



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:41 PM BST

PDB ID : 6SJU
Title : Human kallikrein 7 with aromatic coumarinic ester compound 3 covalently bound to H57
Authors : Hanke, S.; Straeter, N.
Deposited on : 2019-08-13
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

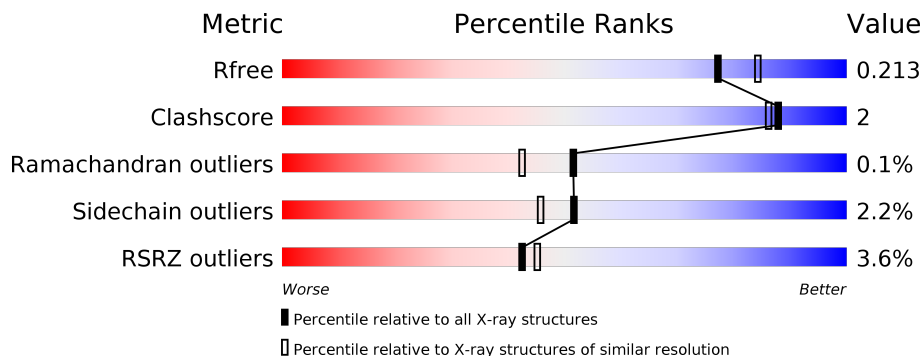
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	224	 2% 94% 6%
1	B	224	 2% 99%
1	C	224	 2% 94% 6%
1	D	224	 2% 92% 7%
1	E	224	 96%
1	F	224	 3% 94% 5%

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Mol	Chain	Length	Quality of chain
1	G	224	
1	H	224	

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	PGE	A	302	-	-	X	-
3	SO4	D	312	-	-	X	X
3	SO4	G	307	-	-	-	X
4	LFW	A	350[A]	-	-	-	X
4	LFW	A	350[B]	-	-	-	X
4	LFW	G	350[A]	-	-	-	X
4	LFW	G	350[B]	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15943 atoms, of which 101 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 Kallikrein-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	Total 1724	C 1074	N 312	O 320	S 18	0	4	0
1	B	224	Total 1699	C 1059	N 303	O 319	S 18	0	4	0
1	C	224	Total 1701	C 1057	N 308	O 318	S 18	0	2	0
1	D	224	Total 1709	C 1064	N 309	O 318	S 18	0	2	0
1	E	224	Total 1701	C 1062	N 304	O 317	S 18	0	3	0
1	F	224	Total 1696	C 1057	N 305	O 316	S 18	0	2	0
1	G	224	Total 1702	C 1059	N 309	O 316	S 18	0	1	0
1	H	224	Total 1697	C 1054	N 307	O 318	S 18	0	1	0

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	24	6	14	4	0	0
2	A	1	24	6	14	4	0	0
2	B	1	24	6	14	4	0	0
2	D	1	24	6	14	4	0	0
2	E	1	24	6	14	4	0	0
2	F	1	24	6	14	4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	C	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0
3	E	1	5	4	1	0	0

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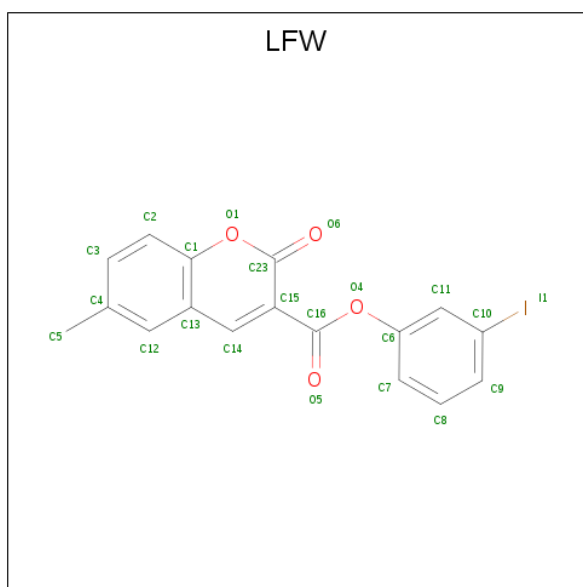
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	E	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0

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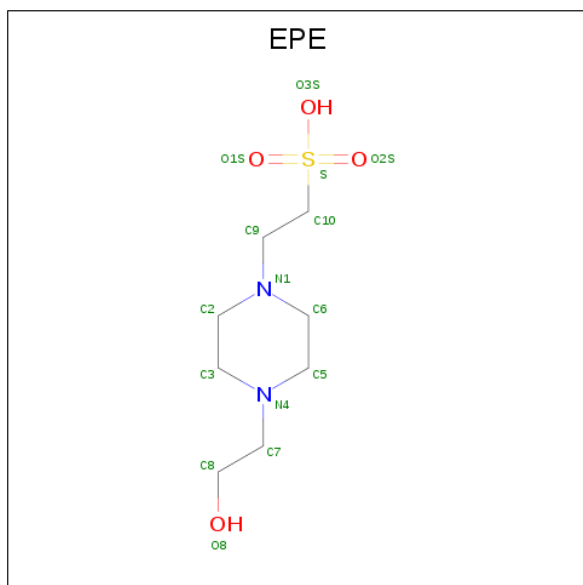
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (3-iodanylphenyl) 6-methyl-2-oxidanylidene-chromene-3-carboxylate (three-letter code: LFW) (formula: C₁₇H₁₁IO₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			30	22	8		
4	B	1	Total	C	O	0	1
			30	22	8		
4	C	1	Total	C	O	0	1
			30	22	8		
4	D	1	Total	C	O	0	1
			30	22	8		
4	E	1	Total	C	O	0	1
			30	22	8		
4	F	1	Total	C	O	0	1
			30	22	8		
4	G	1	Total	C	O	0	1
			30	22	8		
4	H	1	Total	C	O	0	1
			30	22	8		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	H	1	Total	C	N	O	S	0	0	
			15	8	2	4	1			
5	H	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

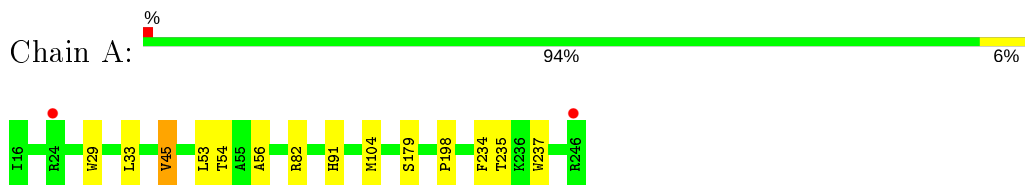
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	198	Total	O	0	0
			198	198		
6	B	177	Total	O	0	1
			177	177		
6	C	206	Total	O	0	1
			206	206		
6	D	190	Total	O	0	0
			190	190		
6	E	195	Total	O	0	1
			195	195		
6	F	207	Total	O	0	0
			207	207		
6	G	137	Total	O	0	0
			137	137		
6	H	123	Total	O	0	0
			123	123		

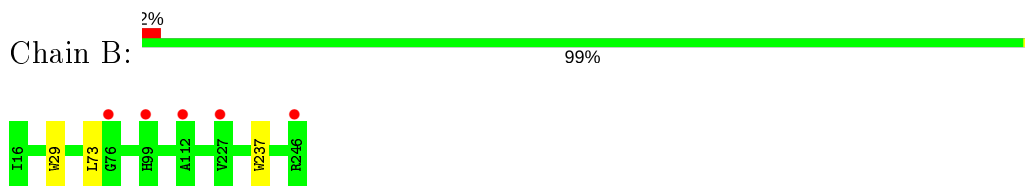
3 Residue-property plots [i](#)

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.

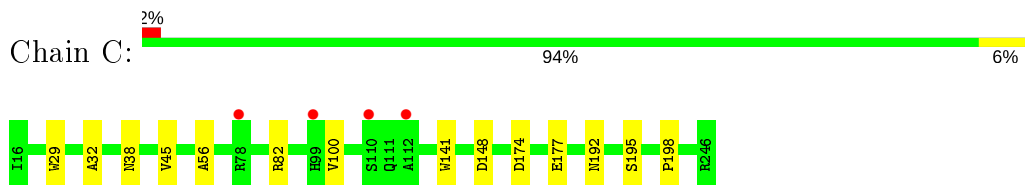
- Molecule 1: Kallikrein-7



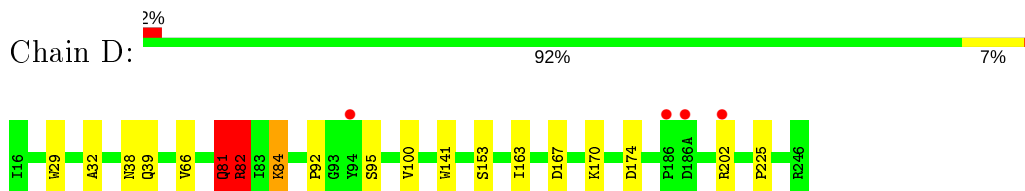
- Molecule 1: Kallikrein-7



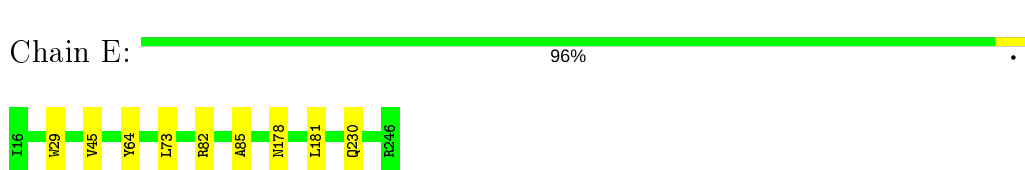
- Molecule 1: Kallikrein-7



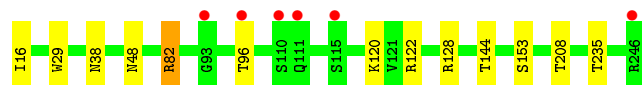
- Molecule 1: Kallikrein-7



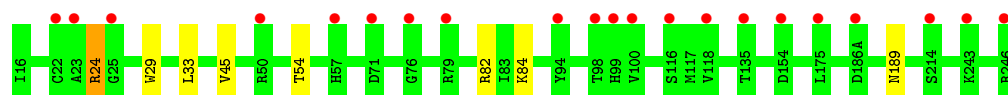
- Molecule 1: Kallikrein-7



- Molecule 1: Kallikrein-7



- Molecule 1: Kallikrein-7



- Molecule 1: Kallikrein-7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.65Å 116.95Å 291.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.08 – 1.97 47.08 – 1.97	Depositor EDS
% Data completeness (in resolution range)	78.4 (47.08-1.97) 78.4 (47.08-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.97Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.221 0.172 , 0.213	Depositor DCC
R_{free} test set	1719 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtrriage
Anisotropy	0.464	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15943	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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: EPE, LFW, PGE, SO4

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	0.73	0/1772	0.76	2/2406 (0.1%)
1	B	0.69	0/1744	0.70	0/2371
1	C	0.70	0/1740	0.69	0/2365
1	D	0.69	0/1751	0.76	2/2379 (0.1%)
1	E	0.71	0/1743	0.71	0/2371
1	F	0.71	0/1738	0.71	0/2364
1	G	0.59	0/1741	0.66	0/2365
1	H	0.64	0/1736	0.68	0/2361
All	All	0.68	0/13965	0.71	4/18982 (0.0%)

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	C	0	2
1	D	0	1
1	H	0	2
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	GLN	O-C-N	-12.43	102.82	122.70
1	A	235[A]	THR	CA-C-O	6.35	133.43	120.10
1	A	235[B]	THR	CA-C-O	6.35	133.43	120.10
1	D	81	GLN	CA-C-N	5.58	129.48	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	56	ALA	Mainchain
1	D	81	GLN	Mainchain
1	H	56	ALA	Mainchain

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	1724	0	1710	12	0
1	B	1699	0	1659	1	0
1	C	1701	0	1661	7	0
1	D	1709	0	1683	14	0
1	E	1701	0	1667	4	0
1	F	1696	0	1659	5	0
1	G	1702	0	1672	3	0
1	H	1697	0	1652	10	0
2	A	20	28	28	8	0
2	B	10	14	14	1	0
2	D	10	14	14	0	0
2	E	10	14	14	0	0
2	F	10	14	14	0	0
3	A	45	0	0	0	0
3	B	60	0	0	0	0
3	C	75	0	0	1	0
3	D	60	0	0	5	0
3	E	45	0	0	0	0
3	F	55	0	0	0	0
3	G	50	0	0	0	0
3	H	60	0	0	0	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
4	C	30	0	0	1	0
4	D	30	0	0	0	0
4	E	30	0	0	0	0
4	F	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	30	0	0	0	0
4	H	30	0	0	0	0
5	H	30	17	34	6	0
6	A	198	0	0	1	0
6	B	177	0	0	0	0
6	C	206	0	0	0	0
6	D	190	0	0	0	0
6	E	195	0	0	1	0
6	F	207	0	0	0	0
6	G	137	0	0	0	0
6	H	123	0	0	1	0
All	All	15842	101	13481	56	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 2.

All (56) 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:D:38:ASN:OD1	1:D:82:ARG:NH2	1.93	1.01
1:D:81:GLN:HA	3:D:312:SO4:O2	1.63	0.98
6:A:410:HOH:O	1:H:39:GLN:HG2	1.67	0.94
1:D:81:GLN:CA	3:D:312:SO4:O2	2.18	0.90
1:A:234:PHE:HA	2:A:302:PGE:H22	1.57	0.85
1:D:81:GLN:C	3:D:312:SO4:O2	2.19	0.82
1:F:38:ASN:OD1	1:F:82:ARG:NH2	2.13	0.82
1:H:91:HIS:HE2	5:H:302:EPE:C3	2.02	0.71
1:D:82:ARG:N	3:D:312:SO4:O2	2.23	0.71
1:D:66:VAL:O	1:D:82:ARG:HA	1.92	0.68
1:A:237:TRP:HB2	2:A:302:PGE:H3	1.77	0.64
1:C:192:ASN:HB3	4:C:350[A]:LFW:O4	1.98	0.64
1:H:91:HIS:HE2	5:H:302:EPE:C2	2.12	0.62
1:B:237:TRP:HB2	2:B:301:PGE:H5	1.84	0.59
1:A:237:TRP:H	2:A:302:PGE:H2	1.66	0.59
1:G:24:ARG:H	1:G:24:ARG:HE	1.49	0.59
1:H:91:HIS:HE2	5:H:302:EPE:H22	1.68	0.58
1:H:237:TRP:HB2	5:H:302:EPE:H31	1.87	0.56
1:A:91:HIS:HE2	2:A:302:PGE:H42	1.72	0.55
1:D:167:ASP:HA	1:D:170:LYS:HD3	1.90	0.54
1:H:233:LYS:HD2	6:H:401:HOH:O	2.08	0.53
1:C:45:VAL:HG11	1:C:198:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:VAL:HG23	1:C:177:GLU:HG3	1.94	0.49
1:C:45:VAL:CG1	1:C:198:PRO:HB3	2.43	0.49
1:D:82:ARG:CD	1:F:128:ARG:HG2	2.43	0.49
1:A:45[A]:VAL:HG11	1:A:198:PRO:HB3	1.96	0.48
1:A:237:TRP:HB2	2:A:302:PGE:C3	2.44	0.48
1:C:38:ASN:OD1	1:C:82:ARG:NH2	2.48	0.47
1:A:45[A]:VAL:HG23	1:A:53:LEU:HB3	1.97	0.47
3:C:314:SO4:O3	3:C:315:SO4:O1	2.32	0.47
1:C:100:VAL:CG2	1:C:177:GLU:HG3	2.45	0.47
1:D:81:GLN:HA	3:D:312:SO4:S	2.52	0.46
1:H:32:ALA:HB2	1:H:141:TRP:CZ3	2.49	0.46
1:H:91:HIS:NE2	5:H:302:EPE:H22	2.31	0.46
1:H:237:TRP:HB2	5:H:302:EPE:C3	2.45	0.46
1:G:33:LEU:HD11	1:G:54:THR:HG21	1.98	0.46
1:E:82:ARG:HD3	6:E:469:HOH:O	2.16	0.45
1:A:45[A]:VAL:CG1	1:A:198:PRO:HB3	2.47	0.45
1:C:32:ALA:HB2	1:C:141:TRP:CZ3	2.50	0.45
1:E:181:LEU:HD22	1:E:230:GLN:HG3	1.99	0.45
1:A:56:ALA:HA	1:A:104:MET:HB2	1.99	0.45
1:D:84:LYS:HE2	1:D:84:LYS:HB3	1.38	0.44
1:E:73:LEU:HD23	1:E:73:LEU:HA	1.80	0.44
1:E:64:TYR:HB2	1:E:85:ALA:HB3	2.01	0.43
1:D:95:SER:HB3	1:D:100:VAL:HG12	2.01	0.42
1:D:32:ALA:HB2	1:D:141:TRP:CZ3	2.55	0.42
2:A:302:PGE:H4	1:D:92:PRO:O	2.20	0.41
1:D:163:ILE:HD12	1:D:225:PRO:HB3	2.02	0.41
1:F:122:ARG:HD2	1:F:208:THR:HG22	2.02	0.41
1:F:48:ASN:HA	1:F:120:LYS:HG2	2.02	0.41
1:A:91:HIS:NE2	2:A:302:PGE:H42	2.35	0.41
1:A:91:HIS:HE2	2:A:302:PGE:C4	2.33	0.41
1:H:103:LEU:HD21	1:H:234:PHE:CD1	2.55	0.41
1:F:16:ILE:O	1:F:144:THR:HA	2.21	0.40
1:G:24:ARG:H	1:G:24:ARG:NE	2.18	0.40
1:A:33:LEU:HD11	1:A:54:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/224 (101%)	223 (99%)	3 (1%)	0	100	100
1	B	225/224 (100%)	222 (99%)	3 (1%)	0	100	100
1	C	223/224 (100%)	220 (99%)	3 (1%)	0	100	100
1	D	224/224 (100%)	220 (98%)	3 (1%)	1 (0%)	34	22
1	E	225/224 (100%)	221 (98%)	4 (2%)	0	100	100
1	F	224/224 (100%)	221 (99%)	3 (1%)	0	100	100
1	G	223/224 (100%)	220 (99%)	3 (1%)	0	100	100
1	H	223/224 (100%)	218 (98%)	5 (2%)	0	100	100
All	All	1793/1792 (100%)	1765 (98%)	27 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	82	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/194 (102%)	192 (98%)	5 (2%)	47	39
1	B	192/194 (99%)	190 (99%)	2 (1%)	76	73
1	C	192/194 (99%)	188 (98%)	4 (2%)	53	47
1	D	194/194 (100%)	187 (96%)	7 (4%)	35	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	192/194 (99%)	188 (98%)	4 (2%)	53	47
1	F	191/194 (98%)	186 (97%)	5 (3%)	46	37
1	G	192/194 (99%)	186 (97%)	6 (3%)	40	28
1	H	191/194 (98%)	189 (99%)	2 (1%)	76	73
All	All	1541/1552 (99%)	1506 (98%)	35 (2%)	52	44

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	TRP
1	A	45[A]	VAL
1	A	45[B]	VAL
1	A	82	ARG
1	A	179	SER
1	B	29	TRP
1	B	73	LEU
1	C	29	TRP
1	C	148	ASP
1	C	174	ASP
1	C	195	SER
1	D	29	TRP
1	D	39	GLN
1	D	82	ARG
1	D	84	LYS
1	D	153	SER
1	D	174	ASP
1	D	202	ARG
1	E	29	TRP
1	E	45[A]	VAL
1	E	45[B]	VAL
1	E	178	ASN
1	F	29	TRP
1	F	82	ARG
1	F	96	THR
1	F	153	SER
1	F	235	THR
1	G	24	ARG
1	G	29	TRP
1	G	45	VAL
1	G	82	ARG
1	G	84	LYS

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Mol	Chain	Res	Type
1	G	189	ASN
1	H	29	TRP
1	H	189	ASN

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

Mol	Chain	Res	Type
1	H	39	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](#)

114 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	$\# Z > 2$
4	LFW	D	314[A]	1	9,16,24	0.99	0	9,23,34	0.49	0
3	SO4	B	307	-	4,4,4	0.20	0	6,6,6	0.16	0
4	LFW	H	350[B]	1	9,16,24	0.91	0	9,23,34	0.47	0
3	SO4	B	302	-	4,4,4	0.58	0	6,6,6	0.18	0
3	SO4	F	307	-	4,4,4	0.26	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	314	-	4,4,4	0.23	0	6,6,6	0.39	0
3	SO4	C	303	-	4,4,4	0.17	0	6,6,6	0.44	0
3	SO4	F	303	-	4,4,4	0.30	0	6,6,6	0.20	0
3	SO4	A	311	-	4,4,4	0.16	0	6,6,6	0.35	0
3	SO4	C	312	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	D	311	-	4,4,4	0.26	0	6,6,6	0.30	0
3	SO4	E	304	-	4,4,4	0.48	0	6,6,6	0.21	0
3	SO4	F	311	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	C	309	-	4,4,4	0.30	0	6,6,6	0.15	0
3	SO4	D	312	-	4,4,4	0.31	0	6,6,6	0.67	0
3	SO4	F	308	-	4,4,4	0.22	0	6,6,6	0.35	0
4	LFW	C	350[B]	1	9,16,24	0.85	0	9,23,34	0.49	0
3	SO4	G	310	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	B	308	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	C	308	-	4,4,4	0.26	0	6,6,6	0.24	0
3	SO4	E	305	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	B	312	-	4,4,4	0.18	0	6,6,6	0.07	0
3	SO4	F	310	-	4,4,4	0.35	0	6,6,6	0.39	0
3	SO4	A	308	-	4,4,4	0.47	0	6,6,6	0.34	0
3	SO4	G	303	-	4,4,4	0.16	0	6,6,6	0.24	0
3	SO4	A	304	-	4,4,4	0.32	0	6,6,6	0.26	0
3	SO4	C	311	-	4,4,4	0.58	0	6,6,6	0.23	0
4	LFW	A	350[B]	1	9,16,24	1.26	1 (11%)	9,23,34	0.44	0
3	SO4	G	305	-	4,4,4	0.30	0	6,6,6	0.42	0
5	EPE	H	302	-	15,15,15	1.01	1 (6%)	18,20,20	0.63	0
3	SO4	C	313	-	4,4,4	0.05	0	6,6,6	0.33	0
3	SO4	A	307	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	H	314	-	4,4,4	0.11	0	6,6,6	0.16	0
3	SO4	D	305	-	4,4,4	0.40	0	6,6,6	0.18	0
2	PGE	F	301	-	9,9,9	0.31	0	8,8,8	0.23	0
3	SO4	H	313	-	4,4,4	0.18	0	6,6,6	0.10	0
2	PGE	D	301	-	9,9,9	0.33	0	8,8,8	0.20	0
4	LFW	G	350[A]	1	9,16,24	0.99	0	9,23,34	0.49	0
3	SO4	C	315	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	F	306	-	4,4,4	0.30	0	6,6,6	0.67	0
3	SO4	B	310	-	4,4,4	0.13	0	6,6,6	0.15	0
3	SO4	D	308	-	4,4,4	0.51	0	6,6,6	0.73	0
4	LFW	G	350[B]	1	9,16,24	1.21	1 (11%)	9,23,34	0.42	0
3	SO4	G	307	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	E	302	-	4,4,4	0.44	0	6,6,6	0.25	0
3	SO4	C	305	-	4,4,4	0.48	0	6,6,6	0.52	0
3	SO4	B	306	-	4,4,4	0.26	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	H	308	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	C	310	-	4,4,4	0.32	0	6,6,6	0.24	0
3	SO4	B	309	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	B	305	-	4,4,4	0.49	0	6,6,6	0.28	0
3	SO4	D	302	-	4,4,4	0.40	0	6,6,6	0.45	0
3	SO4	D	306	-	4,4,4	0.73	0	6,6,6	0.82	0
3	SO4	G	304	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	B	303	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	D	307	-	4,4,4	0.49	0	6,6,6	0.60	0
2	PGE	A	301	-	9,9,9	0.29	0	8,8,8	0.32	0
2	PGE	B	301	-	9,9,9	0.75	0	8,8,8	0.69	0
4	LFW	H	350[A]	1	9,16,24	0.79	0	9,23,34	0.46	0
3	SO4	D	310	-	4,4,4	0.33	0	6,6,6	0.47	0
3	SO4	A	306	-	4,4,4	0.37	0	6,6,6	0.53	0
3	SO4	A	305	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SO4	F	305	-	4,4,4	0.35	0	6,6,6	0.54	0
4	LFW	C	350[A]	1	9,16,24	0.80	0	9,23,34	0.49	0
3	SO4	H	311	-	4,4,4	0.13	0	6,6,6	0.16	0
3	SO4	F	309	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	B	313	-	4,4,4	0.31	0	6,6,6	0.85	0
3	SO4	F	312	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	G	309	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	C	304	-	4,4,4	0.48	0	6,6,6	0.63	0
3	SO4	C	307	-	4,4,4	0.14	0	6,6,6	0.15	0
3	SO4	E	307	-	4,4,4	0.18	0	6,6,6	0.13	0
3	SO4	H	307	-	4,4,4	0.16	0	6,6,6	0.06	0
2	PGE	A	302	-	9,9,9	0.34	0	8,8,8	0.47	0
3	SO4	G	301	-	4,4,4	0.31	0	6,6,6	0.38	0
3	SO4	H	304	-	4,4,4	0.19	0	6,6,6	0.18	0
3	SO4	C	301	-	4,4,4	0.45	0	6,6,6	0.29	0
3	SO4	D	309	-	4,4,4	0.18	0	6,6,6	0.95	0
3	SO4	E	309	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	A	310	-	4,4,4	0.13	0	6,6,6	0.30	0
3	SO4	D	304	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	E	306	-	4,4,4	0.28	0	6,6,6	0.17	0
2	PGE	E	301	-	9,9,9	0.34	0	8,8,8	0.50	0
4	LFW	A	350[A]	1	9,16,24	1.09	0	9,23,34	0.46	0
4	LFW	E	350[B]	1	9,16,24	0.91	0	9,23,34	0.48	0
3	SO4	H	312	-	4,4,4	0.16	0	6,6,6	0.08	0
4	LFW	E	350[A]	1	9,16,24	0.83	0	9,23,34	0.50	0
4	LFW	B	314[A]	1	9,16,24	0.92	0	9,23,34	0.46	0
3	SO4	A	309	-	4,4,4	0.26	0	6,6,6	0.29	0
4	LFW	B	314[B]	1	9,16,24	1.15	1 (11%)	9,23,34	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	304	-	4,4,4	0.42	0	6,6,6	0.90	0
3	SO4	E	308	-	4,4,4	0.29	0	6,6,6	0.77	0
3	SO4	H	303	-	4,4,4	0.37	0	6,6,6	0.42	0
3	SO4	C	306	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	E	303	-	4,4,4	0.20	0	6,6,6	0.31	0
3	SO4	H	309	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	G	308	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	303	-	4,4,4	0.49	0	6,6,6	0.24	0
3	SO4	H	305	-	4,4,4	0.32	0	6,6,6	0.63	0
3	SO4	B	304	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	C	302	-	4,4,4	0.37	0	6,6,6	0.22	0
3	SO4	D	313	-	4,4,4	0.18	0	6,6,6	0.10	0
4	LFW	F	350[B]	1	9,16,24	1.13	1 (11%)	9,23,34	0.47	0
3	SO4	G	302	-	4,4,4	0.15	0	6,6,6	0.22	0
3	SO4	B	311	-	4,4,4	0.16	0	6,6,6	0.16	0
4	LFW	D	314[B]	1	9,16,24	1.12	0	9,23,34	0.46	0
3	SO4	H	306	-	4,4,4	0.14	0	6,6,6	0.23	0
3	SO4	D	303	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	G	306	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	H	310	-	4,4,4	0.14	0	6,6,6	0.14	0
4	LFW	F	350[A]	1	9,16,24	1.07	0	9,23,34	0.48	0
3	SO4	F	302	-	4,4,4	0.32	0	6,6,6	0.32	0
3	SO4	E	310	-	4,4,4	0.21	0	6,6,6	0.61	0
5	EPE	H	301	-	15,15,15	0.80	1 (6%)	18,20,20	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LFW	D	314[A]	1	-	0/0/4/8	0/2/2/3
2	PGE	A	301	-	-	3/7/7/7	-
2	PGE	B	301	-	-	3/7/7/7	-
4	LFW	A	350[B]	1	-	0/0/4/8	0/2/2/3
2	PGE	E	301	-	-	4/7/7/7	-
4	LFW	A	350[A]	1	-	0/0/4/8	0/2/2/3
4	LFW	E	350[B]	1	-	0/0/4/8	0/2/2/3
4	LFW	H	350[B]	1	-	0/0/4/8	0/2/2/3
4	LFW	E	350[A]	1	-	0/0/4/8	0/2/2/3
4	LFW	B	314[A]	1	-	0/0/4/8	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	H	302	-	-	5/9/19/19	0/1/1/1
4	LFW	B	314[B]	1	-	0/0/4/8	0/2/2/3
4	LFW	H	350[A]	1	-	0/0/4/8	0/2/2/3
2	PGE	F	301	-	-	6/7/7/7	-
4	LFW	C	350[A]	1	-	0/0/4/8	0/2/2/3
2	PGE	D	301	-	-	3/7/7/7	-
4	LFW	G	350[A]	1	-	0/0/4/8	0/2/2/3
4	LFW	C	350[B]	1	-	0/0/4/8	0/2/2/3
4	LFW	G	350[B]	1	-	0/0/4/8	0/2/2/3
5	EPE	H	301	-	-	4/9/19/19	0/1/1/1
2	PGE	A	302	-	-	3/7/7/7	-
4	LFW	F	350[A]	1	-	0/0/4/8	0/2/2/3
4	LFW	F	350[B]	1	-	0/0/4/8	0/2/2/3
4	LFW	D	314[B]	1	-	0/0/4/8	0/2/2/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	302	EPE	C10-S	-3.67	1.72	1.77
5	H	301	EPE	C10-S	-2.87	1.73	1.77
4	A	350[B]	LFW	C15-C16	2.55	1.49	1.47
4	G	350[B]	LFW	C15-C16	2.23	1.49	1.47
4	F	350[B]	LFW	C15-C16	2.07	1.49	1.47
4	B	314[B]	LFW	C15-C16	2.05	1.49	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	302	EPE	C10-C9-N1-C6
2	B	301	PGE	O2-C3-C4-O3
2	F	301	PGE	O3-C5-C6-O4
2	F	301	PGE	O2-C3-C4-O3
2	A	301	PGE	O2-C3-C4-O3
2	F	301	PGE	O1-C1-C2-O2
5	H	302	EPE	C8-C7-N4-C5
5	H	301	EPE	C10-C9-N1-C2
2	B	301	PGE	C3-C4-O3-C5
2	A	301	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	H	302	EPE	N4-C7-C8-O8
2	E	301	PGE	C1-C2-O2-C3
5	H	302	EPE	C8-C7-N4-C3
2	D	301	PGE	C3-C4-O3-C5
2	A	302	PGE	C4-C3-O2-C2
2	F	301	PGE	C6-C5-O3-C4
2	B	301	PGE	C4-C3-O2-C2
2	D	301	PGE	C1-C2-O2-C3
2	F	301	PGE	C3-C4-O3-C5
2	D	301	PGE	O2-C3-C4-O3
2	E	301	PGE	C4-C3-O2-C2
5	H	302	EPE	C10-C9-N1-C2
5	H	301	EPE	C10-C9-N1-C6
2	F	301	PGE	C1-C2-O2-C3
2	E	301	PGE	O3-C5-C6-O4
2	A	302	PGE	C6-C5-O3-C4
5	H	301	EPE	C8-C7-N4-C3
2	A	301	PGE	C3-C4-O3-C5
5	H	301	EPE	C8-C7-N4-C5
2	A	302	PGE	C1-C2-O2-C3
2	E	301	PGE	O2-C3-C4-O3

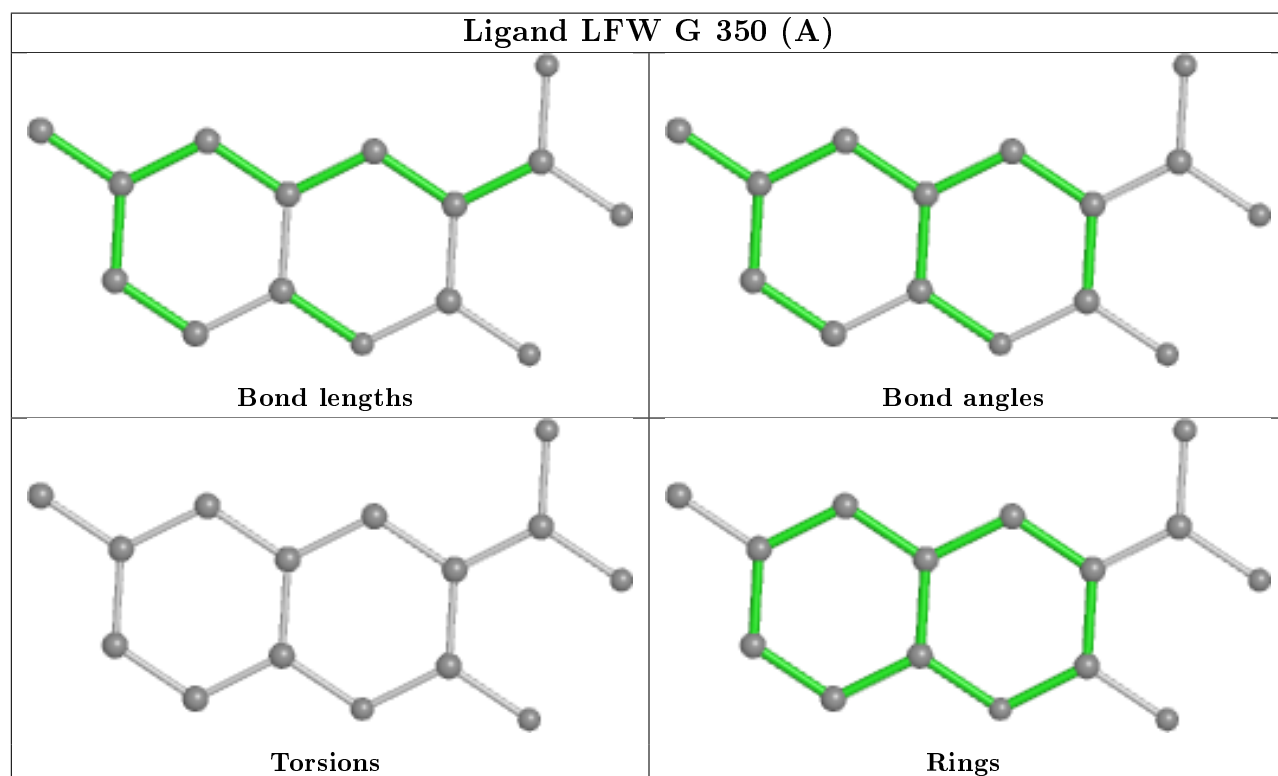
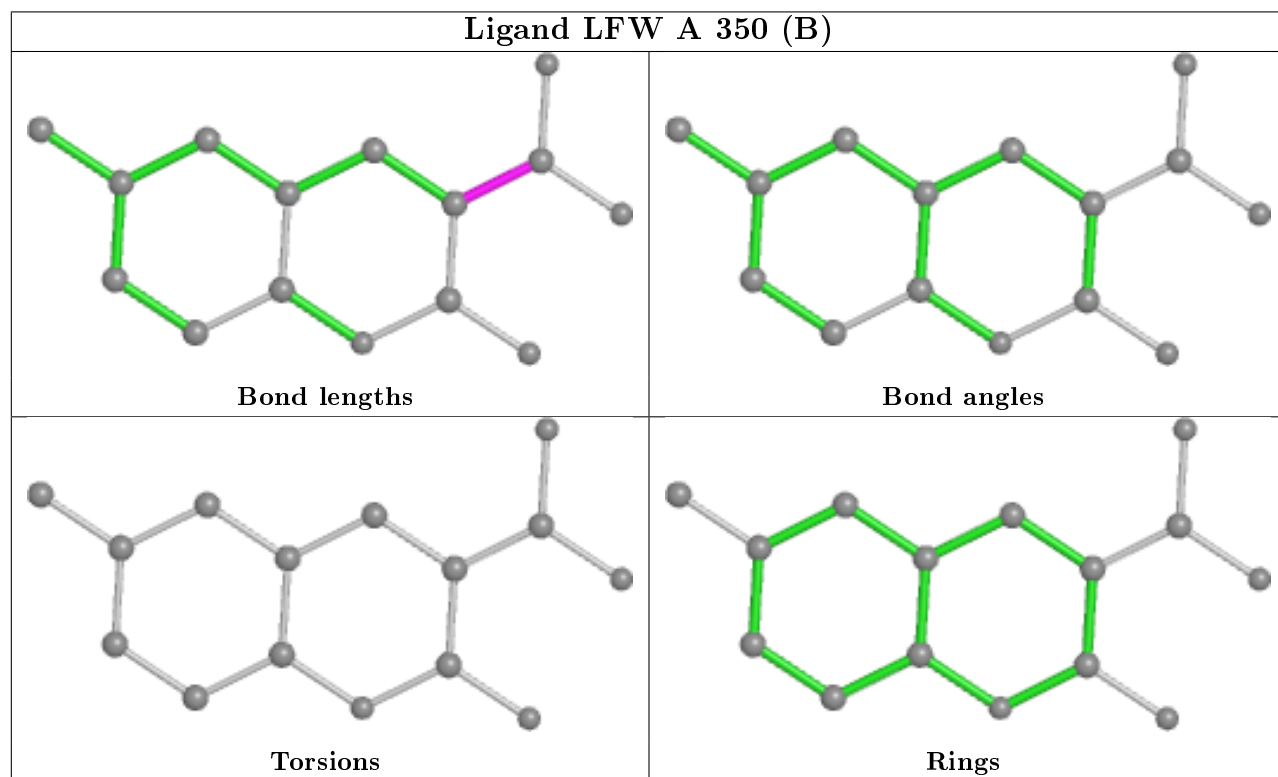
There are no ring outliers.

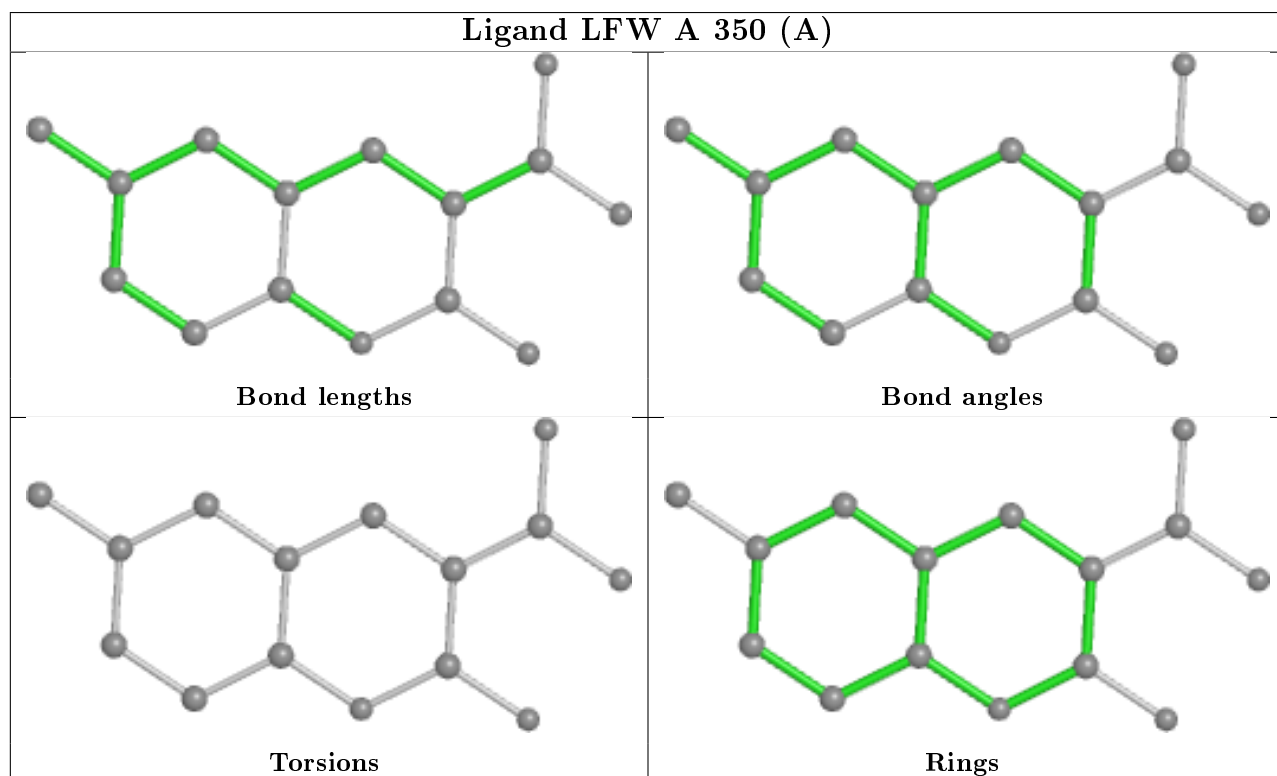
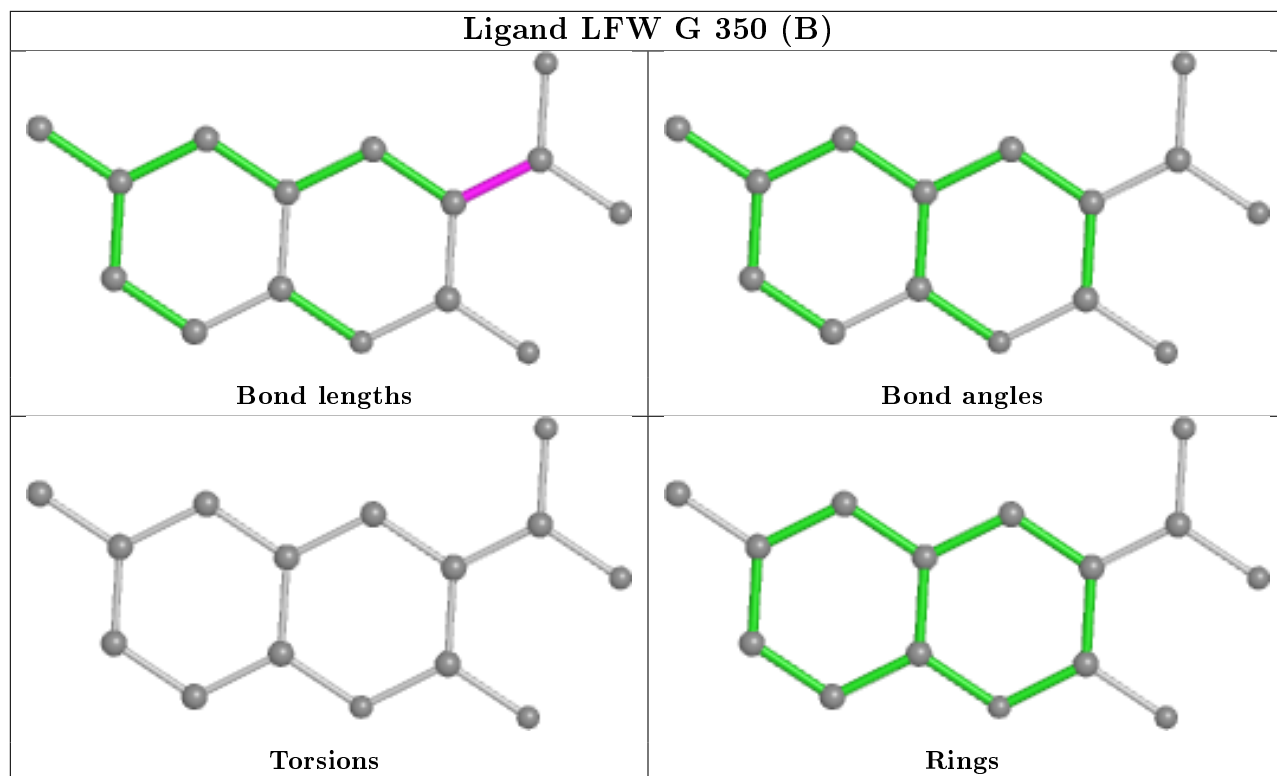
7 monomers are involved in 22 short contacts:

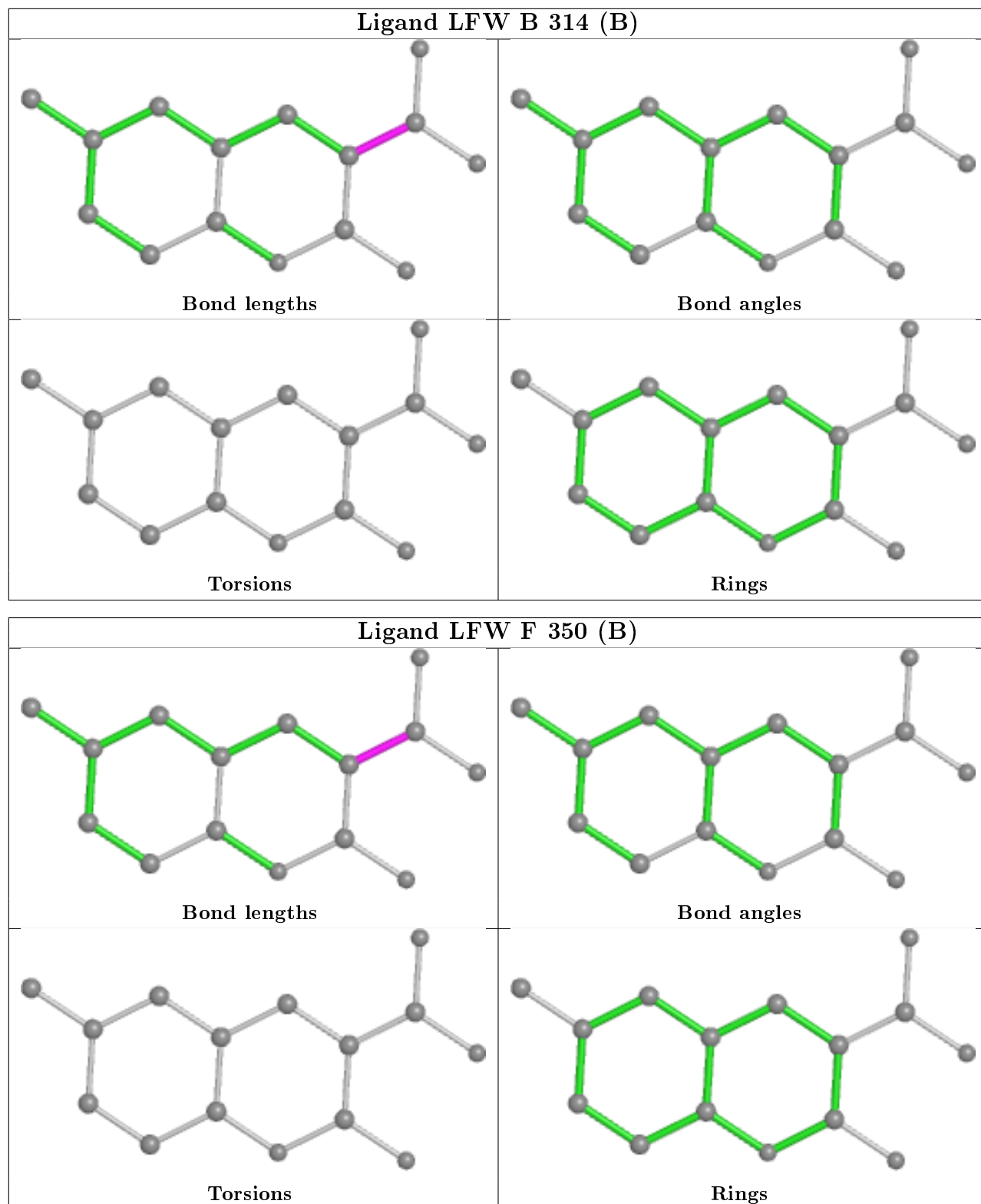
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	314	SO4	1	0
3	D	312	SO4	5	0
5	H	302	EPE	6	0
3	C	315	SO4	1	0
2	B	301	PGE	1	0
4	C	350[A]	LFW	1	0
2	A	302	PGE	8	0

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

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	224/224 (100%)	0.07	2 (0%) 84 85	26, 34, 53, 87	0
1	B	224/224 (100%)	0.09	5 (2%) 62 63	25, 34, 53, 88	1 (0%)
1	C	224/224 (100%)	0.20	4 (1%) 68 69	25, 36, 54, 72	1 (0%)
1	D	224/224 (100%)	0.15	4 (1%) 68 69	27, 39, 60, 75	0
1	E	224/224 (100%)	-0.01	0 100 100	27, 36, 54, 76	0
1	F	224/224 (100%)	0.10	6 (2%) 54 56	27, 37, 54, 77	0
1	G	224/224 (100%)	0.69	21 (9%) 8 9	33, 46, 65, 88	0
1	H	224/224 (100%)	0.70	23 (10%) 6 7	34, 49, 66, 93	0
All	All	1792/1792 (100%)	0.25	65 (3%) 42 45	25, 39, 60, 93	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	186(A)	ASP	5.0
1	B	246	ARG	4.7
1	G	22	CYS	4.3
1	H	186	PRO	4.1
1	B	76	GLY	3.9
1	H	103	LEU	3.7
1	A	246	ARG	3.6
1	G	79	ARG	3.3
1	H	94	TYR	3.2
1	H	25	GLY	3.2
1	G	94	TYR	3.1
1	H	133	GLY	3.0
1	H	135	THR	3.0
1	H	246	ARG	3.0
1	F	96	THR	3.0
1	G	116	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	223	ASN	2.9
1	G	186(A)	ASP	2.9
1	D	94	TYR	2.7
1	H	168	CYS	2.7
1	F	246	ARG	2.7
1	H	220(A)	GLY	2.7
1	G	25	GLY	2.6
1	H	49	GLU	2.6
1	F	111	GLN	2.6
1	H	234	PHE	2.6
1	G	98	THR	2.5
1	G	135	THR	2.5
1	G	246	ARG	2.5
1	B	99[A]	HIS	2.5
1	C	110	SER	2.5
1	B	112	ALA	2.5
1	G	23	ALA	2.5
1	G	175	LEU	2.5
1	A	24	ARG	2.5
1	H	79	ARG	2.5
1	D	202	ARG	2.4
1	H	110	SER	2.4
1	H	16	ILE	2.4
1	D	186(A)	ASP	2.4
1	H	113	ARG	2.3
1	F	93	GLY	2.3
1	G	76	GLY	2.3
1	H	245	HIS	2.3
1	G	214	SER	2.3
1	G	100	VAL	2.2
1	H	186(B)	SER	2.2
1	G	71	ASP	2.2
1	G	99	HIS	2.2
1	G	118	VAL	2.2
1	G	57[A]	HIS	2.2
1	C	78	ARG	2.2
1	H	222	PRO	2.1
1	C	112	ALA	2.1
1	G	243	LYS	2.1
1	F	115	SER	2.1
1	H	78	ARG	2.1
1	H	100	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	101	ASN	2.1
1	F	110	SER	2.1
1	C	99[A]	HIS	2.1
1	D	186	PRO	2.1
1	G	50	ARG	2.1
1	B	227	VAL	2.0
1	G	154	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	G	307	5/5	0.50	0.45	199,199,199,199	0
3	SO4	F	310	5/5	0.53	0.31	170,170,170,170	0
3	SO4	D	312	5/5	0.59	0.62	145,145,145,146	0
2	PGE	B	301	10/10	0.66	0.25	44,46,48,49	0
2	PGE	A	301	10/10	0.71	0.19	58,62,65,65	0
5	EPE	H	302	15/15	0.72	0.33	50,53,76,78	0
3	SO4	A	311	5/5	0.75	0.21	71,75,77,80	0
3	SO4	E	310	5/5	0.75	0.24	105,107,108,109	0
2	PGE	E	301	10/10	0.76	0.20	48,52,56,57	0
3	SO4	C	315	5/5	0.76	0.39	137,137,137,137	0
5	EPE	H	301	15/15	0.77	0.32	85,93,100,100	0
2	PGE	D	301	10/10	0.80	0.29	52,54,57,58	0
4	LFW	G	350[A]	15/22	0.80	0.66	47,49,51,51	15
3	SO4	H	307	5/5	0.80	0.24	131,131,132,132	0
4	LFW	A	350[B]	15/22	0.80	0.46	42,45,50,52	15
4	LFW	A	350[A]	15/22	0.80	0.46	33,35,39,40	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LFW	G	350[B]	15/22	0.80	0.66	35,44,50,52	15
3	SO4	B	307	5/5	0.80	0.25	108,110,110,111	0
3	SO4	C	307	5/5	0.81	0.19	127,127,128,128	0
3	SO4	F	309	5/5	0.81	0.49	101,103,104,106	0
2	PGE	A	302	10/10	0.82	0.16	43,44,46,49	0
4	LFW	C	350[B]	15/22	0.82	0.55	40,48,51,52	15
3	SO4	G	310	5/5	0.82	0.29	123,123,124,124	0
3	SO4	E	307	5/5	0.82	0.19	115,116,117,117	0
4	LFW	C	350[A]	15/22	0.82	0.55	42,45,47,47	15
3	SO4	H	314	5/5	0.83	0.26	128,128,129,129	0
3	SO4	D	309	5/5	0.83	0.22	103,105,105,108	0
2	PGE	F	301	10/10	0.83	0.18	48,50,53,54	0
4	LFW	E	350[B]	15/22	0.84	0.43	32,37,44,47	15
4	LFW	E	350[A]	15/22	0.84	0.43	33,40,43,43	15
3	SO4	H	309	5/5	0.84	0.40	136,136,137,137	0
4	LFW	D	314[B]	15/22	0.84	0.56	42,48,53,55	15
3	SO4	B	312	5/5	0.84	0.32	123,123,123,124	0
4	LFW	D	314[A]	15/22	0.84	0.56	41,45,48,49	15
4	LFW	B	314[A]	15/22	0.85	0.50	35,39,42,44	15
4	LFW	B	314[B]	15/22	0.85	0.50	35,44,47,48	15
3	SO4	B	309	5/5	0.86	0.35	106,106,107,108	0
3	SO4	G	306	5/5	0.86	0.34	123,124,124,124	0
4	LFW	H	350[B]	15/22	0.87	0.62	45,49,51,52	15
3	SO4	G	303	5/5	0.87	0.20	101,102,102,102	0
4	LFW	H	350[A]	15/22	0.87	0.62	41,44,47,48	15
3	SO4	D	313	5/5	0.88	0.27	115,115,115,115	0
4	LFW	F	350[B]	15/22	0.88	0.49	42,47,51,52	15
3	SO4	C	311	5/5	0.88	0.17	70,74,76,76	0
3	SO4	B	306	5/5	0.88	0.20	83,83,86,89	0
4	LFW	F	350[A]	15/22	0.88	0.49	38,39,41,43	15
3	SO4	E	305	5/5	0.88	0.21	93,95,96,96	0
3	SO4	C	309	5/5	0.88	0.22	79,83,84,84	0
3	SO4	B	313	5/5	0.89	0.20	105,105,106,106	0
3	SO4	B	311	5/5	0.90	0.14	115,115,116,116	0
3	SO4	E	306	5/5	0.90	0.26	68,72,76,77	0
3	SO4	A	306	5/5	0.91	0.20	72,75,79,80	0
3	SO4	H	306	5/5	0.91	0.18	77,78,81,82	0
3	SO4	C	312	5/5	0.91	0.23	94,94,97,98	0
3	SO4	H	313	5/5	0.91	0.32	95,96,96,97	0
3	SO4	G	305	5/5	0.91	0.23	95,95,95,96	0
3	SO4	D	310	5/5	0.91	0.26	94,94,96,96	0
3	SO4	B	310	5/5	0.92	0.23	101,102,104,104	0

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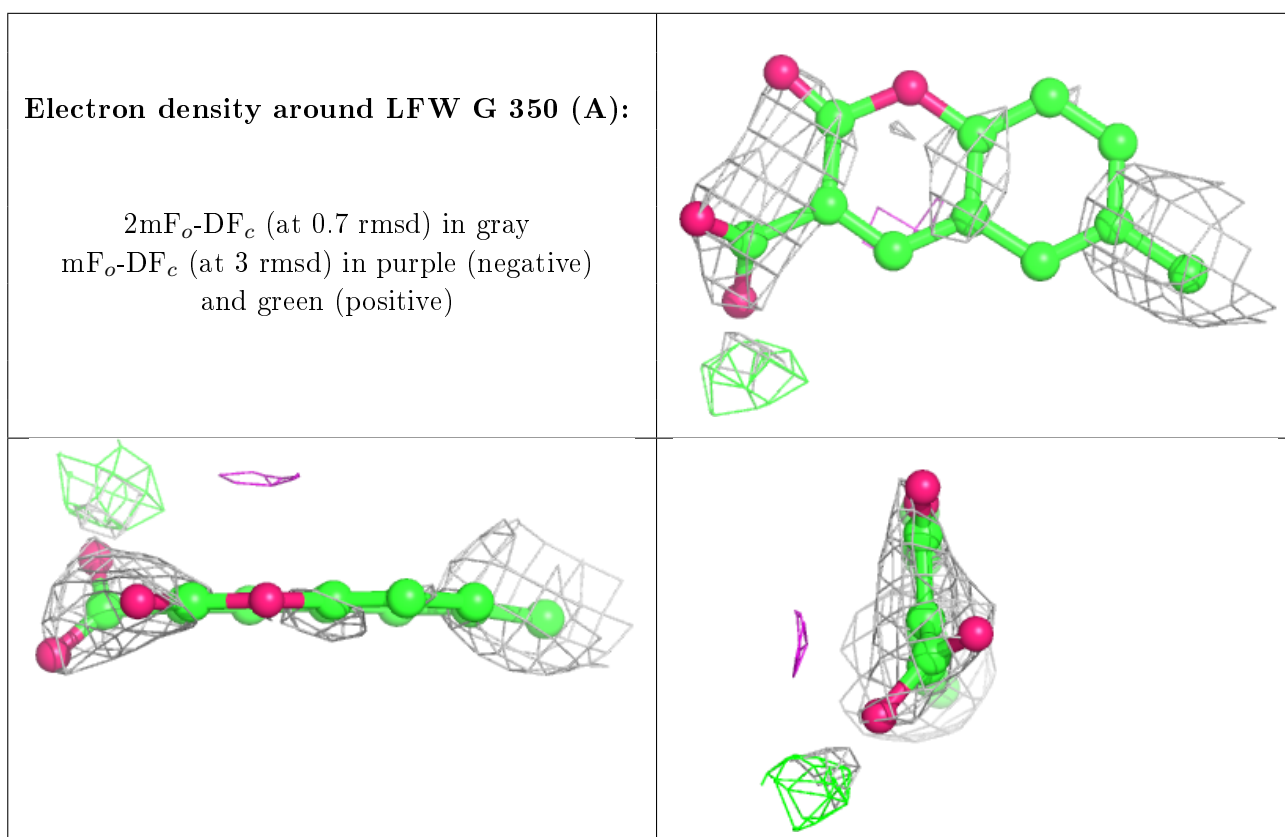
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	H	311	5/5	0.92	0.40	106,107,107,108	0
3	SO4	C	313	5/5	0.92	0.26	81,82,85,87	0
3	SO4	G	308	5/5	0.92	0.32	125,125,126,126	0
3	SO4	H	305	5/5	0.92	0.12	91,92,92,94	0
3	SO4	C	310	5/5	0.92	0.18	69,73,74,75	0
3	SO4	F	312	5/5	0.92	0.28	111,111,111,112	0
3	SO4	A	310	5/5	0.93	0.12	88,89,91,92	0
3	SO4	D	311	5/5	0.93	0.43	91,92,92,93	0
3	SO4	C	303	5/5	0.93	0.12	55,56,60,65	0
3	SO4	H	310	5/5	0.93	0.30	111,111,112,112	0
3	SO4	F	306	5/5	0.93	0.10	65,67,68,70	0
3	SO4	F	304	5/5	0.93	0.30	76,76,77,77	0
3	SO4	E	308	5/5	0.93	0.26	85,85,88,89	0
3	SO4	F	308	5/5	0.94	0.28	112,112,112,113	0
3	SO4	D	308	5/5	0.94	0.28	67,68,69,70	0
3	SO4	E	309	5/5	0.94	0.34	89,89,90,92	0
3	SO4	G	302	5/5	0.94	0.21	85,86,88,89	0
3	SO4	C	308	5/5	0.94	0.19	73,74,76,78	0
3	SO4	C	314	5/5	0.94	0.49	109,110,110,110	0
3	SO4	F	305	5/5	0.95	0.11	67,70,74,76	0
3	SO4	G	304	5/5	0.95	0.18	105,105,106,106	0
3	SO4	G	309	5/5	0.95	0.23	97,97,98,98	0
3	SO4	H	312	5/5	0.95	0.10	104,104,104,105	0
3	SO4	C	304	5/5	0.95	0.10	83,84,85,86	0
3	SO4	D	305	5/5	0.95	0.09	58,61,62,62	0
3	SO4	A	309	5/5	0.95	0.23	65,66,71,72	0
3	SO4	F	311	5/5	0.95	0.21	96,97,97,98	0
3	SO4	B	308	5/5	0.96	0.29	75,76,76,78	0
3	SO4	H	308	5/5	0.96	0.24	98,100,101,102	0
3	SO4	A	305	5/5	0.96	0.21	77,79,79,79	0
3	SO4	F	303	5/5	0.96	0.10	55,59,62,63	0
3	SO4	A	308	5/5	0.96	0.08	55,61,63,64	0
3	SO4	H	304	5/5	0.96	0.08	56,57,62,63	0
3	SO4	E	304	5/5	0.96	0.11	71,72,74,74	0
3	SO4	D	307	5/5	0.96	0.22	65,66,70,70	0
3	SO4	A	304	5/5	0.96	0.11	52,52,56,60	0
3	SO4	C	306	5/5	0.96	0.08	89,89,90,92	0
3	SO4	A	307	5/5	0.96	0.22	76,78,80,81	0
3	SO4	C	305	5/5	0.96	0.19	77,77,78,80	0
3	SO4	D	303	5/5	0.97	0.10	65,67,69,69	0
3	SO4	F	307	5/5	0.97	0.19	69,70,73,76	0
3	SO4	B	305	5/5	0.97	0.07	73,73,75,75	0

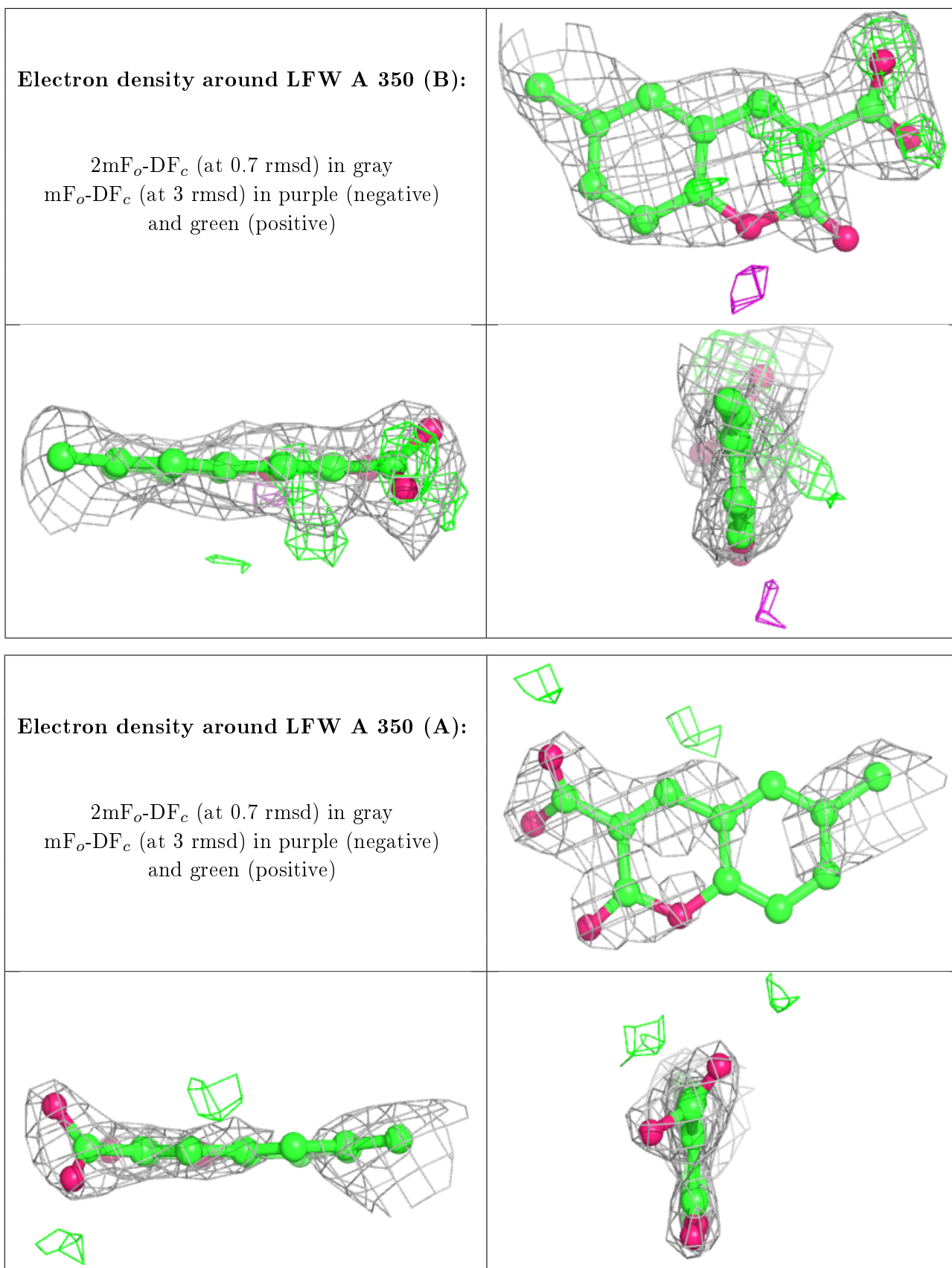
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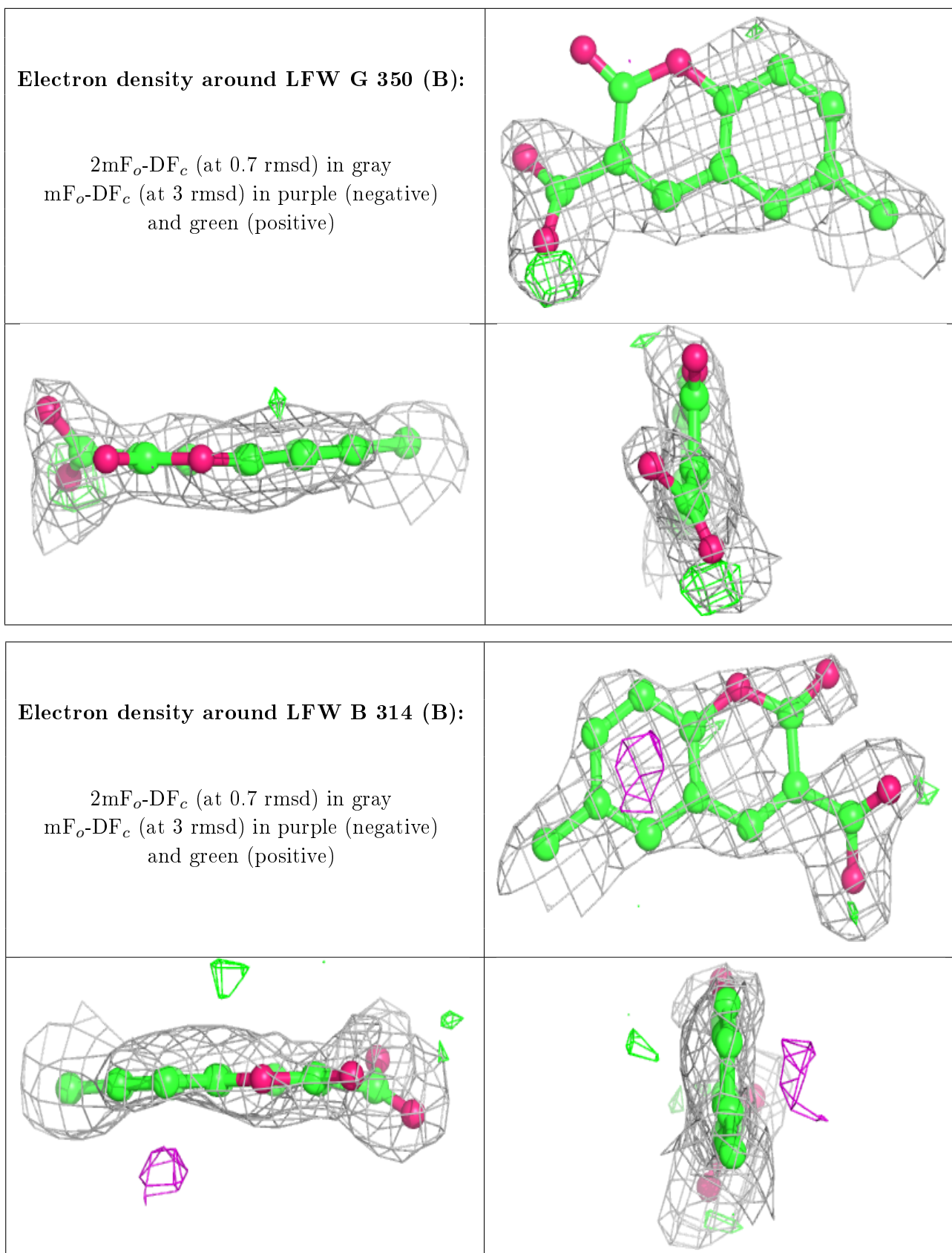
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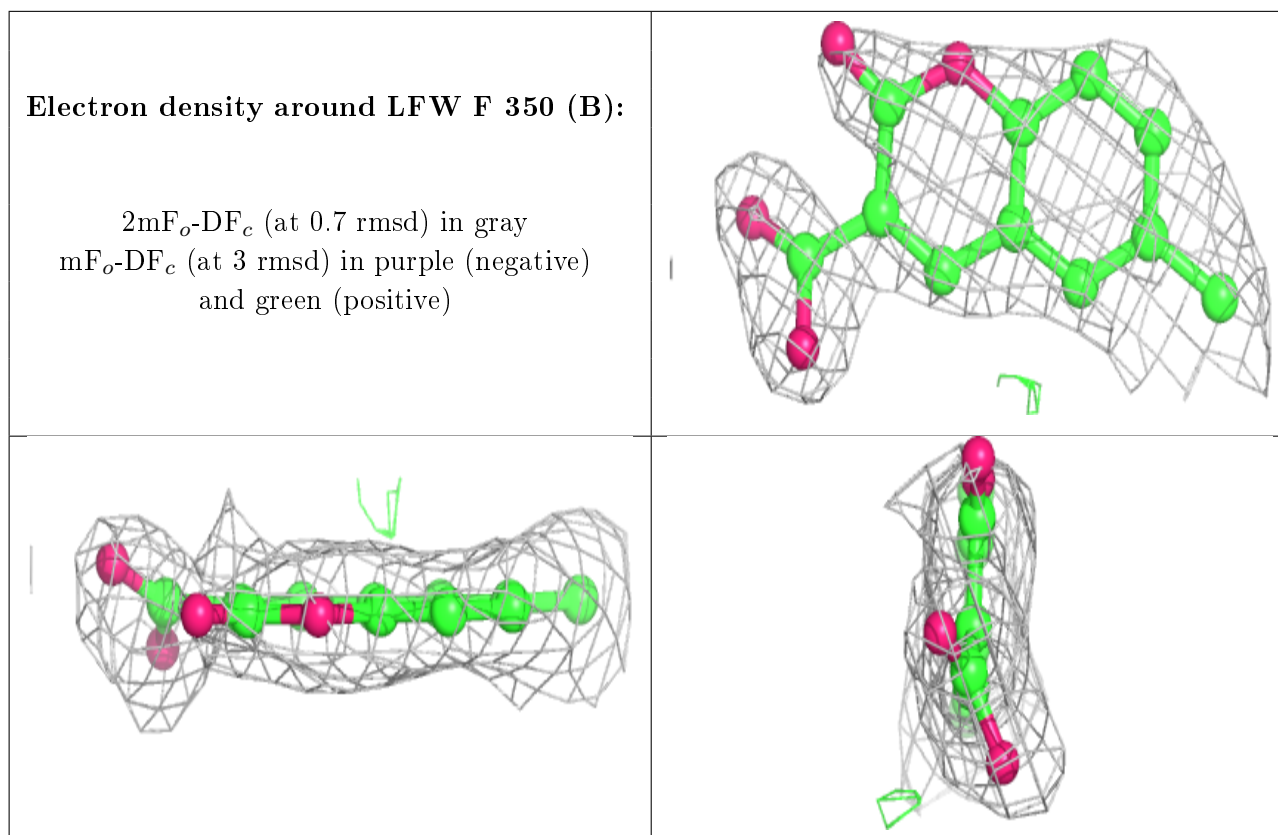
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	D	304	5/5	0.97	0.09	70,73,74,75	0
3	SO4	B	304	5/5	0.97	0.09	67,69,70,74	0
3	SO4	E	303	5/5	0.97	0.08	52,57,61,62	0
3	SO4	D	302	5/5	0.99	0.09	37,38,44,45	0
3	SO4	D	306	5/5	0.99	0.18	58,60,65,66	0
3	SO4	B	302	5/5	0.99	0.10	40,40,47,48	0
3	SO4	G	301	5/5	0.99	0.10	47,47,50,52	0
3	SO4	A	303	5/5	0.99	0.11	42,42,46,46	0
3	SO4	B	303	5/5	0.99	0.06	38,43,45,45	0
3	SO4	C	301	5/5	0.99	0.10	42,43,46,47	0
3	SO4	C	302	5/5	0.99	0.10	36,39,42,42	0
3	SO4	F	302	5/5	0.99	0.11	41,41,44,49	0
3	SO4	E	302	5/5	0.99	0.13	42,43,44,48	0
3	SO4	H	303	5/5	0.99	0.13	45,45,48,48	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.









6.5 Other polymers [i](#)

There are no such residues in this entry.