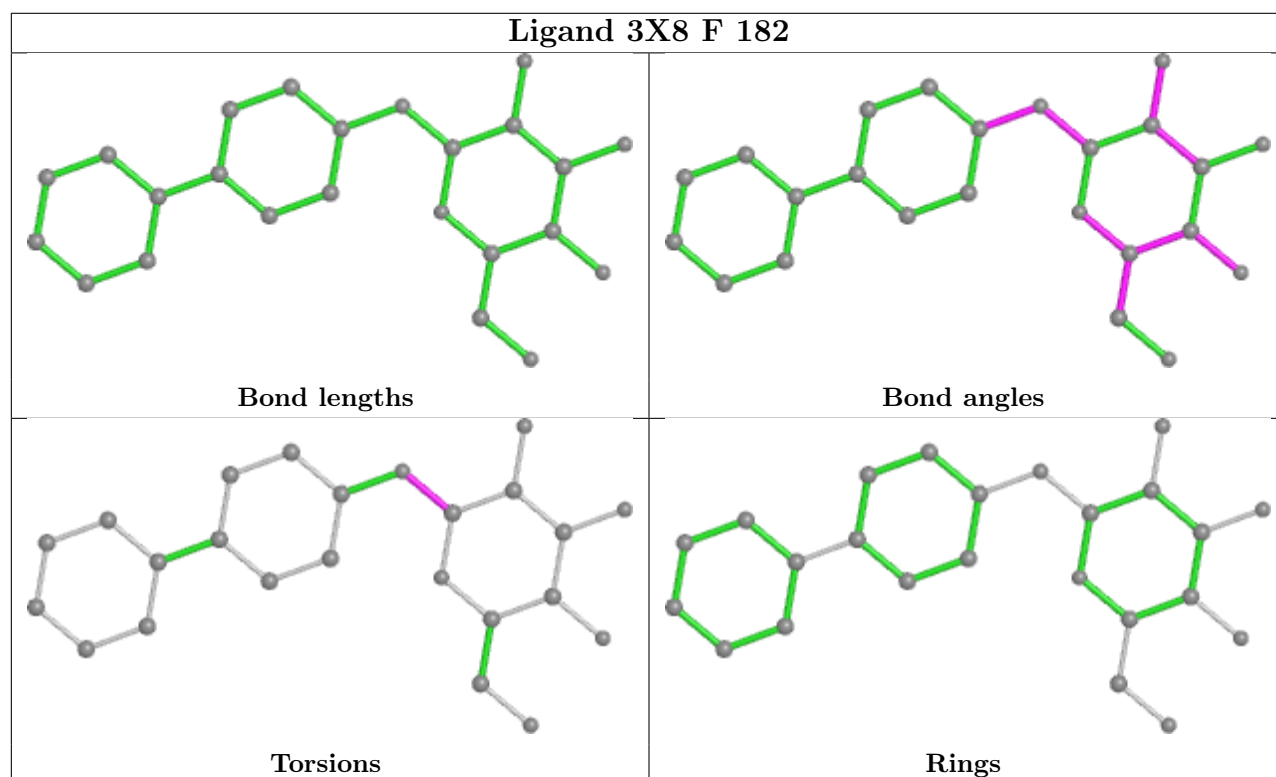
Mol	Chain	Res	Type	Atoms
2	H	182	3X8	O5-C1-O1-CAA
2	C	182	3X8	O5-C1-O1-CAA
2	F	182	3X8	O5-C1-O1-CAA
2	A	182	3X8	O5-C1-O1-CAA
2	E	182	3X8	O5-C1-O1-CAA
2	B	182	3X8	C4-C5-C6-O6
2	B	182	3X8	O5-C5-C6-O6

There are no ring outliers.

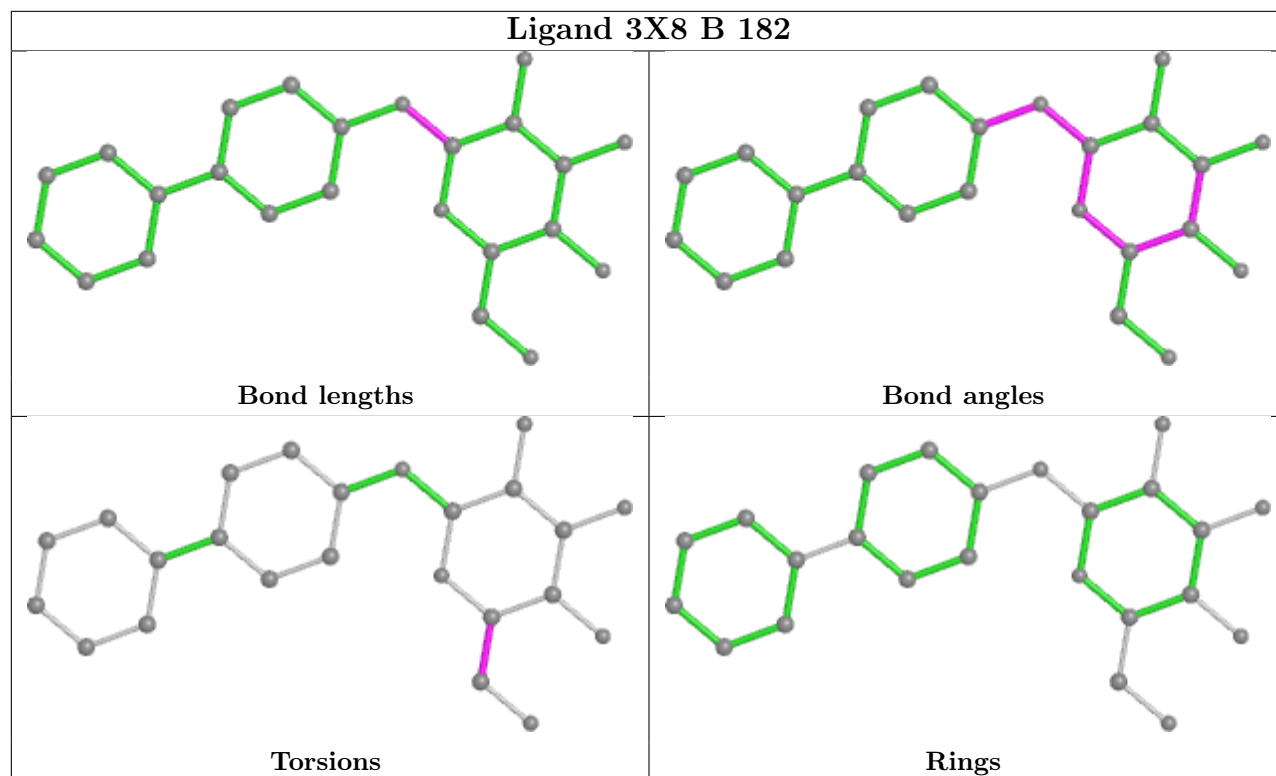
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	182	3X8	1	0
2	A	182	3X8	1	0

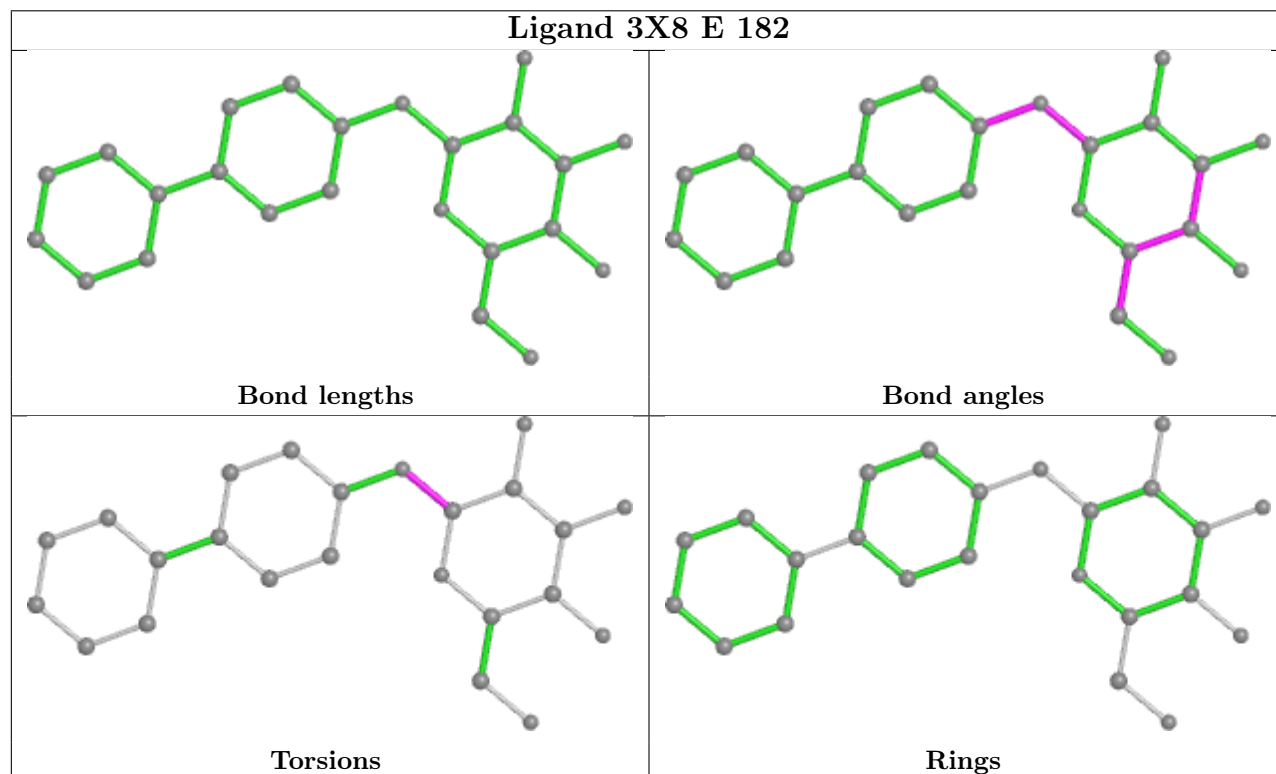
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



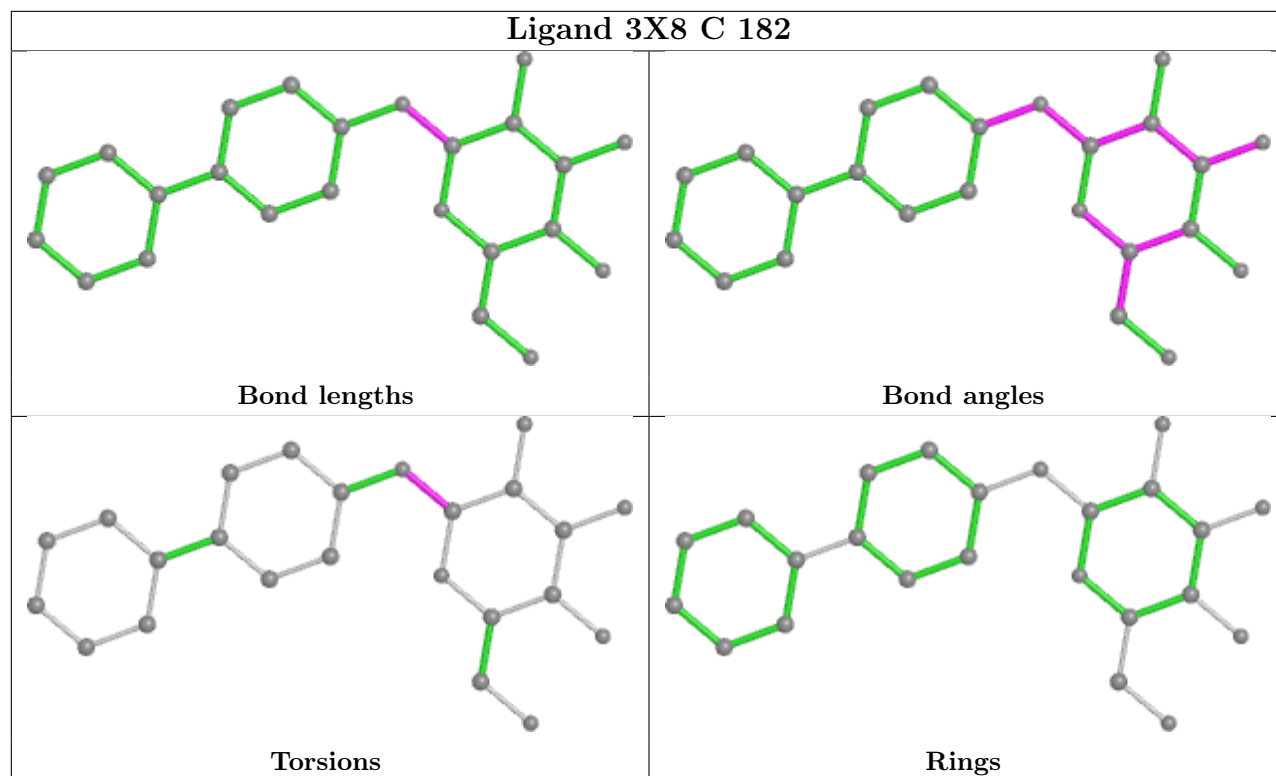
Ligand 3X8 B 182



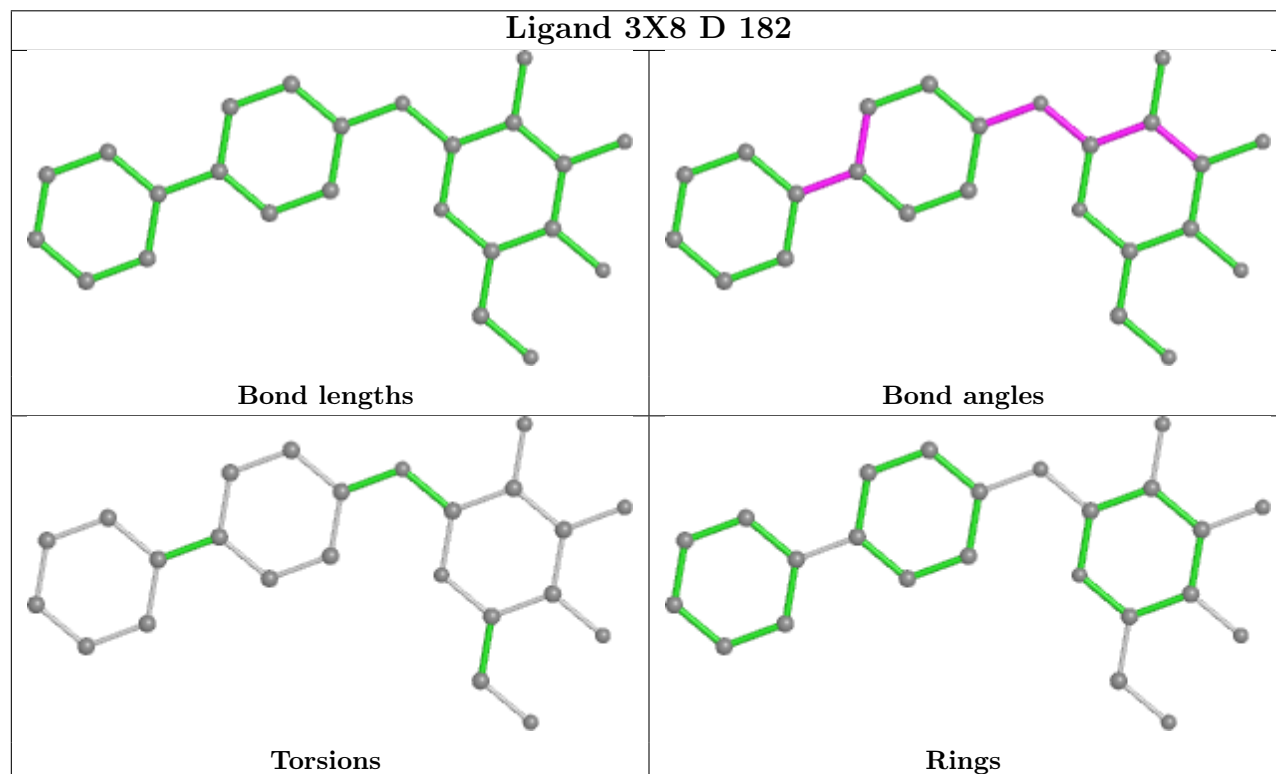
Ligand 3X8 E 182



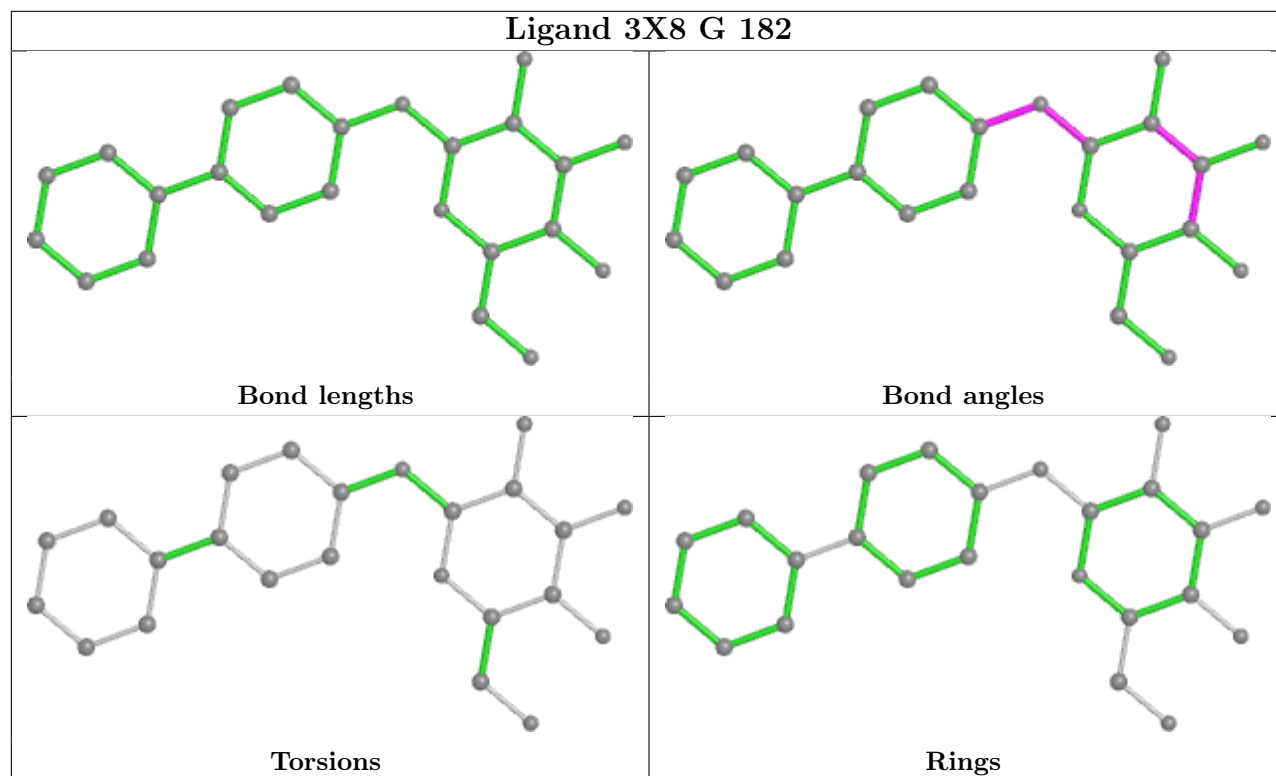
Ligand 3X8 C 182



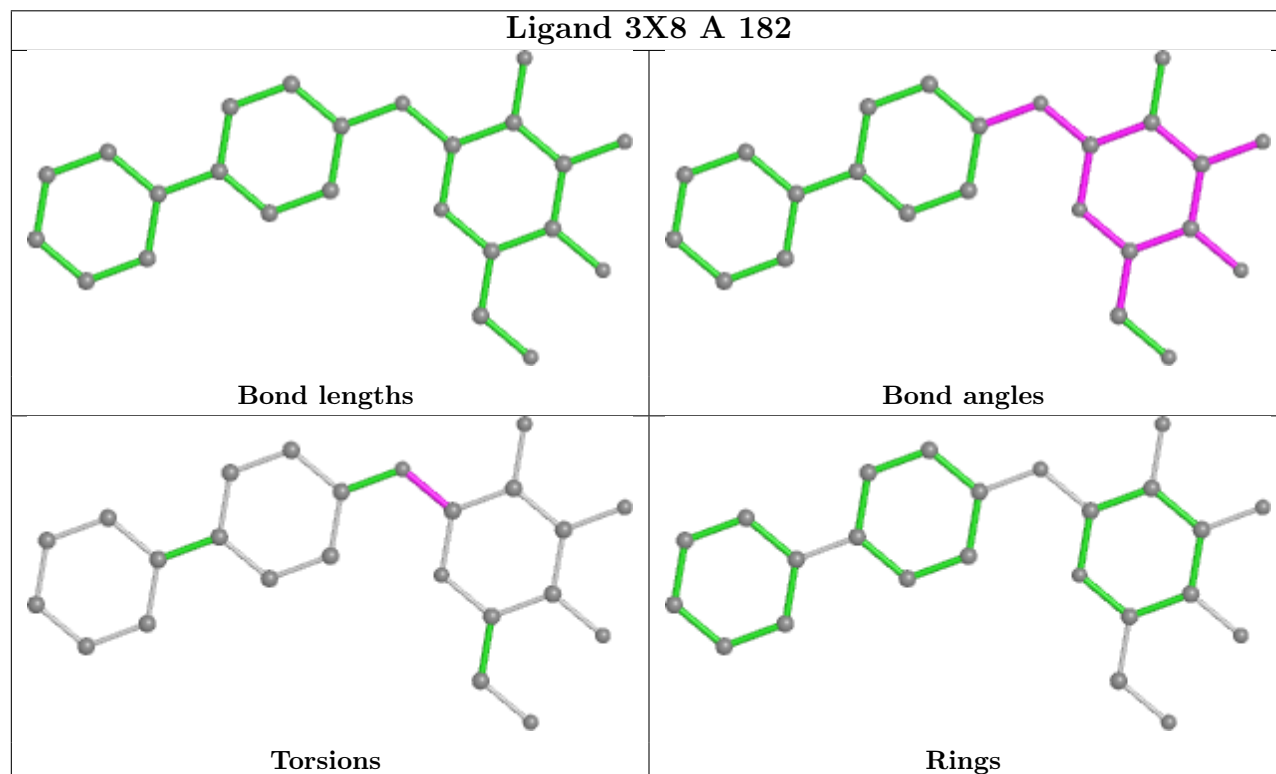
Ligand 3X8 D 182

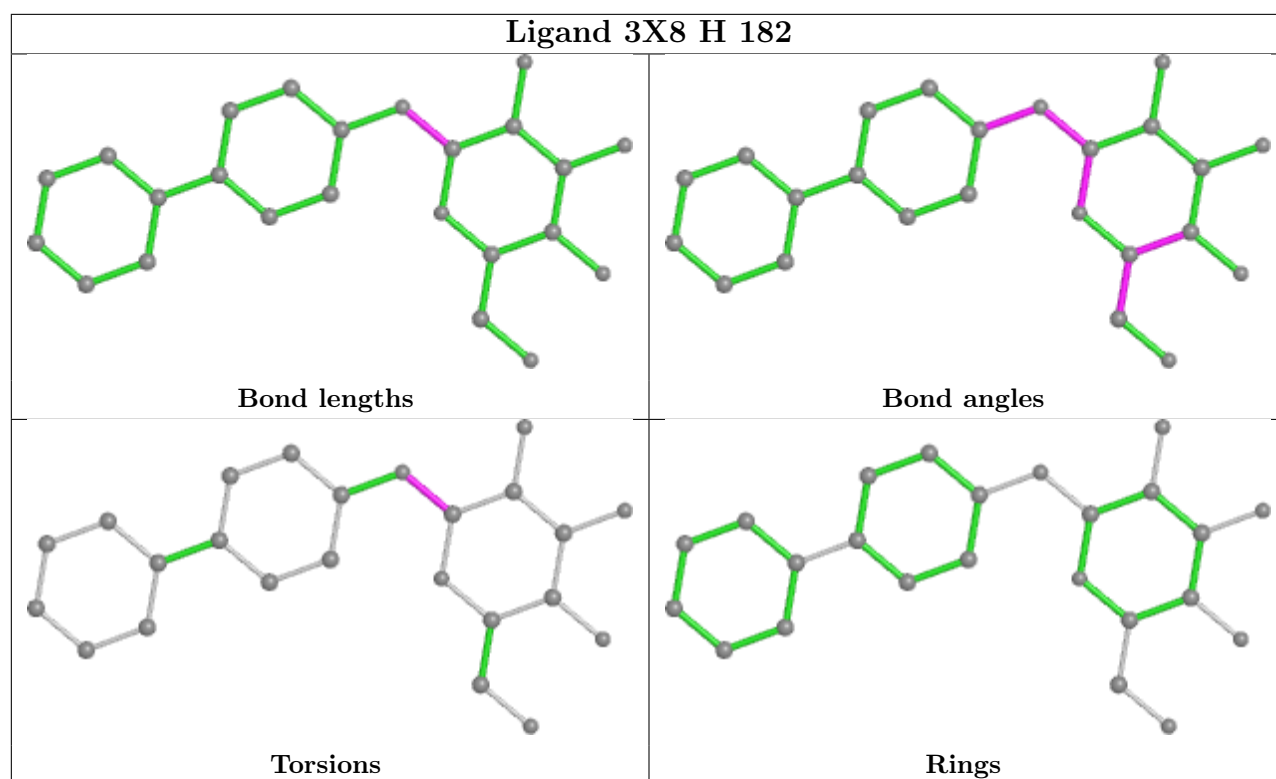


Ligand 3X8 G 182



Ligand 3X8 A 182





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	158/158 (100%)	0.52	4 (2%) 57 64	7, 21, 39, 46	0
1	B	158/158 (100%)	0.36	1 (0%) 89 91	8, 18, 34, 45	0
1	C	158/158 (100%)	0.41	1 (0%) 89 91	6, 18, 33, 40	0
1	D	158/158 (100%)	0.37	2 (1%) 77 81	6, 17, 30, 42	0
1	E	158/158 (100%)	1.12	27 (17%) 1 1	20, 36, 53, 69	0
1	F	158/158 (100%)	1.74	53 (33%) 0 0	26, 43, 64, 73	0
1	G	158/158 (100%)	1.70	54 (34%) 0 0	23, 44, 62, 75	0
1	H	158/158 (100%)	2.10	81 (51%) 0 0	28, 46, 73, 101	0
All	All	1264/1264 (100%)	1.04	223 (17%) 1 1	6, 31, 57, 101	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	79	GLY	9.0
1	H	67	VAL	6.7
1	F	125	LEU	6.6
1	G	112	VAL	6.5
1	H	65	GLY	6.4
1	F	12	PRO	6.1
1	G	158	THR	6.1
1	H	29	ASN	6.0
1	E	99	THR	5.8
1	F	5	THR	5.7
1	H	18	ALA	5.4
1	F	120	ILE	5.2
1	G	21	TYR	5.1
1	G	122	ALA	5.1
1	G	87	THR	4.9
1	G	115	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	85	PRO	4.8
1	H	100	ASP	4.8
1	H	125	LEU	4.7
1	G	125	LEU	4.7
1	F	20	VAL	4.6
1	F	134	THR	4.6
1	H	151	ASN	4.6
1	E	52	ILE	4.5
1	F	87	THR	4.4
1	H	102	PRO	4.4
1	H	115	ALA	4.3
1	G	6	ALA	4.2
1	H	25	ALA	4.2
1	E	137	TYR	4.2
1	F	141	ASP	4.1
1	G	137	TYR	4.1
1	F	22	VAL	4.0
1	H	82	TYR	4.0
1	E	95	TYR	4.0
1	G	154	VAL	4.0
1	H	34	LEU	3.9
1	A	113	SER	3.9
1	G	10	ALA	3.8
1	H	24	LEU	3.8
1	E	93[A]	VAL	3.8
1	D	115	ALA	3.8
1	F	133	GLN	3.8
1	H	139	SER	3.8
1	F	11	ILE	3.7
1	H	35	VAL	3.7
1	H	77[A]	TYR	3.7
1	H	99	THR	3.7
1	G	97	SER	3.7
1	H	6	ALA	3.6
1	F	154	VAL	3.6
1	H	33	ASN	3.6
1	F	21	TYR	3.6
1	A	115	ALA	3.5
1	H	64	TYR	3.5
1	F	112	VAL	3.4
1	H	8	GLY	3.4
1	F	139	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	3	CYS	3.4
1	E	21	TYR	3.4
1	F	9	THR	3.4
1	F	30	VAL	3.4
1	G	113	SER	3.3
1	F	137	TYR	3.3
1	F	8	GLY	3.3
1	F	152	ASN	3.3
1	F	146	TRP	3.3
1	H	20	VAL	3.3
1	F	79	GLY	3.3
1	H	126	ILE	3.2
1	H	28	VAL	3.2
1	G	53	THR	3.2
1	H	131	LEU	3.2
1	H	128	VAL	3.2
1	F	59	GLN	3.2
1	H	86	THR	3.2
1	H	135	ASN	3.1
1	F	10	ALA	3.1
1	F	18	ALA	3.1
1	F	83	PRO	3.0
1	F	158	THR	3.0
1	H	80	SER	3.0
1	F	23	ASN	3.0
1	H	103	TRP	3.0
1	H	61	GLY	3.0
1	H	39	SER	3.0
1	H	111	PRO	3.0
1	E	6	ALA	2.9
1	G	93	VAL	2.9
1	F	115	ALA	2.9
1	E	135	ASN	2.9
1	H	21	TYR	2.9
1	F	13	ILE	2.8
1	E	96	ASN	2.8
1	H	11	ILE	2.8
1	H	101	LYS	2.8
1	H	150	ALA	2.8
1	E	9	THR	2.8
1	C	115	ALA	2.8
1	G	130	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	51	THR	2.8
1	H	3	CYS	2.8
1	H	5	THR	2.8
1	G	16	GLY	2.8
1	G	65	GLY	2.8
1	E	97	SER	2.8
1	H	36	VAL	2.7
1	H	96	ASN	2.7
1	H	148	ILE	2.7
1	F	124	SER	2.7
1	G	124	SER	2.7
1	H	127	ALA	2.7
1	G	68	LEU	2.7
1	H	27	VAL	2.7
1	H	10	ALA	2.7
1	H	98	ARG	2.7
1	F	1	PHE	2.6
1	G	126	ILE	2.6
1	E	84	PHE	2.6
1	F	113	SER	2.6
1	F	55	TYR	2.6
1	H	70	ASN	2.6
1	F	106	ALA	2.6
1	H	114	SER	2.6
1	G	1	PHE	2.6
1	G	55	TYR	2.6
1	E	25	ALA	2.6
1	F	99	THR	2.6
1	G	144[A]	PHE	2.6
1	F	156	VAL	2.5
1	G	155	VAL	2.5
1	G	5	THR	2.5
1	G	73	GLY	2.5
1	F	111	PRO	2.5
1	G	131	LEU	2.5
1	E	114	SER	2.5
1	G	9	THR	2.5
1	H	32	GLN	2.5
1	H	119	ALA	2.5
1	H	7	ASN	2.5
1	H	14	GLY	2.5
1	H	31	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	12	PRO	2.5
1	H	46	ASN	2.5
1	G	123	GLY	2.5
1	G	108	TYR	2.4
1	E	158	THR	2.4
1	F	78	SER	2.4
1	F	42	ILE	2.4
1	A	114	SER	2.4
1	F	34	LEU	2.4
1	G	109	LEU	2.4
1	H	113	SER	2.4
1	F	19	ASN	2.4
1	H	149	TYR	2.4
1	H	132	ARG	2.4
1	H	118	VAL	2.4
1	F	103	TRP	2.4
1	H	51	THR	2.4
1	F	24	LEU	2.3
1	G	58	LEU	2.3
1	G	143[A]	GLN	2.3
1	H	116	GLY	2.3
1	G	136	ASN	2.3
1	H	4	LYS	2.3
1	G	149	TYR	2.3
1	G	33	ASN	2.3
1	F	6	ALA	2.3
1	G	157	PRO	2.3
1	B	79	GLY	2.3
1	F	109	LEU	2.3
1	H	122	ALA	2.3
1	G	51	THR	2.3
1	E	139	SER	2.3
1	E	50	GLU	2.3
1	F	144	PHE	2.2
1	G	27	VAL	2.2
1	H	42	ILE	2.2
1	E	115	ALA	2.2
1	G	95	TYR	2.2
1	G	140	ASP	2.2
1	E	75	VAL	2.2
1	H	93	VAL	2.2
1	F	121	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	57	THR	2.2
1	H	87	THR	2.2
1	H	9	THR	2.2
1	E	138	ASN	2.2
1	G	63	ALA	2.2
1	H	90	THR	2.2
1	E	12	PRO	2.2
1	G	120	ILE	2.1
1	E	35	VAL	2.1
1	H	66	GLY	2.1
1	H	97	SER	2.1
1	G	52	ILE	2.1
1	E	34	LEU	2.1
1	H	75	VAL	2.1
1	G	134	THR	2.1
1	H	110	THR	2.1
1	F	17	SER	2.1
1	E	94	VAL	2.1
1	G	26	PRO	2.1
1	H	1	PHE	2.1
1	H	49	PRO	2.1
1	A	29	ASN	2.1
1	G	135	ASN	2.1
1	H	134	THR	2.1
1	G	82	TYR	2.1
1	G	127	ALA	2.1
1	H	41	GLN	2.1
1	E	42	ILE	2.0
1	H	130	ILE	2.0
1	G	94	VAL	2.0
1	F	142	PHE	2.0
1	H	107	LEU	2.0
1	E	118	VAL	2.0
1	H	71	PHE	2.0
1	F	81	SER	2.0
1	G	99	THR	2.0
1	F	15	GLY	2.0
1	G	22	VAL	2.0
1	H	154	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

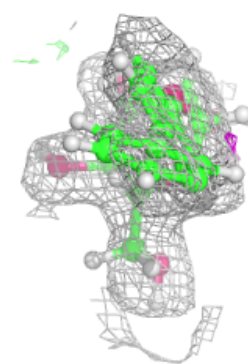
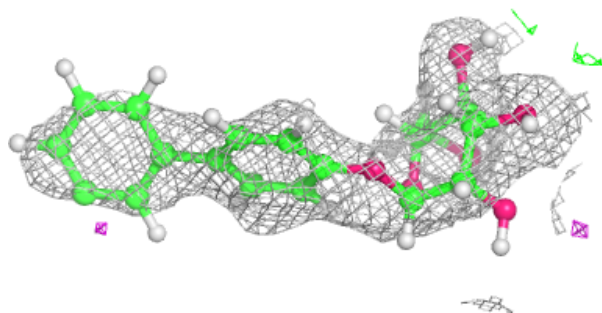
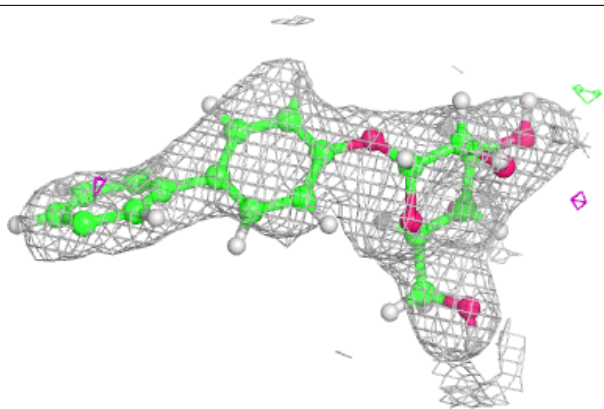
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	3X8	E	182	24/24	0.84	0.22	26,53,75,80	0
2	3X8	H	182	24/24	0.85	0.18	19,43,57,60	0
2	3X8	G	182	24/24	0.88	0.23	24,39,54,64	0
2	3X8	F	182	24/24	0.89	0.16	16,34,54,63	0
2	3X8	B	182	24/24	0.92	0.16	6,20,30,36	0
2	3X8	C	182	24/24	0.92	0.13	7,15,26,31	0
2	3X8	A	182	24/24	0.94	0.13	2,17,29,32	0
2	3X8	D	182	24/24	0.94	0.13	4,18,25,31	0

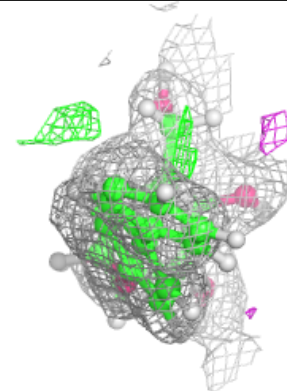
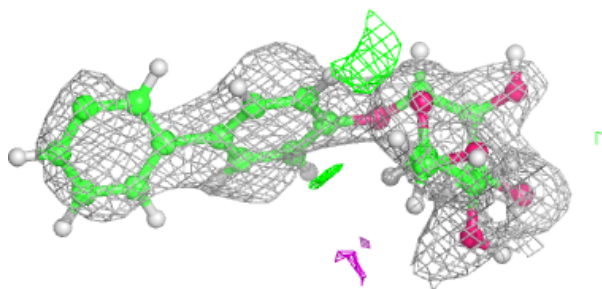
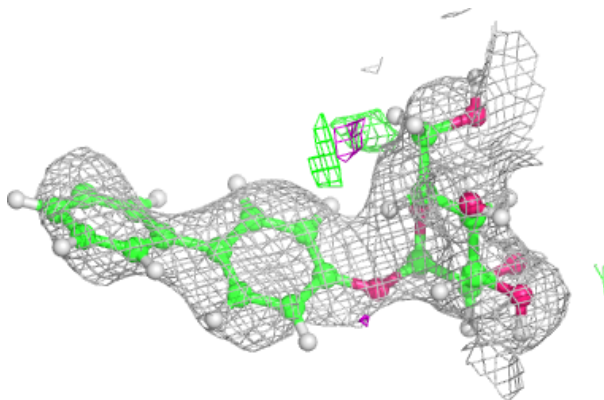
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3X8 E 182:

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

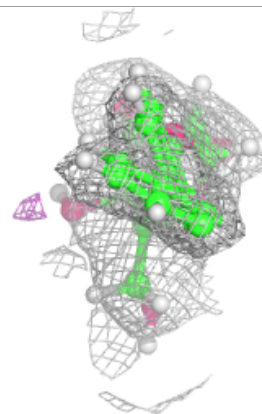
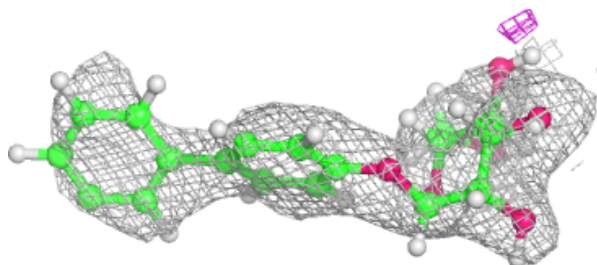
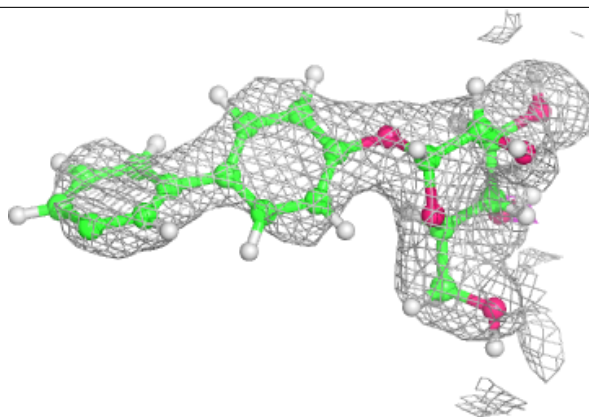
**Electron density around 3X8 H 182:**

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

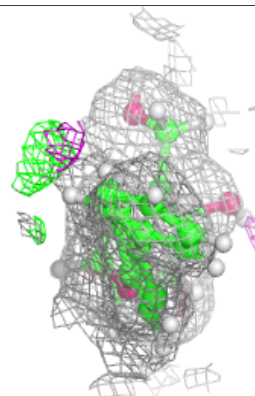
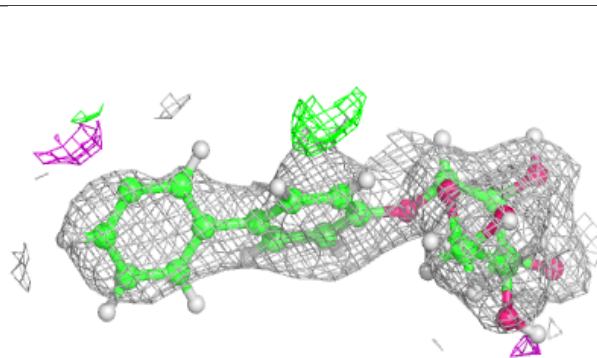
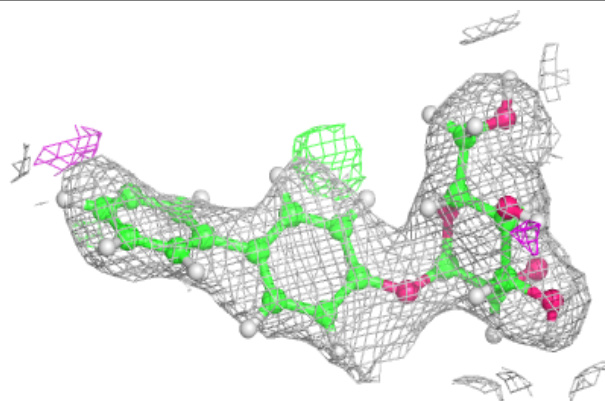


Electron density around 3X8 G 182:

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

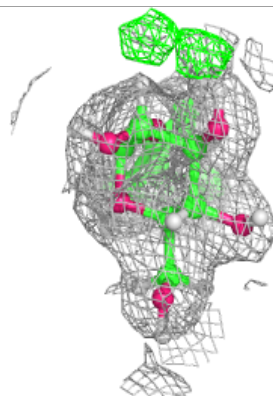
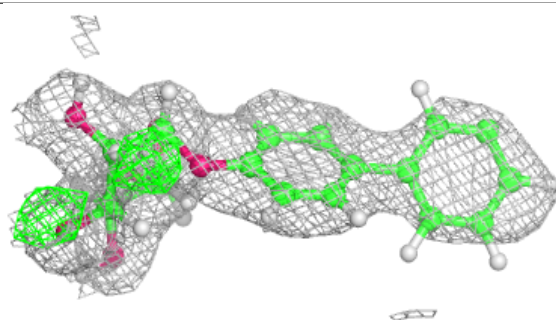
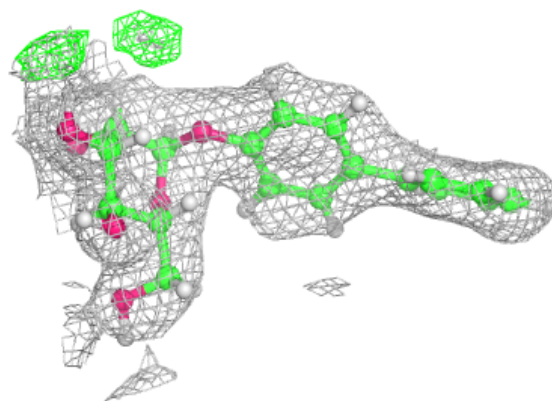
**Electron density around 3X8 F 182:**

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

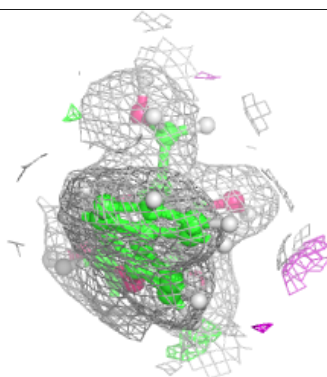
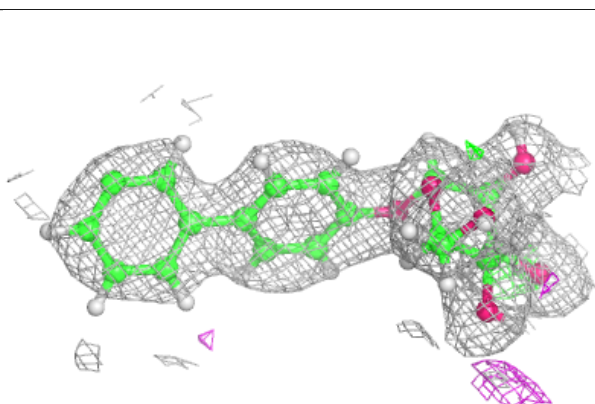
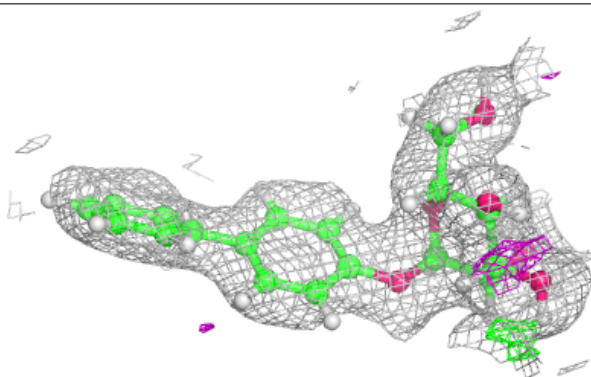


Electron density around 3X8 B 182:

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

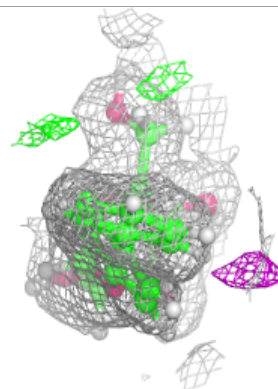
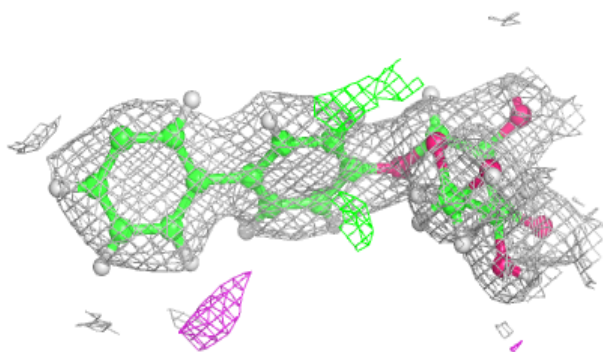
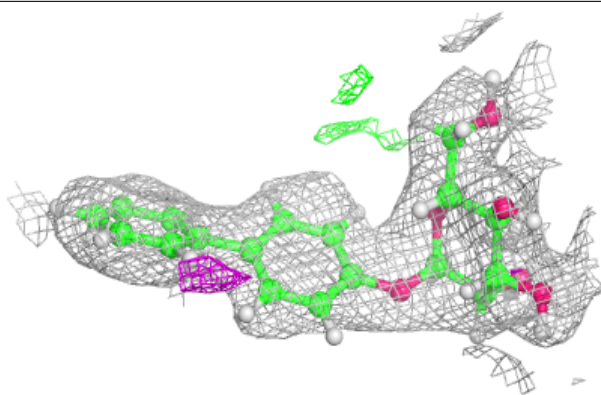
**Electron density around 3X8 C 182:**

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

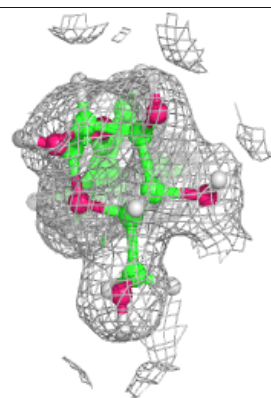
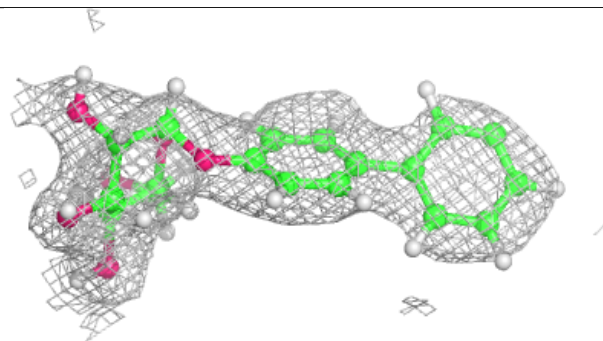
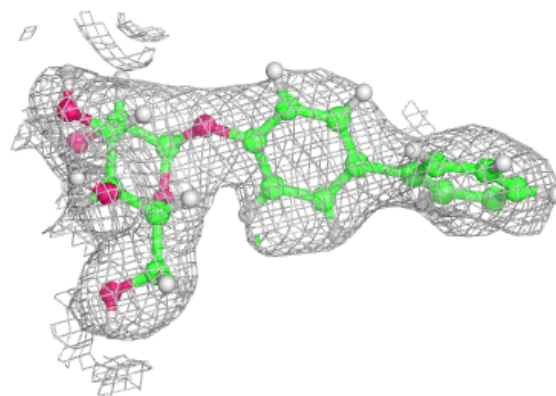


Electron density around 3X8 A 182:

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

**Electron density around 3X8 D 182:**

$2mF_o-DF_c$ (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.