Full wwPDB X-ray Structure Validation Report (i)

Feb 9, 2023 – 02:13 am GMT

PDB ID	:	8BDN
Title	:	VCB in complex with compound 23
Authors	:	Sorrell, F.J.; Mueller, J.E.; Lehmann, M.; Wegener, A.
Deposited on	:	2022-10-19
Resolution	:	2.76 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 (i) 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 (i)) were used in the production of this report:

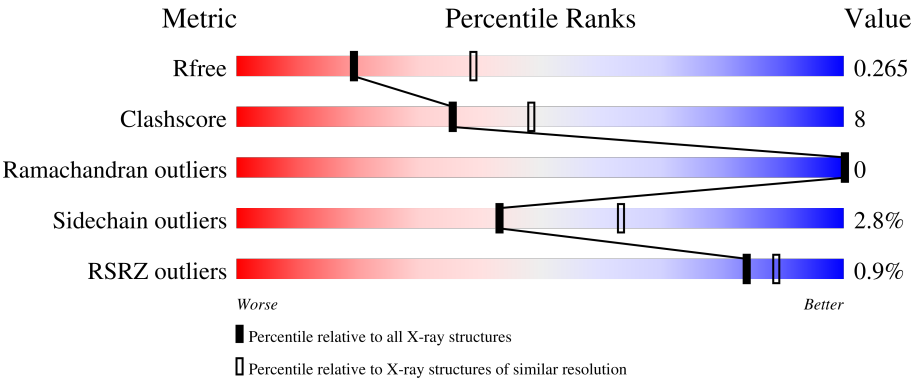
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	104	77% 19%
1	D	104	80% 18%
1	G	104	68% 27%
1	J	104	3% 79% 18%
2	B	97	89% 5% 6%

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Mol	Chain	Length	Quality of chain
2	E	97	79% 12% • 7%
2	H	97	78% 13% • 7%
2	K	97	69% 20% • 9%
3	C	162	% 72% 15% • 10%
3	F	162	% 75% 14% • 10%
3	I	162	% 73% 17% 9%
3	L	162	74% 14% • 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10851 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 Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	104	Total	As	C	N	O	S	0	0	0
			784	1	501	130	148	4			
1	D	104	Total	As	C	N	O	S	0	0	0
			815	1	517	137	155	5			
1	G	104	Total	As	C	N	O	S	0	0	0
			802	1	509	133	155	4			
1	J	103	Total	As	C	N	O	S	0	0	0
			790	1	503	131	151	4			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	S	0	0	0
			715	460	115	134	6			
2	E	90	Total	C	N	O	S	0	0	0
			708	455	114	133	6			
2	H	90	Total	C	N	O	S	0	0	0
			709	456	114	133	6			
2	K	88	Total	C	N	O	S	0	0	0
			695	448	112	129	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369
H	16	MET	-	initiating methionine	UNP Q15369
K	16	MET	-	initiating methionine	UNP Q15369

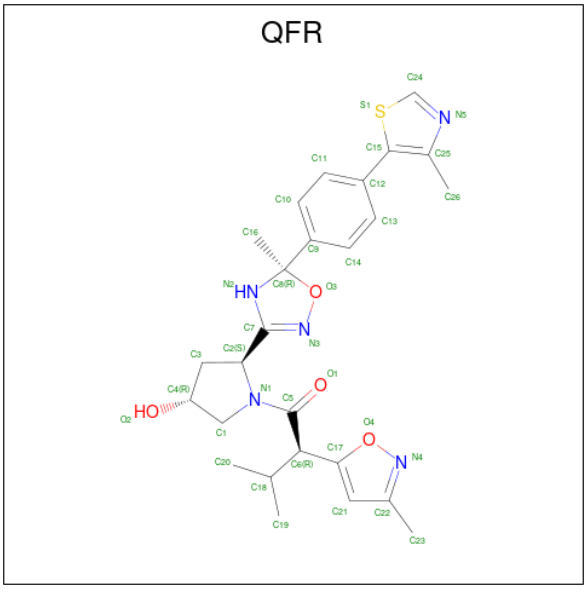
- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	145	Total	As	C	N	O	S	0	1	0
			1156	1	741	205	207	2			
3	F	145	Total	As	C	N	O	S	0	0	0
			1152	1	735	203	211	2			
3	I	147	Total	As	C	N	O	S	0	0	0
			1190	1	757	216	214	2			
3	L	143	Total	As	C	N	O	S	0	1	0
			1150	1	732	206	209	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

- Molecule 4 is (2 {R})-3-methyl-1-[(2 {S},4 {R})-2-[(5 {R})-5-methyl-5-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]-4 {H}-1,2,4-oxadiazol-3-yl]-4-oxidanyl-pyrrolidin-1-yl]-2-(3-methyl-1,2-oxazol-5-yl)butan-1-one (three-letter code: QFR) (formula: $C_{26}H_{31}N_5O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			36	26	5	4	1		
4	F	1	Total	C	N	O	S	0	0
			36	26	5	4	1		
4	I	1	Total	C	N	O	S	0	0
			36	26	5	4	1		
4	L	1	Total	C	N	O	S	0	0
			36	26	5	4	1		

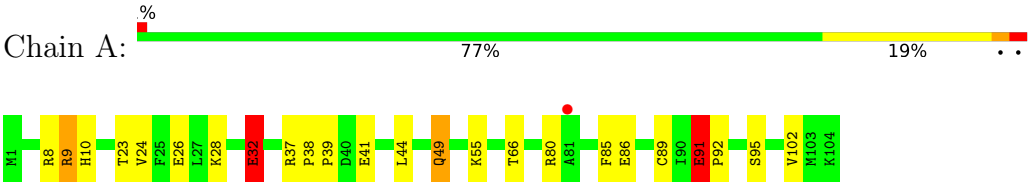
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	3	Total	O	0	0
			3	3		
5	C	3	Total	O	0	0
			3	3		
5	D	6	Total	O	0	0
			6	6		
5	E	4	Total	O	0	0
			4	4		
5	F	6	Total	O	0	0
			6	6		
5	G	3	Total	O	0	0
			3	3		
5	H	3	Total	O	0	0
			3	3		
5	I	6	Total	O	0	0
			6	6		
5	J	1	Total	O	0	0
			1	1		
5	K	1	Total	O	0	0
			1	1		
5	L	2	Total	O	0	0
			2	2		

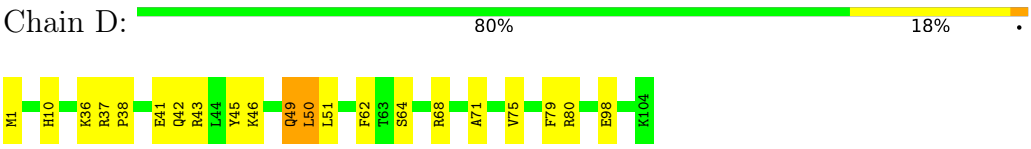
3 Residue-property plots (i)

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.

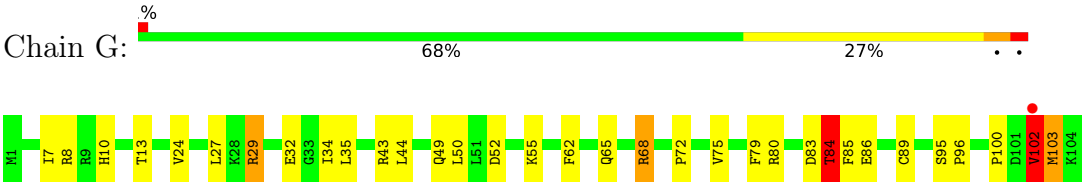
• Molecule 1: Elongin-B



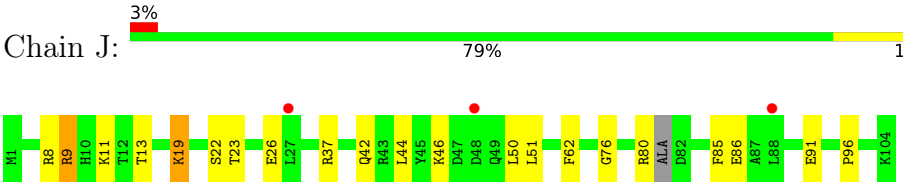
• Molecule 1: Elongin-B



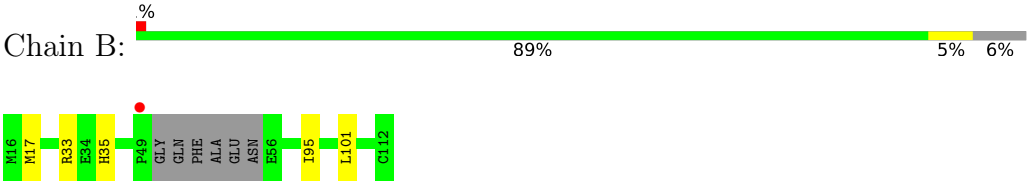
• Molecule 1: Elongin-B



• Molecule 1: Elongin-B

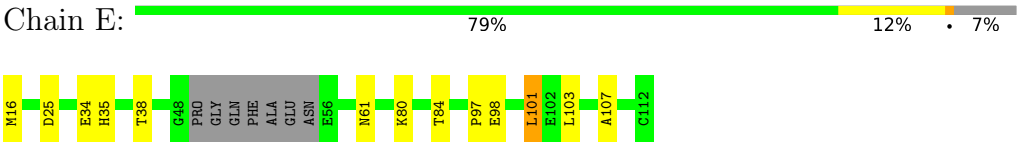


• Molecule 2: Elongin-C



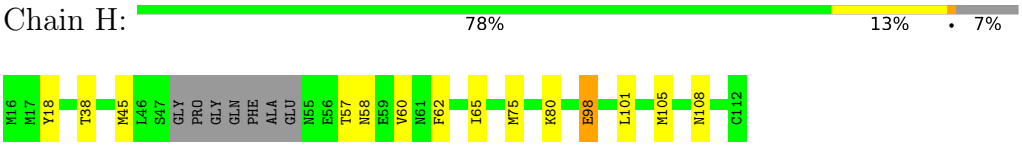
• Molecule 2: Elongin-C

Chain E:



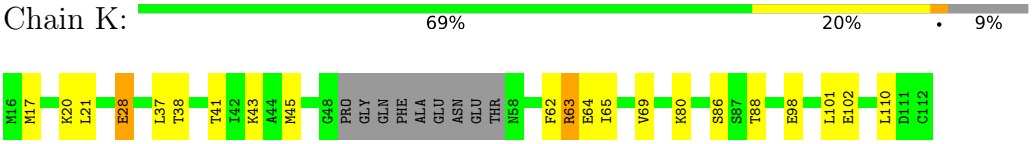
• Molecule 2: Elongin-C

Chain H:



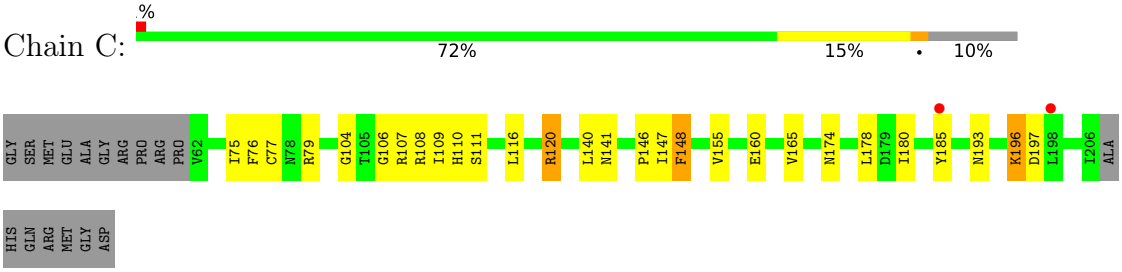
• Molecule 2: Elongin-C

Chain K:



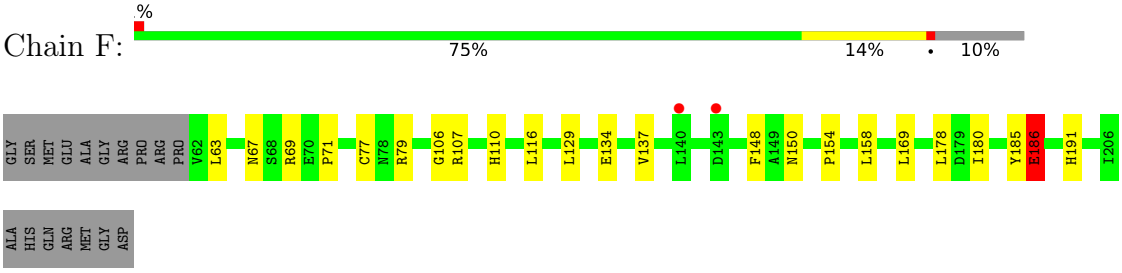
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C:



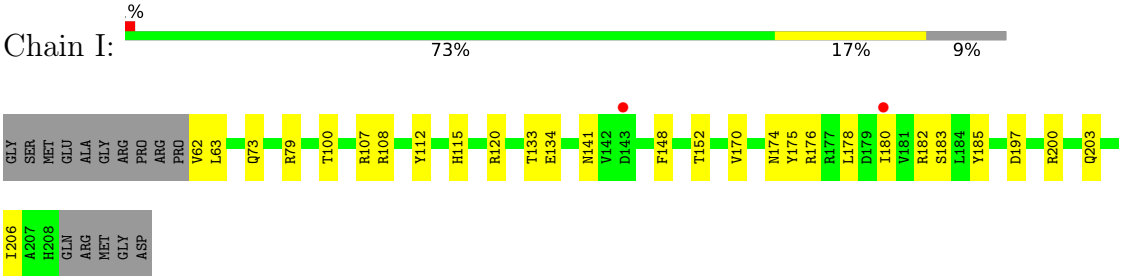
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:



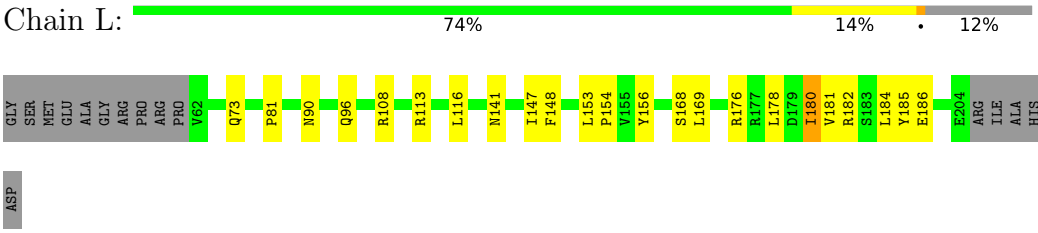
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain I:



• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain L:


74%
14%
12%
GLY SER MET GLU ALA GLY ARG PRO ARG PRO V62 Q73 P81 N90 Q96 R108 R113 L116 N141 I147 F148 L153 P154 V155 Y156 S168 L169 R176 R177 L178 D179 I180 V181 R182 S183 L184 Y185 E186 E204 ARG ILE ALA HIS GLN ARG MET GLY
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.17Å 93.17Å 358.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.88 – 2.76 358.85 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.88-2.76) 92.0 (358.85-2.76)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.209 , 0.263 0.215 , 0.265	Depositor DCC
R_{free} test set	2171 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10851	wwPDB-VP
Average B, all atoms (Å^2)	74.0	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 28.91 % 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 1.6972e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, QFR

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	0.77	3/790 (0.4%)	1.12	5/1072 (0.5%)
1	D	0.44	0/821	0.86	2/1109 (0.2%)
1	G	0.51	1/808 (0.1%)	0.97	8/1095 (0.7%)
1	J	0.47	0/795	0.82	1/1076 (0.1%)
2	B	0.37	0/730	0.61	0/986
2	E	0.45	0/722	0.76	1/974 (0.1%)
2	H	0.42	0/723	0.69	1/977 (0.1%)
2	K	0.48	0/709	0.98	5/956 (0.5%)
3	C	0.42	0/1177	0.85	4/1612 (0.2%)
3	F	0.41	0/1172	0.77	3/1604 (0.2%)
3	I	0.43	0/1210	0.75	0/1652
3	L	0.43	0/1170	0.74	3/1602 (0.2%)
All	All	0.47	4/10827 (0.0%)	0.83	33/14715 (0.2%)

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	3
2	K	0	1
3	F	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CG-CD	8.56	1.64	1.51
1	A	91	GLU	CD-OE2	8.29	1.34	1.25
1	G	102	VAL	CB-CG1	-8.06	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	GLU	CB-CG	-6.05	1.40	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	GLU	CA-CB-CG	-13.86	82.90	113.40
3	C	110	HIS	N-CA-CB	-12.16	88.71	110.60
1	G	102	VAL	CG1-CB-CG2	-10.35	94.34	110.90
1	A	32	GLU	CG-CD-OE2	-10.32	97.65	118.30
1	A	32	GLU	CG-CD-OE1	10.31	138.92	118.30
2	K	17	MET	CG-SD-CE	-9.53	84.95	100.20
2	K	17	MET	CA-CB-CG	9.19	128.93	113.30
3	C	140	LEU	CB-CG-CD1	-8.65	96.30	111.00
2	K	17	MET	CB-CG-SD	-8.41	87.17	112.40
1	G	84	THR	OG1-CB-CG2	-7.68	92.33	110.00
1	G	102	VAL	CA-CB-CG1	-7.54	99.60	110.90
3	L	186	GLU	CA-CB-CG	6.97	128.74	113.40
1	A	91	GLU	CB-CG-CD	6.63	132.09	114.20
3	L	186	GLU	CB-CA-C	-6.48	97.43	110.40
3	F	186	GLU	CA-CB-CG	6.33	127.33	113.40
1	A	32	GLU	N-CA-CB	6.03	121.46	110.60
3	F	186	GLU	OE1-CD-OE2	-5.88	116.24	123.30
3	C	155	VAL	CG1-CB-CG2	-5.85	101.55	110.90
2	E	84	THR	OG1-CB-CG2	-5.67	96.97	110.00
1	G	103	MET	CA-CB-CG	-5.62	103.75	113.30
2	K	110	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	J	19	LYS	CD-CE-NZ	-5.56	98.90	111.70
1	G	35	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	G	84	THR	CA-CB-CG2	-5.42	104.82	112.40
2	H	98	GLU	CB-CA-C	-5.39	99.62	110.40
1	D	49	GLN	CA-CB-CG	-5.38	101.57	113.40
3	L	180	ILE	CG1-CB-CG2	-5.24	99.87	111.40
2	K	28	GLU	CA-CB-CG	-5.22	101.92	113.40
3	C	140	LEU	CA-CB-CG	5.21	127.28	115.30
3	F	186	GLU	CB-CA-C	-5.19	100.03	110.40
1	G	103	MET	N-CA-CB	-5.18	101.28	110.60
1	G	103	MET	CB-CA-C	5.05	120.50	110.40
1	D	50	LEU	CB-CG-CD1	-5.05	102.42	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	GLU	Sidechain
1	A	49	GLN	Sidechain
1	A	91	GLU	Sidechain
3	F	186	GLU	Sidechain
2	K	63	ARG	Sidechain

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	784	0	754	29	0
1	D	815	0	807	16	0
1	G	802	0	778	31	0
1	J	790	0	764	12	0
2	B	715	0	709	4	0
2	E	708	0	702	12	0
2	H	709	0	695	14	0
2	K	695	0	690	15	0
3	C	1156	0	1118	21	0
3	F	1152	0	1106	13	0
3	I	1190	0	1173	22	0
3	L	1150	0	1111	12	0
4	C	36	0	0	0	0
4	F	36	0	0	0	0
4	I	36	0	0	0	0
4	L	36	0	0	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	6	0	0	0	0
5	E	4	0	0	1	0
5	F	6	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
5	I	6	0	0	1	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	2	0	0	0	0
All	All	10851	0	10407	171	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 8.

All (171) 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:A:32:GLU:OE1	1:A:39:PRO:HD3	1.18	1.28
1:A:32:GLU:OE1	1:A:39:PRO:CD	1.90	1.19
1:G:83:ASP:OD1	1:G:84:THR:HG22	1.65	0.94
1:G:29:ARG:NH1	1:G:32:GLU:OE1	2.01	0.92
1:A:91:GLU:HG2	1:A:92:PRO:N	1.91	0.85
3:I:176:ARG:HA	3:I:185:TYR:CE1	2.11	0.85
1:G:102:VAL:HG11	3:I:174:ASN:CB	2.10	0.82
1:A:32:GLU:CD	1:A:39:PRO:HD3	2.00	0.81
1:G:102:VAL:HG11	3:I:174:ASN:HB3	1.62	0.81
1:A:32:GLU:CD	1:A:38:PRO:HA	2.02	0.80
3:F:178:LEU:O	3:F:185:TYR:OH	1.99	0.80
2:E:98:GLU:N	2:E:98:GLU:OE2	2.15	0.79
1:A:91:GLU:HG2	1:A:92:PRO:CD	2.13	0.78
1:A:91:GLU:CG	1:A:92:PRO:HD2	2.13	0.78
2:E:16:MET:N	5:E:201:HOH:O	2.19	0.75
3:I:62:VAL:O	5:I:401:HOH:O	2.06	0.72
1:D:68:ARG:NH2	1:D:71:ALA:HB3	2.06	0.71
1:A:80:ARG:HA	1:A:85:PHE:HA	1.73	0.70
1:A:91:GLU:HG2	1:A:92:PRO:HD2	1.71	0.69
3:L:176:ARG:HA	3:L:185:TYR:CE1	2.28	0.68
1:D:36:LYS:HG3	1:D:36:LYS:O	1.94	0.67
1:G:8:ARG:HG2	1:G:13:THR:HG23	1.76	0.67
1:A:32:GLU:OE2	1:A:38:PRO:HA	1.95	0.66
3:I:100:THR:O	3:I:107:ARG:NH2	2.30	0.65
1:G:103:MET:HG3	3:I:170:VAL:HG22	1.78	0.64
2:K:38:THR:HG23	2:K:80:LYS:HE3	1.80	0.64
1:A:91:GLU:CG	1:A:92:PRO:CD	2.75	0.63
1:G:52:ASP:HB3	1:G:55:LYS:HG3	1.80	0.63
1:J:9:ARG:NH2	1:J:86:GLU:OE2	2.33	0.61
1:D:43:ARG:HD3	1:D:50:LEU:CD1	2.31	0.61
1:A:55:LYS:HG3	1:G:65:GLN:OE1	2.02	0.60
3:I:178:LEU:O	3:I:185:TYR:OH	2.14	0.60
1:A:32:GLU:HB3	1:A:37:ARG:O	2.01	0.60
3:C:120:ARG:NH1	3:C:197:ASP:OD2	2.21	0.59
1:G:72:PRO:HD2	2:H:75:MET:CE	2.32	0.59
3:I:182:ARG:HA	3:I:185:TYR:HD2	1.68	0.59
3:F:79:ARG:HE	3:F:150:ASN:ND2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:62:PHE:HB3	2:K:65:ILE:HD12	1.86	0.58
3:I:175:TYR:O	3:I:185:TYR:HE1	1.86	0.58
1:G:7:ILE:HD11	1:G:27:LEU:HD22	1.86	0.57
2:H:57:THR:O	2:H:58:ASN:HB2	2.05	0.57
1:A:9:ARG:NH1	1:A:86:GLU:OE1	2.38	0.57
3:C:77:CAS:CE2	3:C:106:GLY:HA3	2.35	0.57
1:A:102:VAL:HG11	3:C:174:ASN:HB3	1.86	0.56
1:D:38:PRO:HD2	1:D:41:GLU:OE1	2.04	0.56
3:F:77:CAS:CE2	3:F:106:GLY:HA3	2.35	0.55
1:D:1:MET:SD	1:D:64:SER:HB2	2.46	0.55
1:D:43:ARG:HD3	1:D:50:LEU:HD11	1.89	0.55
1:J:46:LYS:HB3	1:J:51:LEU:HD21	1.89	0.55
3:C:141:ASN:HD22	3:C:141:ASN:N	2.05	0.55
2:B:17:MET:HE3	2:B:33:ARG:HD2	1.89	0.55
1:A:8:ARG:NH2	1:A:91:GLU:O	2.41	0.54
2:K:101:LEU:HD21	3:L:178:LEU:HD22	1.89	0.54
3:C:178:LEU:O	3:C:185:TYR:OH	2.18	0.54
1:J:46:LYS:HD2	1:J:62:PHE:CZ	2.43	0.54
1:J:37:ARG:O	1:J:42:GLN:NE2	2.41	0.53
1:A:38:PRO:HG2	1:A:41:GLU:HG3	1.91	0.53
1:A:32:GLU:OE1	1:A:39:PRO:CG	2.55	0.53
3:I:120:ARG:NH2	3:I:197:ASP:OD2	2.35	0.53
2:K:41:THR:O	2:K:45:MET:HG3	2.09	0.53
3:L:180:ILE:HD12	3:L:184:LEU:HB2	1.90	0.52
1:G:102:VAL:HG11	3:I:174:ASN:CG	2.30	0.52
1:J:19:LYS:O	1:J:22:SER:OG	2.26	0.52
1:G:72:PRO:HD2	2:H:75:MET:HE3	1.92	0.52
2:H:38:THR:HG23	2:H:80:LYS:HD3	1.91	0.52
1:A:23:THR:OG1	1:A:26:GLU:HG3	2.10	0.52
3:I:73:GLN:HB2	3:I:141:ASN:OD1	2.10	0.52
3:C:104:GLY:HA3	2:K:63:ARG:NH1	2.26	0.51
1:G:100:PRO:HD2	1:G:103:MET:HE2	1.93	0.51
3:C:75:ILE:HD11	3:C:146:PRO:HG2	1.92	0.51
3:F:129:LEU:HD13	3:F:154:PRO:HB3	1.93	0.51
2:E:38:THR:CG2	2:E:80:LYS:HD3	2.41	0.50
3:C:109:ILE:CD1	3:C:111:SER:HB2	2.41	0.50
1:J:23:THR:OG1	1:J:26:GLU:HG3	2.12	0.50
1:G:84:THR:OG1	1:G:85:PHE:N	2.40	0.50
3:I:203:GLN:HA	3:I:206:ILE:HD12	1.93	0.49
2:K:21:LEU:HD22	2:K:62:PHE:HE2	1.77	0.49
1:A:66:THR:HA	1:G:49:GLN:HE22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:HIS:O	2:E:38:THR:OG1	2.21	0.49
3:F:79:ARG:HE	3:F:150:ASN:CG	2.16	0.49
2:K:37:LEU:HD22	2:K:43:LYS:HG3	1.93	0.49
1:A:32:GLU:OE1	1:A:39:PRO:N	2.44	0.49
2:E:38:THR:HG21	2:E:80:LYS:HD3	1.95	0.49
3:L:90:ASN:HB3	3:L:96[B]:GLN:HG3	1.94	0.48
1:D:45:TYR:HA	1:D:49:GLN:O	2.12	0.48
3:F:63:LEU:HD12	3:F:63:LEU:HA	1.72	0.48
2:H:45:MET:HE1	2:H:60:VAL:HG13	1.96	0.48
3:I:73:GLN:HE22	3:I:108:ARG:NH1	2.12	0.48
1:D:37:ARG:O	1:D:42:GLN:NE2	2.45	0.48
1:D:43:ARG:HD3	1:D:50:LEU:HD13	1.95	0.48
2:K:86:SER:HB3	2:K:88:THR:HG22	1.95	0.48
3:C:180:ILE:HG12	3:C:185:TYR:CE1	2.48	0.48
1:J:11:LYS:HG3	1:J:91:GLU:HG3	1.94	0.48
1:D:68:ARG:NH2	1:D:71:ALA:CB	2.77	0.47
3:C:193:ASN:OD1	3:C:196:LYS:HB3	2.15	0.47
1:G:79:PHE:O	1:G:86:GLU:HG2	2.15	0.47
2:E:34:GLU:O	2:E:34:GLU:HG2	2.11	0.47
3:L:113:ARG:HH11	3:L:113:ARG:HG2	1.79	0.47
2:E:97:PRO:HB3	3:F:169:LEU:HD13	1.97	0.47
1:J:96:PRO:HB2	2:K:98:GLU:HB3	1.97	0.47
1:A:102:VAL:HG11	3:C:174:ASN:CB	2.46	0.46
1:G:80:ARG:HA	1:G:85:PHE:HA	1.98	0.46
2:H:101:LEU:HD13	2:H:101:LEU:HA	1.74	0.46
3:L:154:PRO:HG2	3:L:156:TYR:CE1	2.50	0.46
3:F:79:ARG:NE	3:F:150:ASN:ND2	2.63	0.46
3:C:76:PHE:CD2	3:C:109:ILE:HG21	2.51	0.46
2:H:62:PHE:HB3	2:H:65:ILE:HD12	1.98	0.45
1:A:49:GLN:NE2	1:G:65:GLN:O	2.49	0.45
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.74	0.45
1:J:8:ARG:HG2	1:J:13:THR:HG23	1.98	0.45
1:A:49:GLN:HE21	1:G:68:ARG:NH1	2.14	0.45
3:L:182:ARG:HA	3:L:185:TYR:CD2	2.51	0.45
1:G:103:MET:HG3	3:I:170:VAL:CG2	2.45	0.45
1:A:23:THR:H	1:A:26:GLU:HG3	1.81	0.44
3:C:196:LYS:HD2	3:C:197:ASP:OD1	2.17	0.44
1:D:62:PHE:CZ	1:D:75:VAL:HG22	2.52	0.44
3:F:180:ILE:HG12	3:F:185:TYR:CE1	2.53	0.44
2:H:101:LEU:N	2:H:101:LEU:HD22	2.31	0.44
3:L:168:SER:O	3:L:169:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:LYS:HD2	1:J:62:PHE:CE1	2.52	0.44
1:J:80:ARG:HB2	1:J:85:PHE:CE1	2.53	0.44
3:I:63:LEU:HD12	3:I:63:LEU:HA	1.70	0.44
3:I:79:ARG:HB2	3:I:152:THR:HG22	2.00	0.44
3:C:141:ASN:ND2	3:C:147:ILE:HG12	2.32	0.44
1:G:10:HIS:CD2	1:G:89:CAS:HB2	2.53	0.44
1:D:42:GLN:HG2	1:D:79:PHE:HE1	1.83	0.43
2:H:105:MET:HG2	3:I:180:ILE:HG22	2.01	0.43
1:A:49:GLN:HE21	1:G:68:ARG:CZ	2.31	0.43
3:C:148:PHE:CE1	2:K:45:MET:HG2	2.52	0.43
1:D:46:LYS:HB3	1:D:51:LEU:HD21	1.99	0.43
2:E:107:ALA:HB2	3:F:158:LEU:HG	2.01	0.43
3:F:116:LEU:HD23	3:F:137:VAL:HG22	2.00	0.43
1:G:72:PRO:HD2	2:H:75:MET:HE2	2.00	0.43
1:J:44:LEU:HA	1:J:76:GLY:O	2.19	0.43
1:D:37:ARG:NH2	1:D:80:ARG:O	2.52	0.42
1:D:98:GLU:H	1:D:98:GLU:CD	2.22	0.42
1:A:24:VAL:HG13	1:A:44:LEU:HD12	2.00	0.42
1:D:68:ARG:CZ	1:D:71:ALA:HB3	2.50	0.42
1:G:102:VAL:HG11	3:I:174:ASN:ND2	2.34	0.42
3:I:112:TYR:HB2	3:I:115:HIS:CE1	2.54	0.42
3:C:116:LEU:HD23	3:C:116:LEU:HA	1.91	0.42
2:K:86:SER:HB3	2:K:88:THR:CG2	2.50	0.42
3:L:73:GLN:OE1	3:L:108:ARG:HD2	2.20	0.42
1:A:91:GLU:CD	1:A:92:PRO:HD2	2.39	0.42
3:F:71:PRO:HB3	3:F:110:HIS:NE2	2.34	0.42
1:G:96:PRO:HB2	2:H:98:GLU:HB3	2.02	0.42
3:I:176:ARG:HA	3:I:185:TYR:HE1	1.78	0.42
2:B:101:LEU:HD11	3:C:178:LEU:HD22	2.01	0.42
3:C:108:ARG:O	3:C:108:ARG:HG3	2.20	0.42
3:L:113:ARG:HG2	3:L:113:ARG:NH1	2.34	0.41
1:G:103:MET:SD	2:H:101:LEU:HD21	2.60	0.41
3:I:133:THR:OG1	3:I:134:GLU:N	2.53	0.41
1:G:34:ILE:HD11	2:H:18:TYR:CZ	2.55	0.41
2:E:103:LEU:HD12	2:E:103:LEU:HA	1.86	0.41
2:E:25:ASP:OD1	2:E:25:ASP:N	2.52	0.41
1:G:24:VAL:HG13	1:G:44:LEU:HD12	2.03	0.41
1:G:62:PHE:CZ	1:G:75:VAL:HG22	2.56	0.41
3:F:106:GLY:O	3:F:107:ARG:HD2	2.21	0.41
2:K:69:VAL:HG21	2:K:102:GLU:HB3	2.03	0.41
2:K:101:LEU:HD12	2:K:101:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HE3	1:A:44:LEU:HG	2.02	0.41
3:L:81:PRO:HD2	3:L:153:LEU:HG	2.03	0.41
2:E:80:LYS:O	2:E:80:LYS:HG2	2.17	0.40
3:L:141:ASN:ND2	3:L:147:ILE:HG12	2.36	0.40
3:C:141:ASN:N	3:C:141:ASN:ND2	2.68	0.40
2:E:101:LEU:HD13	2:E:101:LEU:HA	1.85	0.40
2:B:95:ILE:HB	3:C:165:VAL:HG21	2.04	0.40
1:G:43:ARG:HD2	1:G:50:LEU:CD1	2.51	0.40
1:G:103:MET:HE1	2:H:101:LEU:HD23	2.03	0.40
3:C:107:ARG:NH1	2:K:64:GLU:OE1	2.54	0.40
2:K:20:LYS:HE3	2:K:28:GLU:HB3	2.03	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	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
1	D	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
1	G	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
1	J	98/104 (94%)	96 (98%)	2 (2%)	0	100	100
2	B	87/97 (90%)	87 (100%)	0	0	100	100
2	E	86/97 (89%)	85 (99%)	1 (1%)	0	100	100
2	H	86/97 (89%)	85 (99%)	1 (1%)	0	100	100
2	K	84/97 (87%)	84 (100%)	0	0	100	100
3	C	143/162 (88%)	139 (97%)	4 (3%)	0	100	100
3	F	142/162 (88%)	138 (97%)	4 (3%)	0	100	100
3	I	144/162 (89%)	140 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	141/162 (87%)	138 (98%)	3 (2%)	0	100	100
All	All	1314/1452 (90%)	1283 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	80/91 (88%)	77 (96%)	3 (4%)	33	53
1	D	88/91 (97%)	87 (99%)	1 (1%)	73	84
1	G	85/91 (93%)	80 (94%)	5 (6%)	19	34
1	J	83/91 (91%)	81 (98%)	2 (2%)	49	68
2	B	80/86 (93%)	79 (99%)	1 (1%)	69	81
2	E	79/86 (92%)	77 (98%)	2 (2%)	47	67
2	H	78/86 (91%)	77 (99%)	1 (1%)	69	81
2	K	77/86 (90%)	77 (100%)	0	100	100
3	C	125/147 (85%)	120 (96%)	5 (4%)	31	51
3	F	125/147 (85%)	119 (95%)	6 (5%)	25	44
3	I	132/147 (90%)	129 (98%)	3 (2%)	50	69
3	L	126/147 (86%)	123 (98%)	3 (2%)	49	68
All	All	1158/1296 (89%)	1126 (97%)	32 (3%)	43	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	10	HIS
1	A	95	SER
2	B	35	HIS
3	C	79	ARG

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Mol	Chain	Res	Type
3	C	120	ARG
3	C	148	PHE
3	C	160	GLU
3	C	196	LYS
1	D	10	HIS
2	E	61	ASN
2	E	101	LEU
3	F	67	ASN
3	F	69	ARG
3	F	134	GLU
3	F	148	PHE
3	F	186	GLU
3	F	191	HIS
1	G	29	ARG
1	G	68	ARG
1	G	84	THR
1	G	95	SER
1	G	102	VAL
2	H	108	ASN
3	I	148	PHE
3	I	183	SER
3	I	200	ARG
1	J	9	ARG
1	J	50	LEU
3	L	116	LEU
3	L	148	PHE
3	L	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
3	C	132	GLN
3	F	67	ASN
1	G	49	GLN
3	I	73	GLN
3	L	195	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	CAS	I	77	3	5,8,9	1.02	0	1,9,11	0.57	0
1	CAS	A	89	1	5,8,9	1.12	0	1,9,11	2.41	1 (100%)
3	CAS	C	77	3	5,8,9	1.02	0	1,9,11	0.43	0
3	CAS	L	77	3	5,8,9	1.01	0	1,9,11	0.55	0
3	CAS	F	77	3	5,8,9	0.83	0	1,9,11	1.52	0
1	CAS	D	89	1	5,8,9	1.12	0	1,9,11	1.70	0
1	CAS	G	89	1	5,8,9	1.11	0	1,9,11	1.30	0
1	CAS	J	89	1	5,8,9	1.15	0	1,9,11	0.94	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
3	CAS	I	77	3	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-
1	CAS	G	89	1	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	CAS	CA-CB-SG	-2.41	104.28	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	77	CAS	1	0
3	F	77	CAS	1	0
1	G	89	CAS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	QFR	I	301	-	28,40,40	0.75	1 (3%)	29,60,60	0.80	0
4	QFR	L	301	-	28,40,40	0.75	1 (3%)	29,60,60	0.77	0
4	QFR	F	301	-	28,40,40	0.77	1 (3%)	29,60,60	0.85	0
4	QFR	C	301	-	28,40,40	0.77	1 (3%)	29,60,60	0.75	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	QFR	I	301	-	-	2/25/53/53	0/5/5/5
4	QFR	L	301	-	-	7/25/53/53	0/5/5/5
4	QFR	F	301	-	-	7/25/53/53	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	QFR	C	301	-	-	3/25/53/53	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	QFR	C21-C17	-3.49	1.34	1.39
4	F	301	QFR	C21-C17	-3.45	1.34	1.39
4	L	301	QFR	C21-C17	-3.39	1.34	1.39
4	I	301	QFR	C21-C17	-3.37	1.35	1.39

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	301	QFR	C19-C18-C6-C5
4	F	301	QFR	C20-C18-C6-C5
4	F	301	QFR	C19-C18-C6-C17
4	F	301	QFR	C20-C18-C6-C17
4	L	301	QFR	C19-C18-C6-C5
4	L	301	QFR	C20-C18-C6-C5
4	L	301	QFR	C19-C18-C6-C17
4	L	301	QFR	C20-C18-C6-C17
4	L	301	QFR	O3-C8-C9-C14
4	F	301	QFR	O1-C5-C6-C18
4	C	301	QFR	N2-C8-C9-C14
4	F	301	QFR	N2-C8-C9-C14
4	I	301	QFR	N2-C8-C9-C14
4	C	301	QFR	O3-C8-C9-C10
4	F	301	QFR	O3-C8-C9-C10
4	I	301	QFR	O3-C8-C9-C10
4	L	301	QFR	O3-C8-C9-C10
4	L	301	QFR	O1-C5-C6-C18
4	C	301	QFR	C19-C18-C6-C5

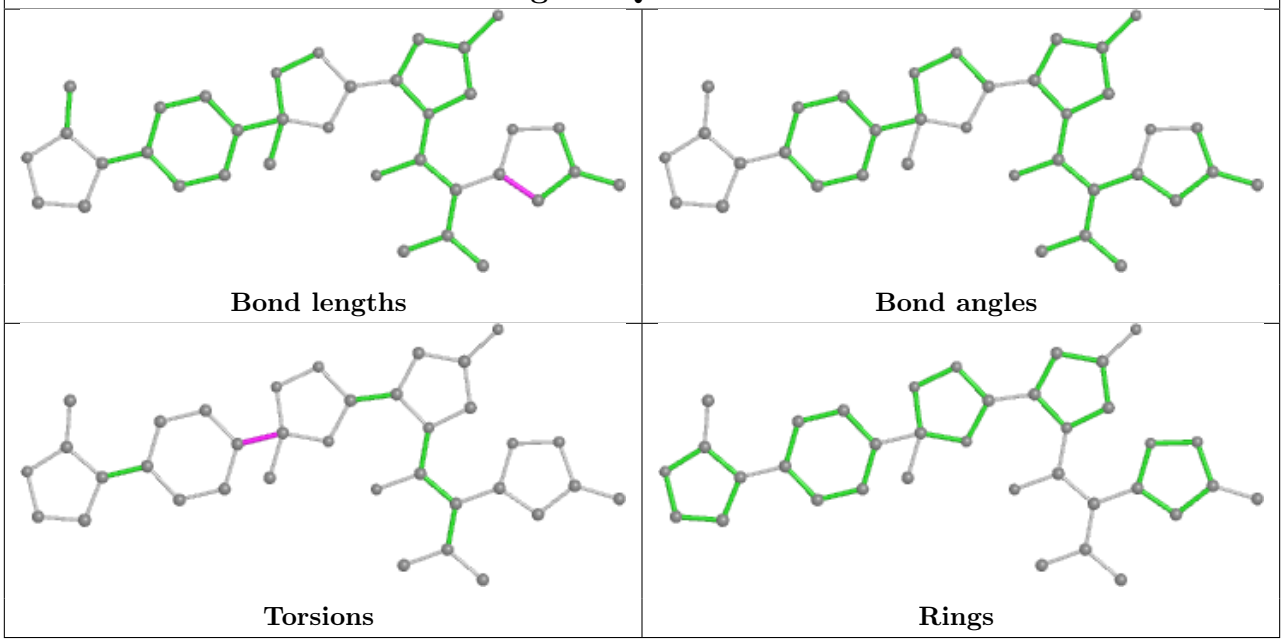
There are no ring outliers.

No monomer is involved in short contacts.

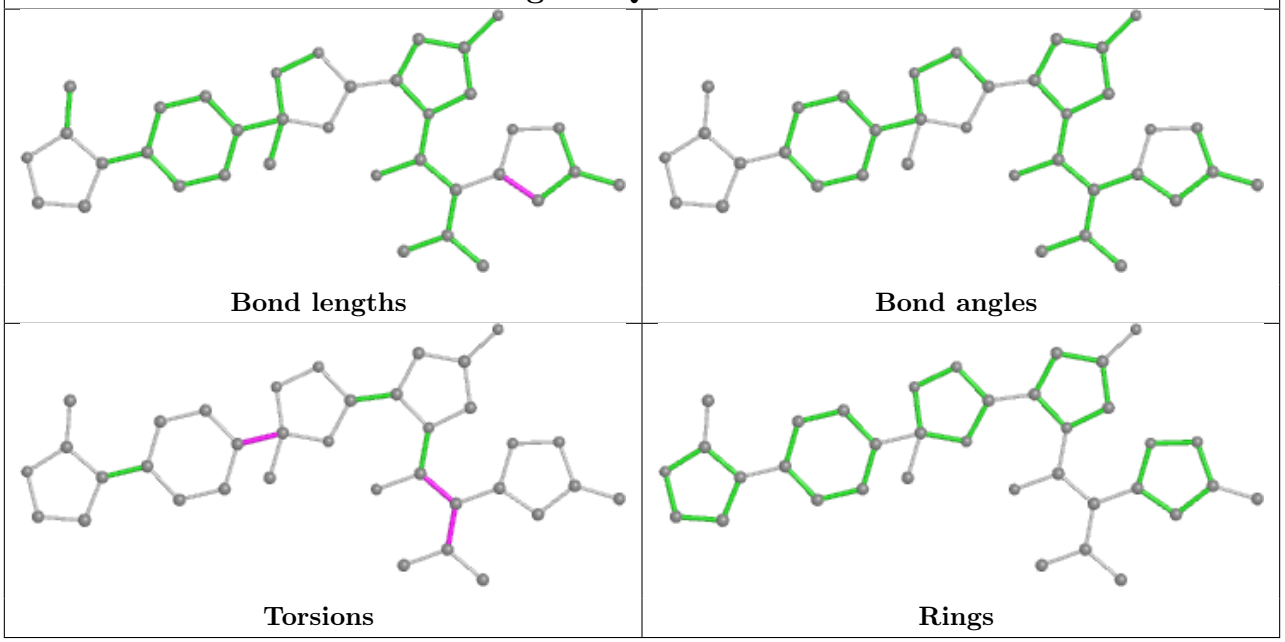
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

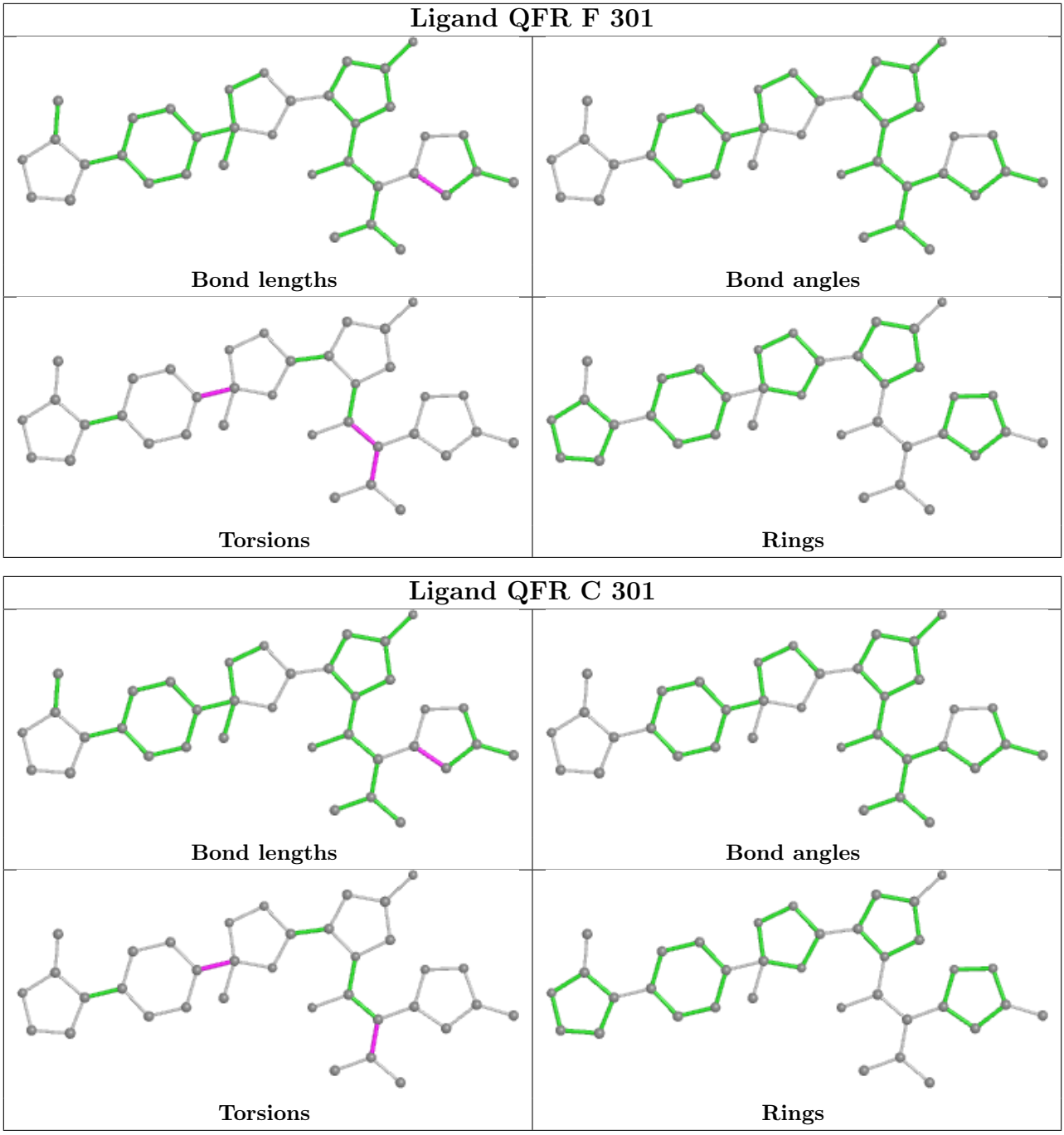
also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 QFR I 301



Ligand QFR L 301





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, 95^{th} 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	103/104 (99%)	0.01	1 (0%) 82 87	59, 80, 110, 122	0
1	D	103/104 (99%)	-0.07	0 100 100	52, 66, 104, 112	0
1	G	103/104 (99%)	-0.04	1 (0%) 82 87	56, 70, 108, 126	0
1	J	102/104 (98%)	0.18	3 (2%) 51 61	62, 86, 113, 124	0
2	B	91/97 (93%)	0.06	1 (1%) 80 86	56, 70, 100, 127	0
2	E	90/97 (92%)	0.08	0 100 100	54, 66, 91, 104	0
2	H	90/97 (92%)	0.01	0 100 100	54, 68, 102, 162	0
2	K	88/97 (90%)	0.24	0 100 100	61, 76, 106, 115	0
3	C	144/162 (88%)	0.16	2 (1%) 75 82	49, 69, 110, 164	0
3	F	144/162 (88%)	0.07	2 (1%) 75 82	48, 66, 120, 149	0
3	I	146/162 (90%)	0.08	2 (1%) 75 82	48, 64, 114, 120	0
3	L	142/162 (87%)	0.11	0 100 100	53, 68, 113, 129	0
All	All	1346/1452 (92%)	0.08	12 (0%) 84 89	48, 70, 111, 164	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	TYR	3.8
1	G	102	VAL	3.5
3	F	140	LEU	3.0
3	C	198	LEU	2.9
1	J	48	ASP	2.6
3	I	180	ILE	2.5
1	J	88	LEU	2.4
3	I	143	ASP	2.3
1	A	81	ALA	2.2
3	F	143	ASP	2.1
1	J	27	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	49	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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
1	CAS	A	89	9/10	0.87	0.16	92,99,156,206	0
1	CAS	D	89	9/10	0.89	0.12	75,82,102,159	0
3	CAS	F	77	9/10	0.92	0.18	57,66,99,101	0
1	CAS	J	89	9/10	0.93	0.14	89,91,132,182	0
1	CAS	G	89	9/10	0.94	0.13	77,85,113,135	0
3	CAS	I	77	9/10	0.95	0.16	50,60,88,96	0
3	CAS	C	77	9/10	0.95	0.13	56,63,100,101	0
3	CAS	L	77	9/10	0.96	0.14	52,61,95,111	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

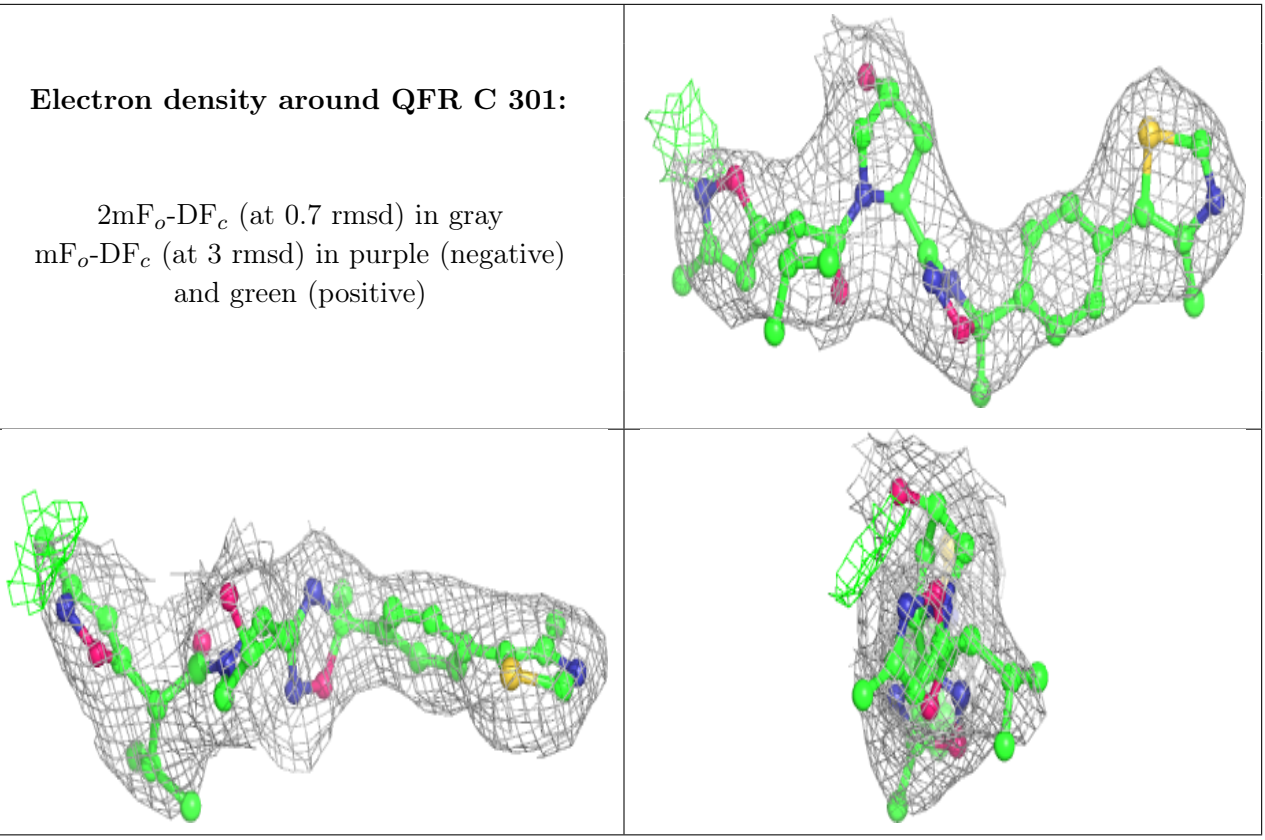
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	QFR	C	301	36/36	0.95	0.20	57,66,83,88	0
4	QFR	F	301	36/36	0.96	0.19	46,60,73,77	0
4	QFR	L	301	36/36	0.96	0.19	51,61,69,71	0
4	QFR	I	301	36/36	0.97	0.18	42,56,63,68	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.

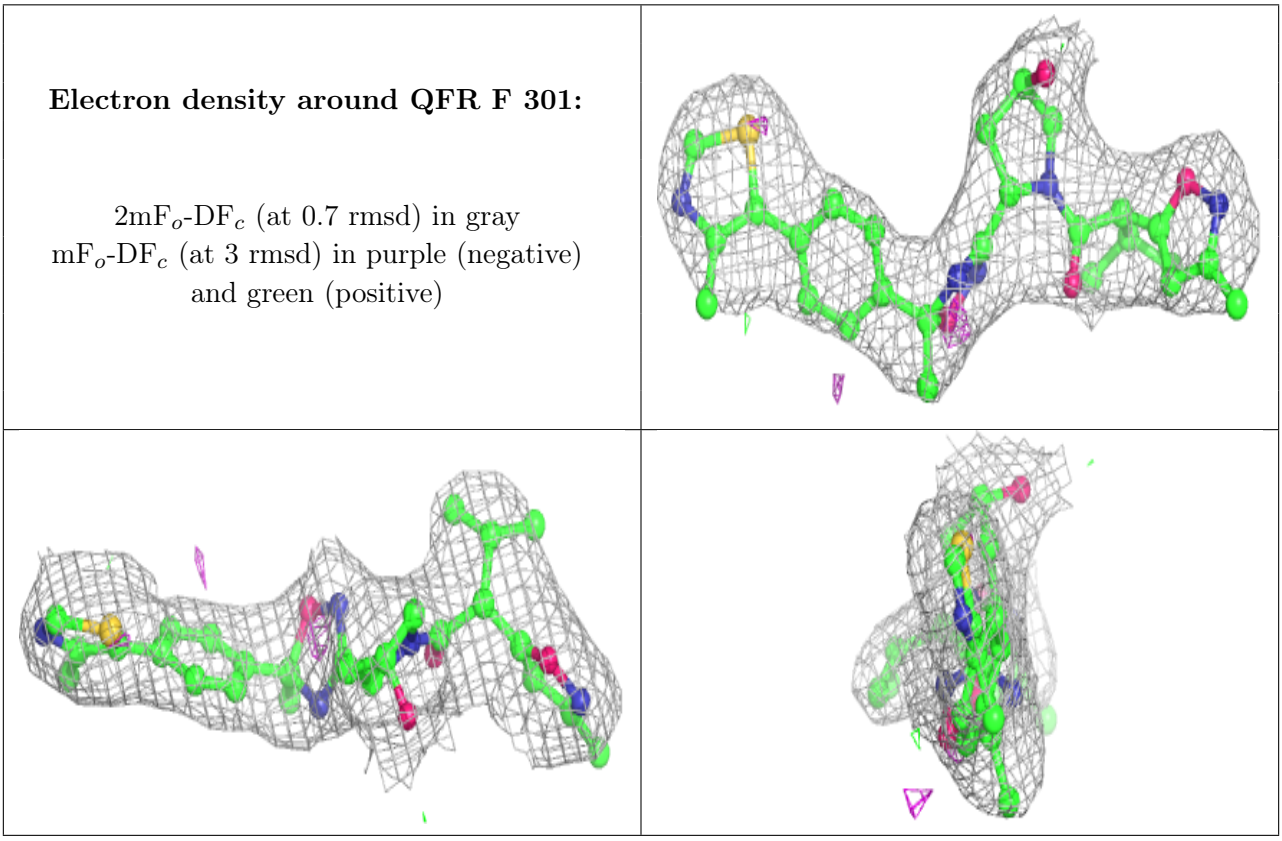
Electron density around QFR C 301:

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



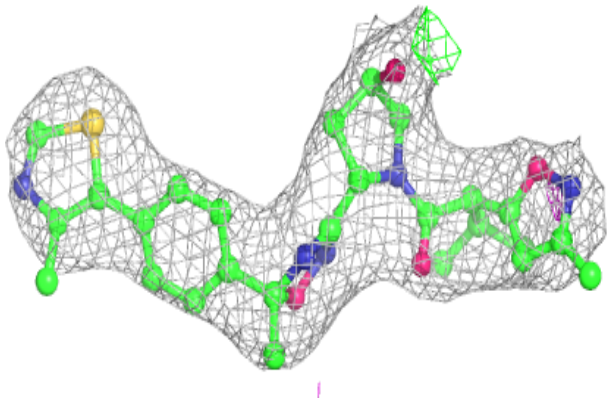
Electron density around QFR F 301:

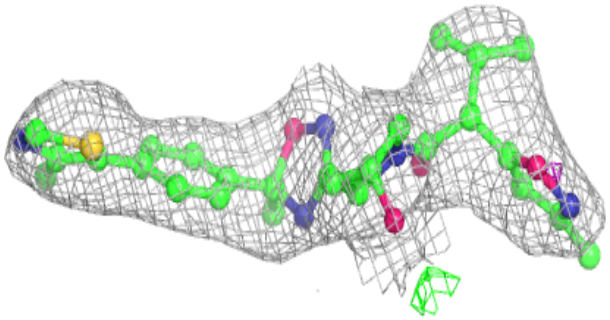
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

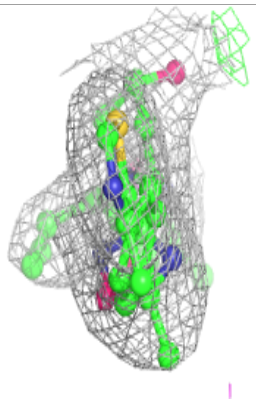


Electron density around QFR L 301:

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

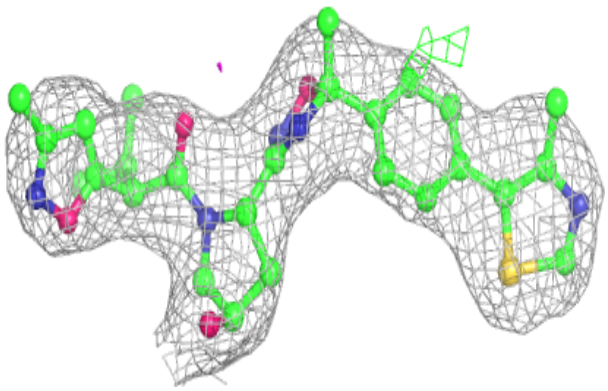


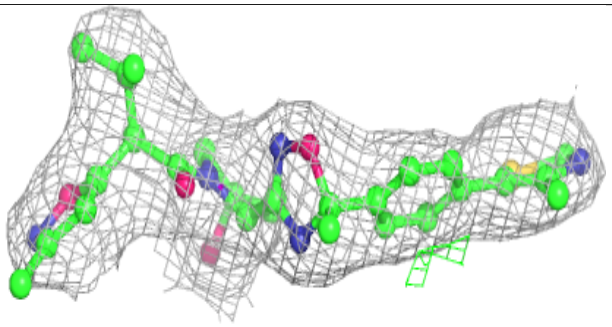


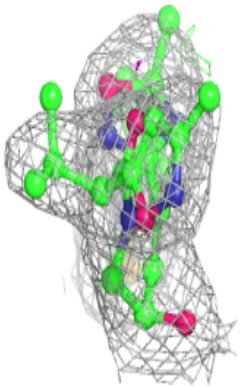


Electron density around QFR I 301:

$2mF_o$-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.