



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2GMH / pdb_00002gmh
Title : Structure of Porcine Electron Transfer Flavoprotein-Ubiquinone Oxidoreductase in Complexed with Ubiquinone
Authors : Zhang, J.; Frerman, F.E.; Kim, J.-J.P.
Deposited on : 2006-04-06
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

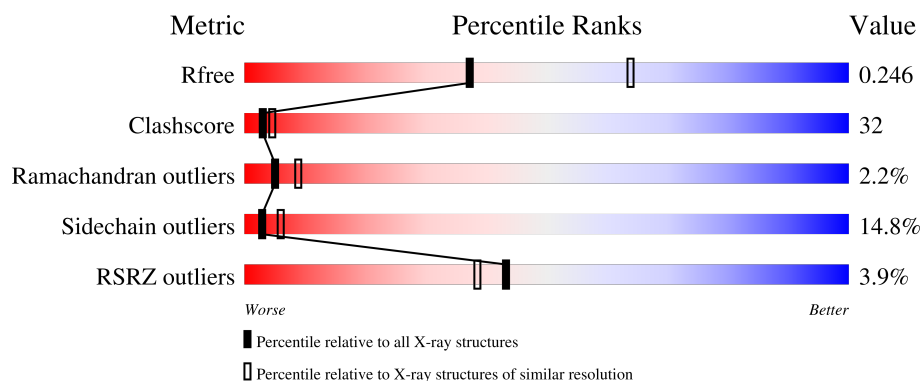
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	584	60% 31% 7% ..
1	B	584	7% 37% 44% 15% ..

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	BHG	A	616	X	-	-	-
2	BHG	A	617	X	-	-	-
2	BHG	B	618	X	-	-	-
7	EDO	A	623	-	-	X	-

2 Entry composition [i](#)

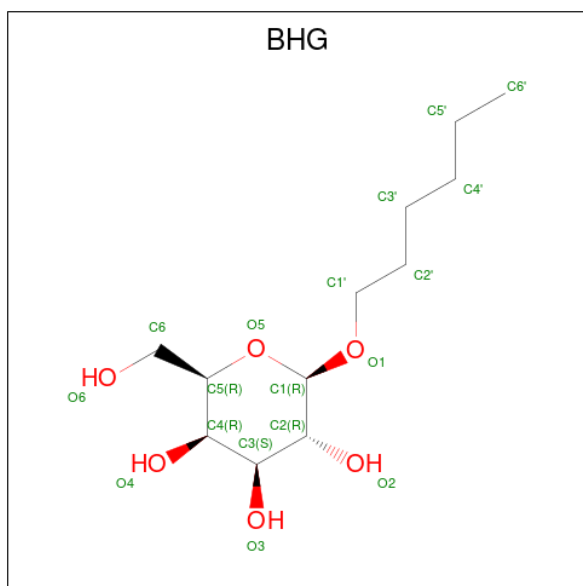
There are 8 unique types of molecules in this entry. The entry contains 9751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Electron transfer flavoprotein-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4558	2910	792	836	20			
1	B	578	Total	C	N	O	S	0	0	0
			4531	2893	787	832	19			

- Molecule 2 is hexyl beta-D-galactopyranoside (CCD ID: BHG) (formula: $C_{12}H_{24}O_6$).

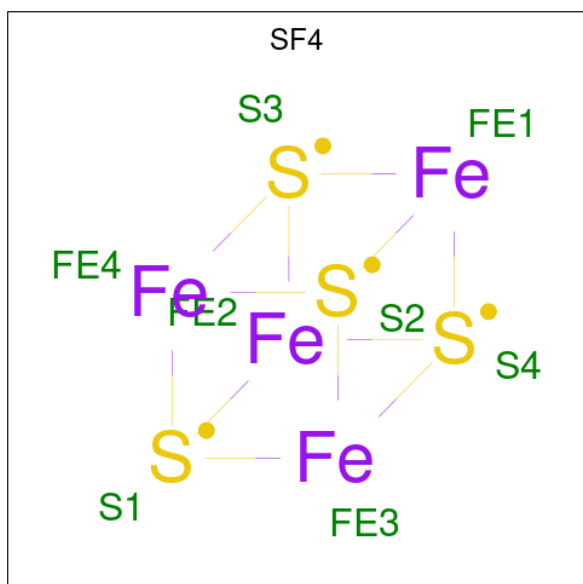


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

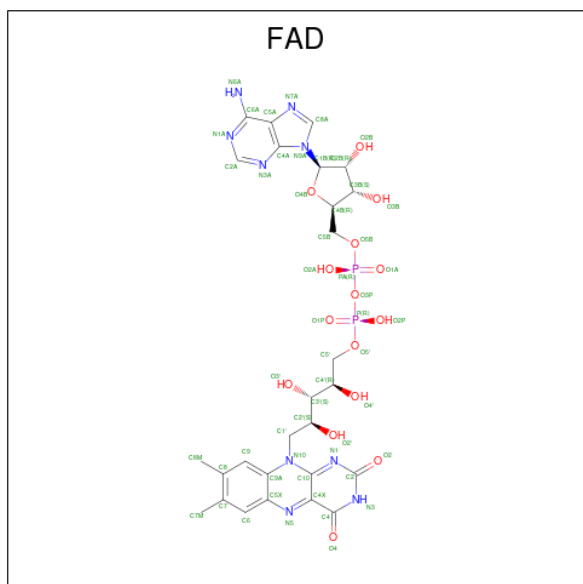
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



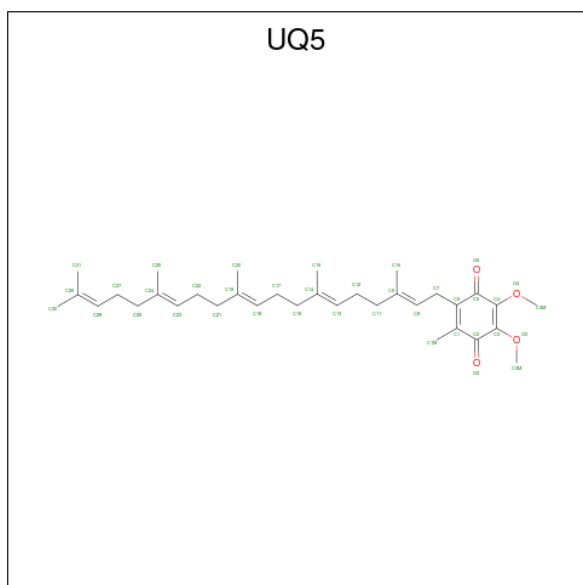
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			38	34	4		
6	B	1	Total	C	O	0	0
			38	34	4		

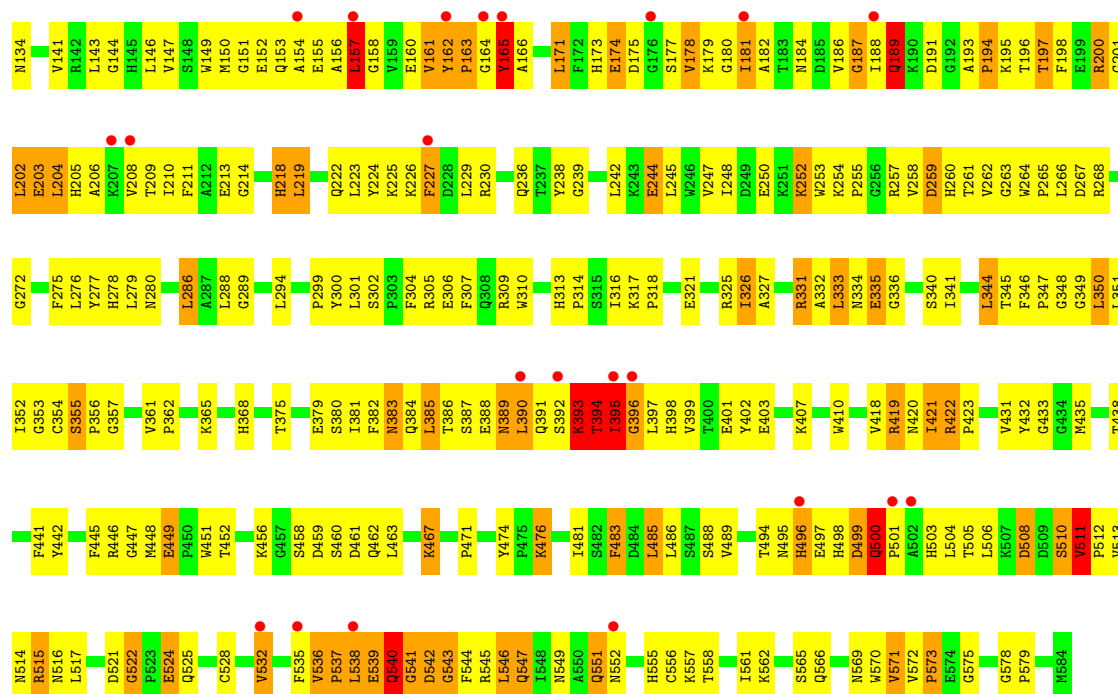
- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	301	Total O 301 301	0	0
8	B	68	Total O 68 68	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.32Å 154.32Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.50 29.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.67-2.50) 98.7 (29.67-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.94 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.254 0.213 , 0.246	Depositor DCC
R_{free} test set	4358 reflections (8.14%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, UQ5, EDO, FAD, BHG, SF4

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	3/4687 (0.1%)	1.32	61/6363 (1.0%)
1	B	0.60	1/4660 (0.0%)	1.31	73/6326 (1.2%)
All	All	0.67	4/9347 (0.0%)	1.32	134/12689 (1.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ARG	CA-C	-6.09	1.45	1.53
1	A	6	VAL	CA-CB	5.97	1.61	1.54
1	A	133	MET	SD-CE	5.60	1.93	1.79
1	B	73	ALA	CA-CB	-5.03	1.45	1.53

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	ASP	N-CA-C	17.99	137.11	113.72
1	A	6	VAL	C-N-CD	-15.72	86.01	120.60
1	A	392	SER	N-CA-C	12.67	124.94	108.34
1	A	6	VAL	CA-C-N	12.59	157.20	127.00
1	A	6	VAL	C-N-CA	12.59	157.20	127.00
1	B	73	ALA	N-CA-C	12.16	124.79	108.38
1	A	388	GLU	N-CA-C	-11.48	90.40	108.30
1	A	5	LYS	N-CA-C	10.73	133.65	110.80
1	B	31	ARG	N-CA-C	10.65	126.32	109.50
1	B	536	VAL	CA-C-N	9.86	132.16	119.84
1	B	536	VAL	C-N-CA	9.86	132.16	119.84
1	A	98	TRP	N-CA-C	9.63	122.98	111.33
1	B	157	LEU	N-CA-C	-9.22	99.31	113.89
1	B	162	TYR	CA-C-N	8.77	133.75	121.91
1	B	162	TYR	C-N-CA	8.77	133.75	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	THR	N-CA-C	-8.59	92.51	110.80
1	B	196	THR	N-CA-C	-8.54	102.64	113.23
1	B	396	GLY	N-CA-C	-8.28	93.55	113.18
1	A	393	LYS	CA-C-N	8.16	137.12	121.54
1	A	393	LYS	C-N-CA	8.16	137.12	121.54
1	B	32	PHE	N-CA-C	-8.11	99.80	110.43
1	A	6	VAL	N-CA-C	8.07	126.31	108.88
1	A	27	VAL	N-CA-C	7.99	120.15	109.37
1	B	166	ALA	N-CA-C	7.78	121.08	108.63
1	A	19	ASP	N-CA-C	-7.74	103.57	113.16
1	A	395	ILE	N-CA-C	-7.61	101.58	111.09
1	B	546	LEU	N-CA-C	7.54	121.02	108.73
1	B	24	TRP	N-CA-C	7.53	122.64	113.38
1	B	121	TYR	N-CA-C	7.48	121.14	110.14
1	B	40	ILE	N-CA-C	7.37	119.00	107.28
1	A	355	SER	N-CA-C	-7.35	102.75	112.75
1	B	500	GLN	CA-C-N	7.32	128.47	119.98
1	B	500	GLN	C-N-CA	7.32	128.47	119.98
1	B	499	ASP	N-CA-C	-7.25	98.94	109.59
1	A	394	THR	N-CA-C	-7.24	95.38	110.80
1	A	541	GLY	N-CA-C	7.21	130.27	113.18
1	A	84	ALA	N-CA-C	7.21	126.15	110.80
1	A	326	ILE	N-CA-C	7.17	119.78	112.90
1	B	528	CYS	CA-C-N	7.14	128.38	120.45
1	B	528	CYS	C-N-CA	7.14	128.38	120.45
1	B	543	GLY	N-CA-C	-7.13	102.80	112.57
1	B	29	MET	N-CA-C	7.09	120.50	107.73
1	B	532	VAL	N-CA-C	7.07	124.05	109.34
1	A	392	SER	CA-C-N	7.06	133.51	122.78
1	A	392	SER	C-N-CA	7.06	133.51	122.78
1	B	163	PRO	N-CA-C	7.01	126.03	113.70
1	B	247	VAL	N-CA-C	-6.97	98.39	108.36
1	A	562	LYS	N-CA-C	6.97	121.87	113.23
1	A	10	THR	N-CA-C	6.96	120.09	108.20
1	B	8	ARG	N-CA-C	-6.89	96.13	110.80
1	B	87	ASP	CA-C-N	6.81	128.35	119.84
1	B	87	ASP	C-N-CA	6.81	128.35	119.84
1	B	7	PRO	CA-C-N	6.81	134.55	121.54
1	B	7	PRO	C-N-CA	6.81	134.55	121.54
1	A	102	GLY	N-CA-C	6.79	125.01	115.43
1	A	83	GLY	N-CA-C	-6.68	97.36	113.18
1	B	93	GLU	N-CA-C	-6.64	103.22	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	THR	N-CA-C	-6.56	99.77	109.81
1	B	203	GLU	N-CA-C	-6.47	98.18	108.73
1	B	497	GLU	N-CA-C	-6.44	100.03	110.20
1	B	86	LEU	N-CA-C	6.38	119.64	109.24
1	B	420	ASN	N-CA-C	6.38	121.06	113.28
1	B	390	LEU	N-CA-C	6.29	119.47	110.10
1	A	121	TYR	N-CA-C	6.26	118.71	109.69
1	A	5	LYS	CA-C-N	6.22	133.63	122.13
1	A	5	LYS	C-N-CA	6.22	133.63	122.13
1	A	85	CYS	N-CA-C	-6.21	97.16	108.02
1	A	338	PHE	N-CA-C	6.21	118.84	111.33
1	B	64	ASP	N-CA-C	6.19	119.28	109.50
1	B	18	ARG	N-CA-C	-6.18	104.61	111.71
1	B	508	ASP	N-CA-C	-6.16	96.90	107.61
1	A	140	VAL	N-CA-C	-6.15	99.56	108.36
1	A	32	PHE	N-CA-C	-6.13	102.28	110.55
1	B	421	ILE	N-CA-C	6.11	116.22	110.30
1	B	65	LEU	N-CA-C	6.08	119.40	109.06
1	A	87	ASP	CA-C-N	6.06	125.74	119.56
1	A	87	ASP	C-N-CA	6.06	125.74	119.56
1	A	390	LEU	N-CA-C	5.97	118.36	109.59
1	B	118	THR	N-CA-C	-5.90	100.37	109.52
1	B	165	TYR	N-CA-C	5.89	120.98	107.48
1	A	185	ASP	N-CA-C	-5.89	102.22	110.35
1	B	511	VAL	CB-CA-C	-5.86	108.14	114.35
1	B	547	GLN	N-CA-C	5.85	119.44	107.69
1	A	343	LYS	N-CA-C	-5.82	101.22	109.96
1	B	326	ILE	CB-CA-C	-5.82	104.72	112.46
1	B	84	ALA	N-CA-C	5.81	123.18	110.80
1	A	86	LEU	N-CA-C	5.81	118.71	109.24
1	A	297	GLN	N-CA-C	5.79	120.48	112.90
1	B	558	THR	N-CA-C	5.78	117.25	111.07
1	B	9	ILE	N-CA-C	-5.69	107.29	111.90
1	B	541	GLY	N-CA-C	5.69	126.67	113.18
1	B	515	ARG	N-CA-C	5.65	119.69	112.12
1	A	382	PHE	N-CA-C	-5.65	104.50	111.33
1	B	25	GLU	N-CA-C	5.62	122.77	110.80
1	A	8	ARG	N-CA-C	-5.61	103.50	111.24
1	B	9	ILE	CB-CA-C	-5.60	105.92	111.30
1	B	193	ALA	N-CA-C	5.59	117.85	110.36
1	A	389	ASN	CA-C-N	5.53	129.20	121.24
1	A	389	ASN	C-N-CA	5.53	129.20	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	LYS	O-C-N	5.49	130.29	123.32
1	A	363	LYS	N-CA-C	-5.46	106.78	113.50
1	B	496	HIS	N-CA-C	-5.46	101.20	108.74
1	B	56	GLN	N-CA-C	-5.42	105.37	111.28
1	B	540	GLN	N-CA-C	5.42	122.34	110.80
1	A	393	LYS	CA-CB-CG	-5.42	103.27	114.10
1	A	492	SER	N-CA-C	-5.37	106.90	113.50
1	B	189	GLN	N-CA-C	5.37	117.34	109.24
1	A	8	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	393	LYS	N-CA-C	-5.35	99.41	110.80
1	A	74	ALA	N-CA-C	-5.34	104.71	111.11
1	B	267	ASP	N-CA-C	-5.32	102.13	110.17
1	B	30	GLU	CA-C-N	-5.32	114.32	122.62
1	B	30	GLU	C-N-CA	-5.32	114.32	122.62
1	A	295	ASP	N-CA-C	-5.32	106.66	112.72
1	B	321	GLU	N-CA-C	-5.29	102.22	110.10
1	A	545	ARG	N-CA-C	-5.29	101.15	109.50
1	B	74	ALA	N-CA-C	5.28	122.04	110.80
1	B	522	GLY	CA-C-N	5.27	125.08	119.28
1	B	522	GLY	C-N-CA	5.27	125.08	119.28
1	A	417	SER	N-CA-C	5.25	117.75	111.71
1	B	34	GLU	N-CA-C	-5.22	100.19	109.06
1	B	433	GLY	N-CA-C	-5.18	106.43	113.37
1	A	497	GLU	N-CA-C	-5.17	102.25	109.96
1	B	59	ALA	N-CA-C	5.17	117.71	111.40
1	A	349	GLY	N-CA-C	5.16	119.12	110.56
1	A	8	ARG	CA-CB-CG	-5.15	103.80	114.10
1	B	544	PHE	N-CA-C	5.12	116.77	109.14
1	A	419	ARG	N-CA-C	5.09	117.56	111.71
1	A	267	ASP	N-CA-C	-5.08	103.82	110.53
1	A	558	THR	N-CA-C	5.07	116.61	111.14
1	B	355	SER	N-CA-C	-5.05	105.58	112.35
1	B	223	LEU	N-CA-C	-5.05	105.67	111.07
1	A	514	ASN	N-CA-C	5.03	116.84	111.36
1	A	361	VAL	N-CA-C	5.00	119.69	108.88

There are no chirality outliers.

There are no planarity outliers.

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	4558	0	4457	211	0
1	B	4531	0	4424	371	0
2	A	36	0	48	5	0
2	B	18	0	24	0	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	53	0	31	2	0
5	B	53	0	31	3	0
6	A	38	0	50	16	0
6	B	38	0	50	13	0
7	A	36	0	54	18	0
7	B	4	0	6	0	0
8	A	301	0	0	8	0
8	B	68	0	0	5	0
All	All	9751	0	9175	588	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 32.

All (588) 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:B:38:VAL:HG12	1:B:67:VAL:HG12	1.26	1.13
1:B:55:LYS:HB2	1:B:157:LEU:HD12	1.30	1.08
1:B:351:LEU:HB3	1:B:356:PRO:HG3	1.43	1.00
1:B:510:SER:O	1:B:514:ASN:HB2	1.62	0.99
1:B:203:GLU:HG2	1:B:205:HIS:CE1	1.97	0.99
1:B:43:ALA:HB3	1:B:71:GLU:HG2	1.46	0.98
1:B:31:ARG:HE	1:B:200:ARG:NH1	1.61	0.98
1:B:34:GLU:HG3	1:B:66:ARG:HH22	1.28	0.98
1:B:12:HIS:ND1	1:B:14:THR:HG23	1.81	0.95
1:A:345:THR:HG22	1:A:398:HIS:CD2	2.03	0.94
1:B:31:ARG:NE	1:B:200:ARG:HH12	1.64	0.93
1:B:208:VAL:HG13	1:B:349:GLY:HA2	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:HB2	1:B:157:LEU:CD1	1.99	0.92
1:B:203:GLU:HG2	1:B:205:HIS:HE1	1.34	0.92
1:A:361:VAL:HG21	1:A:422:ARG:HG3	1.53	0.91
1:B:188:ILE:HG22	1:B:189:GLN:N	1.84	0.90
1:B:209:THR:CG2	1:B:211:PHE:HE1	1.84	0.90
1:B:325:ARG:HH12	1:B:488:SER:HA	1.37	0.90
1:B:38:VAL:HG12	1:B:67:VAL:CG1	2.03	0.89
1:A:5:LYS:HD3	1:A:6:VAL:HG12	1.53	0.89
1:B:325:ARG:HH21	1:B:483:PHE:HB2	1.39	0.88
1:B:508:ASP:HB3	1:B:511:VAL:CG1	2.03	0.88
1:B:209:THR:HG23	1:B:211:PHE:HE1	1.35	0.88
1:B:43:ALA:CB	1:B:71:GLU:HG2	2.04	0.88
1:B:496:HIS:CD2	1:B:578:GLY:H	1.90	0.88
1:B:40:ILE:HB	1:B:69:LEU:HD23	1.56	0.88
1:A:351:LEU:HB3	1:A:356:PRO:HG3	1.53	0.87
1:B:503:HIS:HB2	1:B:571:VAL:O	1.72	0.87
1:B:325:ARG:HH21	1:B:483:PHE:CB	1.87	0.86
1:A:355:SER:HB3	1:A:356:PRO:HD3	1.57	0.86
1:A:551:GLN:H	1:A:551:GLN:HE21	1.23	0.86
1:B:114:PHE:CE1	6:B:615:UQ5:H4M3	2.10	0.86
1:B:188:ILE:HG22	1:B:189:GLN:H	1.38	0.86
1:B:39:VAL:HG23	1:B:206:ALA:HB2	1.56	0.86
1:B:133:MET:HG2	6:B:615:UQ5:H4M1	1.57	0.86
1:B:392:SER:HB2	1:B:394:THR:OG1	1.74	0.86
1:B:72:LYS:HE2	1:B:555:HIS:CD2	2.11	0.86
1:B:248:ILE:HG21	1:B:286:LEU:HD22	1.56	0.85
1:B:188:ILE:CG2	1:B:189:GLN:H	1.89	0.85
1:B:173:HIS:CE1	1:B:179:LYS:HG2	2.12	0.85
1:B:248:ILE:HD13	1:B:286:LEU:HD22	1.55	0.85
1:B:541:GLY:O	1:B:542:ASP:HB2	1.74	0.85
1:A:441:PHE:HB3	1:A:449:GLU:OE2	1.76	0.84
1:B:508:ASP:O	1:B:511:VAL:HG13	1.78	0.84
1:B:361:VAL:HG11	1:B:422:ARG:HG3	1.58	0.83
1:A:353:GLY:O	1:A:356:PRO:HD2	1.77	0.83
1:B:114:PHE:HB2	1:B:127:ILE:HD11	1.61	0.83
1:B:325:ARG:NH2	1:B:483:PHE:HB2	1.94	0.82
1:B:209:THR:HG23	1:B:211:PHE:CE1	2.14	0.82
1:A:551:GLN:H	1:A:551:GLN:NE2	1.78	0.82
1:A:8:ARG:H	1:A:8:ARG:HE	1.28	0.81
1:A:490:ALA:HA	7:A:621:EDO:H21	1.62	0.81
1:B:21:ASP:HB3	1:B:24:TRP:HD1	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HE2	1:B:555:HIS:HD2	1.45	0.81
1:B:171:LEU:HB2	1:B:179:LYS:HB2	1.63	0.81
1:A:117:LEU:CD2	1:A:122:ARG:HG3	2.11	0.80
1:B:81:LEU:HD22	1:B:331:ARG:HB2	1.64	0.80
1:B:498:HIS:CE1	1:B:551:GLN:HB3	2.16	0.80
7:A:621:EDO:H12	8:A:857:HOH:O	1.81	0.80
1:A:34:GLU:HG3	1:A:66:ARG:HH12	1.46	0.80
1:A:443:TRP:O	1:A:446:ARG:NH1	2.15	0.80
1:B:355:SER:HB3	1:B:356:PRO:HD3	1.63	0.79
1:B:15:ILE:HD13	1:B:506:LEU:O	1.83	0.79
1:B:132:PRO:HD3	1:B:442:TYR:CD2	2.18	0.79
1:B:127:ILE:HG22	1:B:127:ILE:O	1.83	0.79
1:A:114:PHE:HE1	6:A:612:UQ5:H4M2	1.48	0.79
1:B:353:GLY:O	1:B:356:PRO:HD2	1.84	0.78
1:B:275:PHE:CE2	1:B:289:GLY:HA3	2.18	0.78
1:B:517:LEU:HA	1:B:522:GLY:N	1.99	0.78
1:B:146:LEU:O	1:B:150:MET:HG3	1.83	0.78
1:A:445:PHE:O	1:A:448:MET:HG3	1.83	0.77
1:A:522:GLY:O	1:A:525:GLN:HG2	1.86	0.76
1:B:227:PHE:HD1	1:B:227:PHE:N	1.82	0.76
1:A:129:PRO:HG2	2:A:617:BHG:H62	1.66	0.76
1:B:73:ALA:CB	1:B:79:HIS:CE1	2.69	0.75
1:B:226:LYS:HB3	1:B:227:PHE:CD1	2.22	0.75
1:B:40:ILE:HB	1:B:69:LEU:CD2	2.16	0.75
1:B:15:ILE:CD1	1:B:505:THR:HB	2.17	0.74
1:B:132:PRO:HD3	1:B:442:TYR:CE2	2.23	0.74
1:B:84:ALA:HB3	1:B:141:VAL:O	1.87	0.73
1:B:334:ASN:HD21	1:B:354:CYS:HB3	1.54	0.73
1:A:361:VAL:HG22	1:A:362:PRO:HD3	1.70	0.73
1:B:512:PRO:CB	1:B:546:LEU:HD22	2.19	0.73
1:B:394:THR:C	1:B:396:GLY:H	1.96	0.72
1:B:508:ASP:HB3	1:B:511:VAL:HG12	1.71	0.72
1:B:73:ALA:HB3	1:B:79:HIS:CE1	2.24	0.72
1:B:227:PHE:N	1:B:227:PHE:CD1	2.55	0.72
1:B:15:ILE:HD11	1:B:505:THR:HB	1.72	0.72
1:B:72:LYS:NZ	1:B:79:HIS:ND1	2.37	0.72
1:B:538:LEU:HB2	1:B:543:GLY:O	1.90	0.72
1:B:522:GLY:O	1:B:525:GLN:HG2	1.89	0.72
1:A:117:LEU:HD23	1:A:122:ARG:HG3	1.72	0.71
6:B:615:UQ5:H153	6:B:615:UQ5:H4M2	1.70	0.71
1:A:345:THR:CG2	1:A:398:HIS:CD2	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD11	1:A:385:LEU:HD13	1.71	0.71
1:A:345:THR:HG22	1:A:398:HIS:HD2	1.54	0.71
1:B:76:ILE:HD11	1:B:161:VAL:HG21	1.71	0.71
1:A:345:THR:CG2	1:A:398:HIS:HD2	2.04	0.70
1:B:173:HIS:ND1	1:B:179:LYS:HG2	2.05	0.70
1:B:393:LYS:HE3	1:B:393:LYS:HA	1.72	0.70
1:B:512:PRO:HB3	1:B:546:LEU:HD22	1.73	0.70
1:B:260:HIS:HB3	6:B:615:UQ5:H3M2	1.73	0.70
1:B:186:VAL:HG12	1:B:187:GLY:N	2.07	0.70
1:A:32:PHE:HA	7:A:628:EDO:H21	1.73	0.70
1:B:21:ASP:OD1	1:B:23:ARG:HD3	1.90	0.70
6:A:612:UQ5:H3M2	6:A:612:UQ5:H4M3	1.74	0.70
1:B:97:ASP:OD2	1:B:101:LYS:HD2	1.92	0.70
1:B:344:LEU:HD12	1:B:403:GLU:OE1	1.92	0.70
1:A:8:ARG:H	1:A:8:ARG:NE	1.90	0.69
1:A:5:LYS:HZ2	1:A:8:ARG:NH1	1.89	0.69
1:B:403:GLU:HG2	1:B:407:LYS:HE3	1.74	0.69
1:A:150:MET:HE1	1:A:371:MET:HE2	1.74	0.69
1:B:210:ILE:HG12	1:B:350:LEU:HD21	1.75	0.69
1:B:310:TRP:CZ2	1:B:316:ILE:HD13	2.28	0.69
1:B:334:ASN:ND2	1:B:354:CYS:HB3	2.08	0.69
1:A:5:LYS:NZ	1:A:8:ARG:NH1	2.40	0.68
1:B:230:ARG:NH2	8:B:1009:HOH:O	2.18	0.68
1:A:8:ARG:N	1:A:8:ARG:CD	2.56	0.68
1:A:490:ALA:HA	7:A:621:EDO:C2	2.22	0.68
1:A:505:THR:HA	7:A:623:EDO:H12	1.74	0.68
1:A:53:ARG:NH1	1:A:57:LEU:HD13	2.09	0.68
1:A:260:HIS:HB3	6:A:612:UQ5:C4M	2.24	0.67
1:B:97:ASP:O	1:B:101:LYS:HB2	1.95	0.67
1:B:432:TYR:HA	1:B:435:MET:HE3	1.76	0.67
1:B:214:GLY:O	1:B:355:SER:HA	1.96	0.66
1:A:31:ARG:HG2	1:A:200:ARG:HD3	1.78	0.66
1:B:498:HIS:HE1	1:B:551:GLN:HB3	1.60	0.65
1:B:40:ILE:O	1:B:70:VAL:HG23	1.96	0.65
1:B:189:GLN:HB3	1:B:499:ASP:OD2	1.96	0.65
1:B:503:HIS:CD2	1:B:573:PRO:HD3	2.32	0.65
1:A:8:ARG:N	1:A:8:ARG:HD2	2.11	0.65
1:B:208:VAL:HA	1:B:348:GLY:O	1.96	0.65
1:B:227:PHE:HD2	1:B:346:PHE:HB2	1.60	0.65
1:B:394:THR:O	1:B:396:GLY:N	2.28	0.65
1:B:34:GLU:CG	1:B:66:ARG:HH22	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:HIS:CE1	1:B:551:GLN:CB	2.80	0.65
1:B:252:LYS:HE2	1:B:318:PRO:O	1.97	0.64
1:B:276:LEU:O	1:B:277:TYR:HD1	1.81	0.64
1:B:512:PRO:O	1:B:516:ASN:HB2	1.97	0.64
1:A:272:GLY:H	6:A:612:UQ5:C1M	2.11	0.64
1:A:132:PRO:O	1:A:363:LYS:HG3	1.98	0.64
1:B:242:LEU:N	1:B:242:LEU:HD12	2.13	0.64
1:A:401:GLU:CD	1:A:401:GLU:H	2.04	0.63
1:B:276:LEU:C	1:B:277:TYR:HD1	2.07	0.63
1:B:70:VAL:HG12	1:B:165:TYR:O	1.99	0.63
1:B:18:ARG:HG3	1:B:29:MET:HE1	1.79	0.63
1:B:79:HIS:CD2	1:B:579:PRO:HD2	2.33	0.63
1:B:257:ARG:HD3	1:B:259:ASP:OD1	1.98	0.63
1:B:52:THR:HG21	1:B:95:PHE:CZ	2.33	0.63
1:A:128:LEU:HD23	2:A:617:BHG:O3	1.99	0.63
1:A:9:ILE:HG22	1:A:548:ILE:HD12	1.81	0.63
1:A:5:LYS:HE3	1:A:8:ARG:HD3	1.80	0.63
1:B:244:GLU:HG2	1:B:307:PHE:HZ	1.63	0.63
1:B:310:TRP:CE2	1:B:316:ILE:HD13	2.34	0.63
1:B:61:HIS:C	1:B:63:LYS:H	2.05	0.62
1:B:117:LEU:HD22	1:B:313:HIS:CE1	2.34	0.62
1:B:347:PRO:HB3	1:B:394:THR:HG21	1.80	0.62
1:A:6:VAL:HG13	1:A:8:ARG:CZ	2.29	0.62
1:A:6:VAL:HG13	1:A:8:ARG:NH2	2.14	0.62
1:A:350:LEU:HD12	1:A:381:ILE:HD11	1.81	0.62
1:A:5:LYS:HE3	1:A:8:ARG:CD	2.30	0.62
1:B:382:PHE:O	1:B:386:THR:HG23	2.00	0.62
1:A:170:ILE:HD13	1:A:223:LEU:HD13	1.82	0.62
1:B:393:LYS:HA	1:B:393:LYS:CE	2.29	0.62
1:B:31:ARG:HE	1:B:200:ARG:HH12	0.79	0.61
1:B:242:LEU:HD22	1:B:304:PHE:HA	1.82	0.61
1:B:180:GLY:HA3	1:B:204:LEU:O	2.00	0.61
1:B:242:LEU:CD2	1:B:304:PHE:HA	2.31	0.61
1:B:248:ILE:HD13	1:B:286:LEU:CD2	2.27	0.61
1:B:483:PHE:N	1:B:483:PHE:HD2	1.98	0.61
1:A:5:LYS:HD3	1:A:6:VAL:CG1	2.27	0.61
1:A:517:LEU:HA	1:A:522:GLY:H	1.66	0.61
1:A:39:VAL:HG23	1:A:206:ALA:HB2	1.81	0.61
1:B:352:ILE:HG22	1:B:402:TYR:OH	2.00	0.61
1:B:365:LYS:HB3	1:B:368:HIS:CE1	2.36	0.61
1:B:14:THR:HG21	1:B:571:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:LEU:O	1:B:489:VAL:HG23	2.01	0.60
1:A:173:HIS:CE1	1:A:179:LYS:HG3	2.36	0.60
1:B:517:LEU:O	1:B:521:ASP:HA	2.01	0.60
1:B:226:LYS:HB3	1:B:227:PHE:HD1	1.63	0.60
1:B:447:GLY:HA2	1:B:449:GLU:OE2	2.01	0.60
1:B:517:LEU:HA	1:B:522:GLY:H	1.65	0.60
1:A:426:HIS:CE1	1:A:456:LYS:HD2	2.36	0.59
1:B:299:PRO:HG3	1:B:463:LEU:HD22	1.84	0.59
1:B:483:PHE:N	1:B:483:PHE:CD2	2.68	0.59
1:A:539:GLU:H	1:A:539:GLU:CD	2.09	0.59
1:B:22:LYS:O	1:B:25:GLU:OE2	2.20	0.59
1:A:8:ARG:NE	1:A:8:ARG:N	2.51	0.59
1:B:244:GLU:HG2	1:B:307:PHE:CZ	2.38	0.59
1:B:325:ARG:NH2	1:B:483:PHE:CB	2.57	0.59
1:A:335:GLU:HA	1:A:361:VAL:CG1	2.33	0.59
1:B:84:ALA:CB	1:B:141:VAL:O	2.50	0.59
1:A:497:GLU:H	7:A:619:EDO:H12	1.68	0.59
1:B:375:THR:HG22	1:B:379:GLU:OE2	2.03	0.59
1:B:218:HIS:CD2	1:B:572:VAL:HG13	2.38	0.58
1:A:335:GLU:HA	1:A:361:VAL:HG11	1.84	0.58
1:B:160:GLU:HB3	1:B:162:TYR:CE1	2.39	0.58
1:B:499:ASP:O	1:B:500:GLN:HB3	2.01	0.58
1:A:352:ILE:HG22	1:A:402:TYR:OH	2.04	0.58
1:B:345:THR:HB	1:B:398:HIS:NE2	2.18	0.58
1:B:344:LEU:HD12	1:B:403:GLU:CD	2.27	0.58
1:B:72:LYS:NZ	1:B:72:LYS:HB3	2.18	0.58
1:B:86:LEU:HD22	1:B:87:ASP:N	2.18	0.58
1:B:99:LYS:H	1:B:99:LYS:HD2	1.66	0.58
1:B:186:VAL:CG1	1:B:187:GLY:N	2.66	0.58
1:B:476:LYS:CE	1:B:476:LYS:H	2.17	0.58
1:A:15:ILE:HD13	1:A:506:LEU:O	2.04	0.57
1:B:25:GLU:HG2	1:B:26:GLY:N	2.18	0.57
1:A:517:LEU:HA	1:A:522:GLY:N	2.19	0.57
1:B:60:GLN:HG3	1:B:61:HIS:CE1	2.40	0.57
1:A:40:ILE:HB	1:A:69:LEU:HD22	1.86	0.57
1:A:538:LEU:HB2	1:A:543:GLY:O	2.04	0.57
1:A:10:THR:HA	7:A:623:EDO:C2	2.34	0.57
1:B:348:GLY:N	1:B:397:LEU:O	2.34	0.57
1:A:107:THR:HG23	1:A:280:ASN:HB3	1.87	0.57
1:B:209:THR:CG2	1:B:211:PHE:CE1	2.75	0.56
1:B:226:LYS:HD2	1:B:227:PHE:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:C	1:B:277:TYR:CD1	2.82	0.56
1:B:224:TYR:HA	1:B:229:LEU:HD12	1.88	0.56
1:B:294:LEU:O	1:B:459:ASP:HB3	2.06	0.56
1:B:300:TYR:CE2	1:B:471:PRO:HG3	2.41	0.56
1:A:497:GLU:H	7:A:619:EDO:C1	2.17	0.56
1:B:61:HIS:C	1:B:63:LYS:N	2.64	0.56
1:B:300:TYR:CZ	1:B:471:PRO:HG3	2.41	0.56
1:B:317:LYS:HG3	1:B:481:ILE:HD13	1.87	0.56
1:A:107:THR:HB	1:A:140:VAL:HB	1.86	0.56
1:A:372:LYS:HE3	1:A:376:LEU:HD21	1.86	0.56
1:B:499:ASP:O	1:B:500:GLN:CB	2.53	0.56
1:B:260:HIS:HB3	6:B:615:UQ5:C3M	2.34	0.56
1:B:335:GLU:OE2	1:B:422:ARG:NH1	2.36	0.56
1:A:8:ARG:C	1:A:10:THR:N	2.61	0.56
1:B:85:CYS:HB3	1:B:365:LYS:HE3	1.89	0.55
1:B:202:LEU:HD12	1:B:204:LEU:HG	1.88	0.55
1:A:260:HIS:HB3	6:A:612:UQ5:H4M1	1.89	0.55
1:B:317:LYS:HE3	1:B:481:ILE:HD12	1.87	0.55
1:B:25:GLU:HG2	1:B:26:GLY:H	1.72	0.55
1:B:83:GLY:O	1:B:84:ALA:HB3	2.06	0.55
1:B:218:HIS:NE2	1:B:219:LEU:HD13	2.21	0.55
1:A:551:GLN:HE21	1:A:551:GLN:N	1.98	0.55
1:B:422:ARG:N	1:B:423:PRO:HD2	2.21	0.55
1:B:445:PHE:O	1:B:448:MET:HG2	2.07	0.55
1:B:127:ILE:O	1:B:127:ILE:CG2	2.54	0.55
1:B:171:LEU:O	1:B:179:LYS:N	2.33	0.55
1:B:248:ILE:HG21	1:B:286:LEU:CD2	2.34	0.55
1:B:275:PHE:CZ	1:B:289:GLY:HA3	2.41	0.55
1:A:15:ILE:HD12	1:A:505:THR:HB	1.89	0.55
1:A:508:ASP:HB3	1:A:511:VAL:CG1	2.37	0.55
1:B:143:LEU:O	1:B:144:GLY:C	2.50	0.55
1:B:211:PHE:CE2	1:B:219:LEU:HD23	2.42	0.55
1:B:326:ILE:O	1:B:327:ALA:HB2	2.06	0.54
1:A:24:TRP:CE3	1:A:29:MET:HE1	2.42	0.54
1:B:72:LYS:HB3	1:B:72:LYS:HZ3	1.72	0.54
1:B:173:HIS:HB2	1:B:175:ASP:OD1	2.07	0.54
1:B:476:LYS:H	1:B:476:LYS:HE2	1.73	0.54
1:A:29:MET:C	1:A:200:ARG:HD2	2.33	0.54
1:A:6:VAL:HG22	1:A:6:VAL:O	2.07	0.54
1:B:209:THR:HG21	1:B:211:PHE:HE1	1.67	0.54
1:B:505:THR:C	1:B:506:LEU:HD12	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:CG	1:A:200:ARG:HD3	2.37	0.54
1:A:218:HIS:CE1	1:A:219:LEU:HD13	2.43	0.54
1:B:245:LEU:HB2	1:B:327:ALA:HB3	1.90	0.54
1:A:202:LEU:HD12	1:A:203:GLU:N	2.22	0.54
1:B:178:VAL:HG22	1:B:348:GLY:HA3	1.89	0.54
1:B:545:ARG:HG3	1:B:545:ARG:HH11	1.72	0.54
1:B:98:TRP:HB2	1:B:103:ALA:CB	2.38	0.54
1:B:226:LYS:HB3	1:B:227:PHE:CE1	2.42	0.54
1:B:347:PRO:HB3	1:B:394:THR:CG2	2.38	0.54
1:B:389:ASN:H	1:B:389:ASN:ND2	2.04	0.54
1:B:73:ALA:HB2	1:B:79:HIS:CE1	2.42	0.54
1:B:227:PHE:CD2	1:B:346:PHE:HB2	2.43	0.54
1:B:498:HIS:HE1	1:B:551:GLN:CB	2.19	0.54
1:B:38:VAL:CG1	1:B:67:VAL:CG1	2.84	0.53
1:B:81:LEU:CD2	1:B:331:ARG:HB2	2.36	0.53
1:B:341:ILE:HG12	1:B:357:GLY:O	2.08	0.53
1:B:151:GLY:O	1:B:154:ALA:HB3	2.07	0.53
1:B:210:ILE:HD11	1:B:381:ILE:CD1	2.38	0.53
1:B:387:SER:O	1:B:388:GLU:HB2	2.07	0.53
1:A:350:LEU:CD1	1:A:381:ILE:HD11	2.38	0.53
1:B:55:LYS:NZ	1:B:158:GLY:O	2.42	0.53
1:B:177:SER:HB3	1:B:394:THR:HG22	1.90	0.53
1:B:394:THR:C	1:B:396:GLY:N	2.65	0.53
1:B:435:MET:HG3	6:B:615:UQ5:H112	1.90	0.53
1:B:43:ALA:HB3	1:B:71:GLU:CG	2.29	0.53
1:B:301:LEU:HD23	1:B:302:SER:N	2.23	0.53
1:A:500:GLN:OE1	1:A:574:GLU:HG3	2.09	0.53
1:B:441:PHE:CD2	1:B:449:GLU:HG2	2.43	0.53
1:B:208:VAL:CG2	1:B:397:LEU:HB2	2.39	0.53
1:A:271:TYR:HE1	6:A:612:UQ5:H103	1.74	0.53
1:B:15:ILE:HD12	1:B:505:THR:HB	1.90	0.52
1:B:114:PHE:HD2	1:B:125:VAL:HB	1.75	0.52
1:B:385:LEU:HD21	1:B:397:LEU:CD1	2.39	0.52
1:A:230:ARG:HA	1:A:233:CYS:SG	2.49	0.52
1:A:345:THR:HG22	1:A:398:HIS:NE2	2.25	0.52
1:A:355:SER:HB3	1:A:356:PRO:CD	2.35	0.52
1:B:335:GLU:HA	1:B:361:VAL:CG2	2.39	0.52
1:A:497:GLU:N	7:A:619:EDO:H12	2.24	0.52
1:B:85:CYS:H	5:B:614:FAD:C4	2.22	0.52
1:B:188:ILE:CG2	1:B:189:GLN:N	2.46	0.52
1:A:272:GLY:H	6:A:612:UQ5:H1M2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:CG1	1:B:67:VAL:HG12	2.19	0.52
1:B:254:LYS:H	1:B:278:HIS:CE1	2.28	0.52
1:B:517:LEU:HD22	1:B:535:PHE:CD2	2.43	0.52
1:A:246:TRP:O	1:A:285:LEU:HD12	2.10	0.52
1:A:272:GLY:N	6:A:612:UQ5:H1M1	2.25	0.52
1:A:29:MET:CA	1:A:200:ARG:HD2	2.40	0.52
1:A:335:GLU:OE2	1:A:422:ARG:NH1	2.43	0.52
1:B:262:VAL:HG12	1:B:263:GLY:H	1.75	0.51
1:B:76:ILE:HD11	1:B:161:VAL:CG2	2.40	0.51
1:B:208:VAL:HG23	1:B:397:LEU:HB2	1.90	0.51
1:B:300:TYR:CD2	1:B:471:PRO:HA	2.46	0.51
1:B:302:SER:HB3	1:B:305:ARG:HB2	1.92	0.51
1:A:10:THR:HG23	7:A:623:EDO:H11	1.92	0.51
1:A:150:MET:HE1	1:A:371:MET:CE	2.41	0.51
1:A:539:GLU:OE1	1:A:539:GLU:N	2.38	0.51
1:A:181:ILE:HD12	1:A:181:ILE:C	2.36	0.51
1:A:43:ALA:HB2	1:A:69:LEU:HD11	1.92	0.51
1:A:117:LEU:HD21	1:A:122:ARG:HG3	1.92	0.51
1:B:262:VAL:HG12	1:B:263:GLY:N	2.25	0.51
1:B:538:LEU:HG	1:B:543:GLY:C	2.36	0.51
1:B:13:TYR:HB2	1:B:18:ARG:HD2	1.93	0.50
1:A:29:MET:HA	1:A:200:ARG:HD2	1.94	0.50
1:B:12:HIS:ND1	1:B:14:THR:CG2	2.65	0.50
1:B:40:ILE:O	1:B:69:LEU:CD2	2.60	0.50
1:A:393:LYS:O	1:A:394:THR:HG23	2.10	0.50
1:B:98:TRP:CZ3	1:B:105:LEU:HB2	2.46	0.50
1:B:118:THR:O	1:B:119:GLU:C	2.55	0.50
1:B:335:GLU:HA	1:B:361:VAL:HG22	1.94	0.50
1:B:48:LEU:HD13	1:B:150:MET:HB2	1.93	0.50
1:A:420:ASN:ND2	1:A:449:GLU:OE1	2.45	0.50
1:B:33:ALA:HA	1:B:203:GLU:O	2.11	0.50
1:B:257:ARG:HG2	1:B:258:VAL:N	2.25	0.50
1:B:43:ALA:HB2	1:B:69:LEU:HD13	1.94	0.50
1:B:43:ALA:HB1	1:B:71:GLU:HG2	1.92	0.50
1:B:107:THR:OG1	1:B:280:ASN:HB3	2.12	0.50
1:B:538:LEU:O	1:B:540:GLN:N	2.45	0.50
1:A:282:GLY:HA2	7:A:627:EDO:H21	1.94	0.49
1:B:86:LEU:O	1:B:88:PRO:HD3	2.11	0.49
1:B:213:GLU:OE2	1:B:219:LEU:HB2	2.12	0.49
1:A:5:LYS:HZ2	1:A:6:VAL:CG1	2.25	0.49
1:A:34:GLU:HG3	1:A:66:ARG:NH1	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:THR:O	1:B:379:GLU:HG3	2.12	0.49
1:A:299:PRO:O	1:A:526:ARG:HD2	2.13	0.49
1:A:388:GLU:O	1:A:389:ASN:C	2.56	0.49
1:B:399:VAL:HG13	1:B:401:GLU:OE1	2.12	0.49
1:A:557:LYS:HE2	1:A:570:TRP:CE3	2.47	0.49
1:B:210:ILE:HA	1:B:350:LEU:HD23	1.95	0.49
1:B:545:ARG:HG3	1:B:545:ARG:NH1	2.27	0.49
1:B:203:GLU:CG	1:B:205:HIS:HE1	2.17	0.49
1:A:213:GLU:OE2	1:A:219:LEU:HB2	2.12	0.49
1:B:55:LYS:O	1:B:58:ALA:HB3	2.12	0.49
1:B:75:HIS:ND1	1:B:76:ILE:N	2.60	0.49
1:B:151:GLY:O	1:B:155:GLU:HG3	2.12	0.49
1:B:494:THR:HA	1:B:578:GLY:O	2.13	0.49
1:A:129:PRO:HG2	2:A:617:BHG:C6	2.42	0.49
1:A:65:LEU:HD11	1:A:385:LEU:CD1	2.39	0.49
1:A:273:GLY:C	6:A:612:UQ5:H3M3	2.38	0.49
1:A:333:LEU:HD23	1:A:333:LEU:H	1.76	0.49
1:A:333:LEU:HD23	1:A:333:LEU:N	2.27	0.49
1:B:24:TRP:CE2	1:B:194:PRO:HD3	2.48	0.49
1:B:31:ARG:HD2	1:B:203:GLU:OE1	2.13	0.48
1:B:257:ARG:NH1	8:B:1039:HOH:O	2.44	0.48
1:A:511:VAL:N	1:A:512:PRO:HD2	2.29	0.48
1:B:438:THR:CB	6:B:615:UQ5:H13	2.43	0.48
1:A:227:PHE:HB2	1:A:229:LEU:HD21	1.94	0.48
1:B:85:CYS:SG	1:B:258:VAL:HG11	2.53	0.48
1:B:419:ARG:NH1	1:B:451:TRP:O	2.46	0.48
1:A:5:LYS:HD2	1:A:7:PRO:HA	1.94	0.48
1:B:174:GLU:OE1	1:B:174:GLU:HA	2.13	0.48
1:B:557:LYS:HE2	1:B:570:TRP:CE3	2.49	0.48
1:A:128:LEU:HD23	2:A:617:BHG:HO3	1.79	0.48
1:B:161:VAL:HG23	1:B:163:PRO:HD3	1.94	0.48
1:B:385:LEU:HD21	1:B:397:LEU:HD11	1.95	0.48
1:A:5:LYS:NZ	1:A:6:VAL:HG12	2.28	0.48
1:A:72:LYS:HE3	5:A:611:FAD:O2B	2.14	0.48
1:B:61:HIS:O	1:B:63:LYS:N	2.47	0.48
1:A:73:ALA:HB1	1:A:78:ALA:HB3	1.96	0.48
1:B:236:GLN:OE1	1:B:336:GLY:HA3	2.14	0.48
1:B:264:TRP:CG	1:B:265:PRO:HA	2.49	0.48
1:B:362:PRO:HG3	1:B:418:VAL:HB	1.95	0.48
1:A:438:THR:CB	6:A:612:UQ5:H13	2.43	0.47
1:A:438:THR:OG1	6:A:612:UQ5:H13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:HG12	1:B:350:LEU:CD2	2.43	0.47
1:A:46:ALA:HB1	1:A:352:ILE:HD12	1.96	0.47
1:B:160:GLU:HB3	1:B:162:TYR:HE1	1.78	0.47
1:A:243:LYS:HG2	1:A:244:GLU:N	2.29	0.47
1:A:186:VAL:HG12	1:A:199:GLU:HB2	1.96	0.47
1:B:494:THR:HG21	1:B:552:ASN:O	2.15	0.47
1:A:258:VAL:HG13	1:A:277:TYR:CE2	2.49	0.47
1:A:299:PRO:HG3	1:A:464:LYS:O	2.14	0.47
1:B:40:ILE:CG2	1:B:69:LEU:HD21	2.45	0.47
1:B:99:LYS:C	1:B:101:LYS:H	2.22	0.47
1:A:7:PRO:HD2	1:A:9:ILE:CG1	2.44	0.47
1:A:252:LYS:HD3	1:A:319:THR:HA	1.97	0.47
1:A:272:GLY:O	6:A:612:UQ5:H1M2	2.14	0.47
1:B:316:ILE:HG22	1:B:316:ILE:O	2.15	0.47
1:B:362:PRO:HG3	1:B:421:ILE:HD12	1.96	0.47
1:B:456:LYS:HE3	8:B:918:HOH:O	2.15	0.47
1:B:53:ARG:HD2	1:B:375:THR:HG23	1.97	0.47
1:A:515:ARG:HG3	8:A:1020:HOH:O	2.14	0.47
1:B:40:ILE:O	1:B:69:LEU:HD22	2.15	0.47
1:B:99:LYS:C	1:B:101:LYS:N	2.71	0.47
1:B:114:PHE:CZ	6:B:615:UQ5:H4M3	2.49	0.46
1:B:149:TRP:O	1:B:153:GLN:HG2	2.14	0.46
1:B:244:GLU:HA	1:B:327:ALA:O	2.15	0.46
1:B:317:LYS:HB3	1:B:318:PRO:HD3	1.97	0.46
1:A:29:MET:O	1:A:200:ARG:HD2	2.15	0.46
1:B:306:GLU:CD	1:B:474:TYR:HE2	2.23	0.46
1:B:384:GLN:OE1	1:B:397:LEU:HD22	2.16	0.46
1:A:31:ARG:HG2	1:A:200:ARG:HB3	1.98	0.46
1:B:202:LEU:HD13	1:B:203:GLU:N	2.29	0.46
1:B:549:ASN:HB3	1:B:551:GLN:OE1	2.15	0.46
1:B:80:THR:HG21	1:B:147:VAL:HG21	1.98	0.46
1:B:226:LYS:C	1:B:227:PHE:HD1	2.23	0.46
1:A:239:GLY:O	1:A:333:LEU:HD23	2.16	0.46
1:A:40:ILE:HD12	1:A:51:ALA:HB2	1.98	0.46
1:B:505:THR:O	1:B:506:LEU:HD12	2.15	0.46
1:A:185:ASP:OD1	1:A:201:GLY:N	2.40	0.46
1:B:72:LYS:CE	1:B:555:HIS:HD2	2.23	0.46
1:B:97:ASP:OD2	1:B:101:LYS:CD	2.63	0.46
1:B:388:GLU:OE1	1:B:388:GLU:HA	2.16	0.46
6:B:615:UQ5:H162	6:B:615:UQ5:H203	1.98	0.46
1:B:34:GLU:HG3	1:B:66:ARG:NH2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:VAL:CG1	1:B:187:GLY:H	2.29	0.46
1:B:210:ILE:HA	1:B:350:LEU:CD2	2.46	0.46
1:B:383:ASN:HD22	1:B:383:ASN:HA	1.51	0.46
1:A:399:VAL:HA	1:A:401:GLU:OE1	2.15	0.45
1:B:95:PHE:O	1:B:98:TRP:HD1	1.99	0.45
1:A:21:ASP:OD1	1:A:24:TRP:HD1	1.99	0.45
1:A:211:PHE:HB2	1:A:351:LEU:HD23	1.97	0.45
1:A:495:ASN:C	1:A:495:ASN:HD22	2.25	0.45
1:A:5:LYS:HE3	1:A:8:ARG:HD2	1.99	0.45
1:A:97:ASP:OD2	1:A:101:LYS:HE3	2.15	0.45
1:A:182:ALA:HA	1:A:202:LEU:O	2.16	0.45
1:A:502:ALA:HB3	7:A:623:EDO:H21	1.98	0.45
1:B:175:ASP:OD2	1:B:394:THR:HA	2.16	0.45
1:A:72:LYS:HD3	1:A:572:VAL:HG12	1.98	0.45
6:A:612:UQ5:H251	6:A:612:UQ5:H272	1.45	0.45
1:B:261:THR:HG23	8:B:719:HOH:O	2.15	0.45
1:A:114:PHE:CE1	6:A:612:UQ5:H4M2	2.39	0.45
1:A:87:ASP:HA	1:A:138:ASN:OD1	2.16	0.45
1:B:210:ILE:HD11	1:B:381:ILE:HD12	1.98	0.45
1:B:460:SER:OG	1:B:566:GLN:HG2	2.17	0.45
1:B:260:HIS:CD2	6:B:615:UQ5:H3M1	2.52	0.45
1:B:344:LEU:HD12	1:B:344:LEU:H	1.82	0.45
1:B:361:VAL:HG11	1:B:422:ARG:CG	2.38	0.45
1:A:107:THR:HG23	1:A:280:ASN:CB	2.46	0.44
1:A:218:HIS:NE2	7:A:622:EDO:O1	2.49	0.44
1:B:188:ILE:HG21	1:B:501:PRO:HG3	1.99	0.44
1:A:407:LYS:NZ	8:A:806:HOH:O	2.50	0.44
1:A:502:ALA:O	7:A:623:EDO:H21	2.17	0.44
1:B:392:SER:CB	1:B:394:THR:OG1	2.56	0.44
1:A:126:PRO:HB3	1:B:123:ILE:CG2	2.47	0.44
1:A:230:ARG:HB3	8:A:1015:HOH:O	2.16	0.44
1:B:198:PHE:HZ	1:B:200:ARG:HD3	1.82	0.44
1:B:52:THR:HG21	1:B:95:PHE:HZ	1.82	0.44
1:B:182:ALA:HA	1:B:202:LEU:O	2.18	0.44
1:B:189:GLN:NE2	1:B:191:ASP:OD1	2.41	0.44
1:B:238:TYR:CG	1:B:561:ILE:HD13	2.53	0.44
1:B:344:LEU:HB2	1:B:402:TYR:HE1	1.80	0.44
1:A:360:ASN:ND2	1:A:363:LYS:HD3	2.32	0.44
1:B:307:PHE:O	1:B:307:PHE:CD1	2.70	0.44
1:A:272:GLY:H	6:A:612:UQ5:H1M1	1.82	0.44
1:B:272:GLY:C	6:B:615:UQ5:H1M2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:O	1:B:395:ILE:HG23	2.17	0.44
1:A:15:ILE:CD1	1:A:506:LEU:O	2.65	0.44
1:A:557:LYS:HE2	1:A:570:TRP:CZ3	2.53	0.44
1:B:213:GLU:CD	1:B:219:LEU:HB2	2.42	0.44
1:A:8:ARG:HD3	1:A:8:ARG:HH11	1.55	0.44
1:A:391:GLN:HB3	8:A:805:HOH:O	2.18	0.44
1:B:214:GLY:O	1:B:355:SER:CA	2.65	0.44
1:B:331:ARG:HD2	1:B:332:ALA:H	1.83	0.44
1:A:5:LYS:HD3	1:A:6:VAL:N	2.32	0.44
1:A:333:LEU:HD12	1:A:359:MET:HE2	2.00	0.44
1:B:129:PRO:HA	1:B:134:ASN:ND2	2.33	0.44
1:B:239:GLY:O	1:B:333:LEU:HD23	2.17	0.44
1:A:5:LYS:NZ	1:A:8:ARG:HH11	2.15	0.43
1:A:24:TRP:CZ3	1:A:29:MET:HE1	2.52	0.43
1:B:55:LYS:HA	1:B:58:ALA:CB	2.48	0.43
1:B:165:TYR:HD2	1:B:165:TYR:HA	1.49	0.43
1:B:390:LEU:HA	1:B:390:LEU:HD13	1.56	0.43
1:B:516:ASN:HB3	1:B:524:GLU:OE2	2.18	0.43
1:A:113:ARG:HB2	1:A:259:ASP:OD1	2.19	0.43
1:A:161:VAL:HG12	1:A:163:PRO:HD3	2.00	0.43
1:A:214:GLY:O	1:A:355:SER:HA	2.18	0.43
1:B:325:ARG:NH2	1:B:483:PHE:CD1	2.87	0.43
1:B:547:GLN:O	1:B:547:GLN:HG2	2.19	0.43
1:B:556:CYS:O	1:B:557:LYS:HB2	2.18	0.43
1:A:361:VAL:CG2	1:A:362:PRO:HD3	2.46	0.43
1:A:572:VAL:HG23	7:A:622:EDO:O2	2.18	0.43
1:B:181:ILE:HG23	1:B:182:ALA:N	2.33	0.43
1:A:29:MET:HG3	1:A:200:ARG:NE	2.32	0.43
1:A:419:ARG:HG2	1:A:420:ASN:N	2.34	0.43
1:B:157:LEU:HD22	1:B:157:LEU:HA	1.78	0.43
1:B:181:ILE:HD11	1:B:211:PHE:CZ	2.54	0.43
1:B:272:GLY:O	6:B:615:UQ5:H1M2	2.19	0.43
1:B:236:GLN:NE2	1:B:340:SER:CB	2.82	0.43
1:B:387:SER:OG	1:B:389:ASN:ND2	2.51	0.43
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.90	0.43
1:A:293:GLY:C	1:A:295:ASP:H	2.26	0.43
1:A:403:GLU:HG2	1:A:407:LYS:NZ	2.34	0.43
1:B:253:TRP:CD2	1:B:255:PRO:HD3	2.54	0.43
1:A:81:LEU:CD1	1:A:329:GLY:HA3	2.49	0.43
1:A:5:LYS:HZ1	1:A:8:ARG:NH1	2.15	0.42
1:A:128:LEU:CD2	2:A:617:BHG:O3	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:CD2	1:A:435:MET:CE	3.02	0.42
1:B:130:GLY:O	1:B:446:ARG:NH1	2.46	0.42
1:A:13:TYR:OH	7:A:622:EDO:H22	2.18	0.42
1:A:146:LEU:HG	1:A:150:MET:HE2	2.00	0.42
1:B:365:LYS:HA	5:B:614:FAD:C2	2.49	0.42
1:A:5:LYS:CE	1:A:8:ARG:HD3	2.46	0.42
1:A:241:GLY:O	1:A:330:ALA:HA	2.20	0.42
1:A:503:HIS:HB2	1:A:571:VAL:O	2.20	0.42
1:B:154:ALA:C	1:B:156:ALA:N	2.76	0.42
1:B:307:PHE:CD1	1:B:307:PHE:C	2.97	0.42
1:B:387:SER:O	1:B:388:GLU:CB	2.68	0.42
1:A:150:MET:CE	1:A:371:MET:HE2	2.47	0.42
1:A:300:TYR:CG	1:A:471:PRO:HA	2.54	0.42
1:A:552:ASN:ND2	8:A:857:HOH:O	2.52	0.42
1:B:7:PRO:HG2	1:B:9:ILE:HD11	2.02	0.42
1:B:120:LYS:HE3	8:B:913:HOH:O	2.18	0.42
1:A:533:TYR:HB3	1:A:546:LEU:HD11	2.01	0.42
1:A:555:HIS:CD2	1:A:555:HIS:N	2.88	0.42
1:B:31:ARG:NH1	1:B:203:GLU:OE1	2.49	0.42
1:A:325:ARG:HD3	1:A:483:PHE:CE1	2.55	0.42
6:A:612:UQ5:H162	6:A:612:UQ5:H203	2.01	0.42
1:A:5:LYS:HZ2	1:A:8:ARG:CZ	2.33	0.42
1:A:7:PRO:HD2	1:A:9:ILE:HG13	2.02	0.42
1:A:96:PRO:HD2	1:A:97:ASP:OD1	2.20	0.42
1:B:155:GLU:HG2	1:B:161:VAL:HG11	2.01	0.42
1:B:268:ARG:O	1:B:431:VAL:HG13	2.19	0.42
1:A:220:ALA:HA	1:A:223:LEU:HB2	2.02	0.41
1:B:103:ALA:HA	1:B:104:PRO:HD2	1.87	0.41
1:B:128:LEU:HB3	1:B:129:PRO:HD2	2.01	0.41
1:B:294:LEU:O	1:B:562:LYS:NZ	2.43	0.41
1:A:449:GLU:H	1:A:449:GLU:HG2	1.51	0.41
1:B:111:GLU:HG2	1:B:257:ARG:HG3	2.02	0.41
1:B:384:GLN:C	1:B:386:THR:H	2.27	0.41
1:A:335:GLU:CA	1:A:361:VAL:HG11	2.48	0.41
1:B:89:ARG:HD3	1:B:410:TRP:CE2	2.55	0.41
1:B:188:ILE:CG2	1:B:501:PRO:HG3	2.50	0.41
1:B:224:TYR:OH	1:B:355:SER:O	2.38	0.41
1:A:86:LEU:HD22	1:A:87:ASP:N	2.36	0.41
1:A:573:PRO:HA	8:A:1028:HOH:O	2.21	0.41
1:A:10:THR:HA	7:A:623:EDO:H22	2.00	0.41
1:A:21:ASP:OD1	1:A:24:TRP:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG23	1:A:138:ASN:O	2.21	0.41
1:A:538:LEU:HD12	1:A:538:LEU:HA	1.91	0.41
1:B:200:ARG:HB3	1:B:201:GLY:H	1.57	0.41
1:B:516:ASN:ND2	1:B:565:SER:OG	2.48	0.41
1:B:569:ASN:O	1:B:571:VAL:HG23	2.20	0.41
1:A:84:ALA:HB3	1:A:141:VAL:O	2.21	0.41
1:B:59:ALA:C	1:B:61:HIS:H	2.29	0.41
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.72	0.41
1:B:99:LYS:O	1:B:101:LYS:N	2.54	0.41
1:B:184:ASN:ND2	1:B:575:GLY:H	2.19	0.41
1:B:236:GLN:NE2	1:B:340:SER:HB2	2.36	0.41
1:B:355:SER:N	1:B:356:PRO:CD	2.83	0.41
1:B:536:VAL:HA	1:B:537:PRO:HD3	1.68	0.41
6:B:615:UQ5:H251	6:B:615:UQ5:H272	1.73	0.41
1:A:5:LYS:HZ2	1:A:6:VAL:HG12	1.85	0.41
1:A:8:ARG:HE	1:A:8:ARG:N	2.01	0.41
1:B:177:SER:OG	1:B:394:THR:O	2.31	0.41
1:B:184:ASN:CG	1:B:575:GLY:H	2.28	0.41
1:A:5:LYS:HD3	1:A:6:VAL:H	1.87	0.40
1:A:305:ARG:O	1:A:309:ARG:HB3	2.20	0.40
1:A:388:GLU:HB3	1:A:389:ASN:H	1.63	0.40
1:B:42:GLY:O	1:B:43:ALA:HB3	2.21	0.40
1:B:94:LEU:HD13	1:B:95:PHE:CE1	2.56	0.40
1:B:258:VAL:HG12	1:B:277:TYR:CD1	2.57	0.40
1:B:562:LYS:O	1:B:562:LYS:HG3	2.21	0.40
1:A:5:LYS:HZ1	1:A:8:ARG:HH11	1.69	0.40
1:B:56:GLN:O	1:B:60:GLN:HG2	2.21	0.40
1:B:72:LYS:HB2	5:B:614:FAD:C4A	2.50	0.40
1:B:306:GLU:CD	1:B:309:ARG:HH21	2.29	0.40
1:A:294:LEU:O	1:A:459:ASP:HB3	2.21	0.40
1:A:365:LYS:HA	5:A:611:FAD:C2	2.52	0.40
1:B:21:ASP:HB3	1:B:24:TRP:CD1	2.37	0.40
1:B:129:PRO:HA	1:B:134:ASN:HD22	1.85	0.40
1:B:200:ARG:HB3	1:B:200:ARG:HH11	1.87	0.40
1:A:15:ILE:CD1	1:A:505:THR:HB	2.52	0.40
1:A:133:MET:HA	8:A:710:HOH:O	2.20	0.40
1:A:538:LEU:N	1:A:543:GLY:O	2.43	0.40
1:B:198:PHE:CZ	1:B:200:ARG:HD3	2.56	0.40
1:B:244:GLU:CG	1:B:307:PHE:HZ	2.32	0.40
1:A:10:THR:OG1	7:A:623:EDO:H11	2.22	0.40
1:B:195:LYS:HB3	1:B:197:THR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLY:O	1:B:264:TRP:C	2.64	0.40
1:B:467:LYS:H	1:B:467:LYS:HG2	1.58	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	579/584 (99%)	544 (94%)	31 (5%)	4 (1%)	18	34
1	B	576/584 (99%)	493 (86%)	62 (11%)	21 (4%)	2	3
All	All	1155/1168 (99%)	1037 (90%)	93 (8%)	25 (2%)	5	9

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	B	74	ALA
1	B	84	ALA
1	B	99	LYS
1	B	391	GLN
1	B	395	ILE
1	B	500	GLN
1	B	532	VAL
1	B	539	GLU
1	B	62	GLU
1	B	187	GLY
1	B	385	LEU
1	A	6	VAL
1	A	394	THR
1	A	541	GLY
1	B	314	PRO

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Mol	Chain	Res	Type
1	A	7	PRO
1	B	23	ARG
1	B	164	GLY
1	B	542	ASP
1	B	17	PRO
1	B	133	MET
1	B	573	PRO
1	B	537	PRO
1	B	194	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/486 (99%)	426 (88%)	57 (12%)	5	11
1	B	479/486 (99%)	394 (82%)	85 (18%)	2	3
All	All	962/972 (99%)	820 (85%)	142 (15%)	3	6

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	ARG
1	A	18	ARG
1	A	19	ASP
1	A	21	ASP
1	A	22	LYS
1	A	27	VAL
1	A	29	MET
1	A	57	LEU
1	A	62	GLU
1	A	69	LEU
1	A	72	LYS
1	A	81	LEU
1	A	85	CYS

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Mol	Chain	Res	Type
1	A	86	LEU
1	A	128	LEU
1	A	133	MET
1	A	157	LEU
1	A	174	GLU
1	A	200	ARG
1	A	202	LEU
1	A	219	LEU
1	A	223	LEU
1	A	225	LYS
1	A	226	LYS
1	A	244	GLU
1	A	266	LEU
1	A	279	LEU
1	A	286	LEU
1	A	320	LEU
1	A	321	GLU
1	A	331	ARG
1	A	333	LEU
1	A	342	PRO
1	A	359	MET
1	A	361	VAL
1	A	363	LYS
1	A	383	ASN
1	A	390	LEU
1	A	391	GLN
1	A	393	LYS
1	A	401	GLU
1	A	419	ARG
1	A	422	ARG
1	A	449	GLU
1	A	456	LYS
1	A	461	ASP
1	A	462	GLN
1	A	467	LYS
1	A	482	SER
1	A	495	ASN
1	A	511	VAL
1	A	515	ARG
1	A	526	ARG
1	A	529	PRO
1	A	539	GLU

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Mol	Chain	Res	Type
1	A	551	GLN
1	B	8	ARG
1	B	11	THR
1	B	18	ARG
1	B	20	GLN
1	B	23	ARG
1	B	27	VAL
1	B	29	MET
1	B	30	GLU
1	B	31	ARG
1	B	53	ARG
1	B	60	GLN
1	B	64	ASP
1	B	65	LEU
1	B	69	LEU
1	B	70	VAL
1	B	71	GLU
1	B	72	LYS
1	B	80	THR
1	B	85	CYS
1	B	86	LEU
1	B	94	LEU
1	B	99	LYS
1	B	133	MET
1	B	152	GLU
1	B	157	LEU
1	B	161	VAL
1	B	165	TYR
1	B	171	LEU
1	B	174	GLU
1	B	178	VAL
1	B	181	ILE
1	B	189	GLN
1	B	197	THR
1	B	200	ARG
1	B	202	LEU
1	B	204	LEU
1	B	218	HIS
1	B	219	LEU
1	B	222	GLN
1	B	225	LYS
1	B	227	PHE

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Mol	Chain	Res	Type
1	B	244	GLU
1	B	250	GLU
1	B	252	LYS
1	B	259	ASP
1	B	266	LEU
1	B	279	LEU
1	B	286	LEU
1	B	288	LEU
1	B	331	ARG
1	B	333	LEU
1	B	335	GLU
1	B	344	LEU
1	B	350	LEU
1	B	380	SER
1	B	383	ASN
1	B	389	ASN
1	B	393	LYS
1	B	394	THR
1	B	395	ILE
1	B	419	ARG
1	B	422	ARG
1	B	449	GLU
1	B	452	THR
1	B	458	SER
1	B	461	ASP
1	B	462	GLN
1	B	467	LYS
1	B	476	LYS
1	B	483	PHE
1	B	485	LEU
1	B	486	LEU
1	B	495	ASN
1	B	500	GLN
1	B	504	LEU
1	B	510	SER
1	B	511	VAL
1	B	513	VAL
1	B	515	ARG
1	B	524	GLU
1	B	538	LEU
1	B	539	GLU
1	B	540	GLN

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Mol	Chain	Res	Type
1	B	551	GLN
1	B	571	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	61	HIS
1	A	173	HIS
1	A	280	ASN
1	A	334	ASN
1	A	384	GLN
1	A	495	ASN
1	A	525	GLN
1	A	551	GLN
1	A	552	ASN
1	B	60	GLN
1	B	205	HIS
1	B	334	ASN
1	B	383	ASN
1	B	389	ASN
1	B	426	HIS
1	B	462	GLN
1	B	498	HIS
1	B	516	ASN
1	B	525	GLN
1	B	552	ASN
1	B	582	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	628	-	3,3,3	0.80	0	2,2,2	0.37	0
7	EDO	A	623	-	3,3,3	0.47	0	2,2,2	0.64	0
6	UQ5	A	612	-	38,38,38	2.64	16 (42%)	48,49,49	2.40	17 (35%)
6	UQ5	B	615	-	38,38,38	2.66	17 (44%)	48,49,49	2.20	22 (45%)
5	FAD	B	614	-	58,58,58	2.34	14 (24%)	85,89,89	1.72	12 (14%)
7	EDO	A	621	-	3,3,3	0.57	0	2,2,2	0.46	0
5	FAD	A	611	-	58,58,58	2.45	17 (29%)	85,89,89	1.39	12 (14%)
4	SF4	A	610	1	0,12,12	-	-	-	-	-
4	SF4	B	613	1	0,12,12	-	-	-	-	-
7	EDO	A	622	-	3,3,3	0.67	0	2,2,2	0.11	0
7	EDO	A	627	-	3,3,3	0.79	0	2,2,2	0.48	0
7	EDO	B	620	-	3,3,3	0.59	0	2,2,2	0.60	0
2	BHG	A	617	-	18,18,18	1.39	4 (22%)	23,23,23	2.45	5 (21%)
7	EDO	A	619	-	3,3,3	0.59	0	2,2,2	0.46	0
2	BHG	B	618	-	18,18,18	1.04	1 (5%)	23,23,23	2.95	3 (13%)
2	BHG	A	616	-	18,18,18	1.09	2 (11%)	23,23,23	3.68	4 (17%)
7	EDO	A	625	-	3,3,3	0.67	0	2,2,2	0.49	0
7	EDO	A	626	-	3,3,3	0.75	0	2,2,2	0.53	0
7	EDO	A	624	-	3,3,3	0.59	0	2,2,2	0.62	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
7	EDO	A	628	-	-	0/1/1/1	-
7	EDO	A	623	-	-	1/1/1/1	-
6	UQ5	A	612	-	-	19/33/57/57	0/1/1/1
6	UQ5	B	615	-	-	17/33/57/57	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	B	614	-	-	6/34/50/50	0/6/6/6
7	EDO	A	621	-	-	1/1/1/1	-
5	FAD	A	611	-	-	3/34/50/50	0/6/6/6
4	SF4	A	610	1	-	-	0/6/5/5
4	SF4	B	613	1	-	-	0/6/5/5
7	EDO	A	622	-	-	1/1/1/1	-
7	EDO	A	627	-	-	0/1/1/1	-
7	EDO	B	620	-	-	1/1/1/1	-
2	BHG	A	617	-	1/1/5/5	5/9/29/29	0/1/1/1
7	EDO	A	619	-	-	1/1/1/1	-
2	BHG	B	618	-	1/1/5/5	5/9/29/29	0/1/1/1
2	BHG	A	616	-	1/1/5/5	7/9/29/29	0/1/1/1
7	EDO	A	625	-	-	1/1/1/1	-
7	EDO	A	626	-	-	0/1/1/1	-
7	EDO	A	624	-	-	1/1/1/1	-

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	FAD	PA-O3P	-9.61	1.49	1.59
5	B	614	FAD	PA-O3P	-8.09	1.50	1.59
6	B	615	UQ5	C28-C29	7.37	1.54	1.32
6	A	612	UQ5	C28-C29	7.06	1.53	1.32
5	A	611	FAD	C6-C5X	6.34	1.49	1.40
6	A	612	UQ5	C8-C9	5.67	1.46	1.33
6	A	612	UQ5	C18-C19	5.50	1.45	1.33
5	B	614	FAD	C4X-N5	5.42	1.42	1.30
6	B	615	UQ5	C18-C19	5.35	1.45	1.33
5	B	614	FAD	C10-N10	5.34	1.48	1.37
6	A	612	UQ5	O3-C3	5.30	1.49	1.36
6	B	615	UQ5	C8-C9	5.25	1.45	1.33
5	B	614	FAD	C6-C5X	4.96	1.47	1.40
6	B	615	UQ5	C7-C8	-4.66	1.43	1.50
5	B	614	FAD	C1'-C2'	-4.63	1.46	1.52
5	B	614	FAD	C9A-C5X	4.43	1.48	1.41
6	B	615	UQ5	C25-C24	4.34	1.61	1.50
5	A	611	FAD	C1'-C2'	-4.19	1.46	1.52
5	B	614	FAD	C5'-C4'	4.18	1.57	1.51
5	B	614	FAD	C4A-N3A	4.11	1.42	1.34
5	A	611	FAD	C4X-N5	4.11	1.39	1.30
5	A	611	FAD	C8-C7	4.08	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	FAD	C1'-N10	-4.03	1.38	1.47
6	B	615	UQ5	C22-C23	-3.92	1.38	1.50
6	A	612	UQ5	C21-C19	3.84	1.59	1.51
5	A	611	FAD	C10-N10	3.76	1.45	1.37
5	A	611	FAD	C5'-C4'	-3.67	1.46	1.51
6	A	612	UQ5	C23-C24	3.64	1.41	1.33
5	A	611	FAD	P-O5'	-3.50	1.45	1.59
5	A	611	FAD	C9-C9A	3.49	1.45	1.39
6	A	612	UQ5	C7-C8	-3.44	1.45	1.50
6	A	612	UQ5	C22-C23	-3.40	1.40	1.50
6	B	615	UQ5	C13-C14	3.33	1.40	1.33
6	B	615	UQ5	C6-C5	3.30	1.55	1.46
6	A	612	UQ5	C13-C14	3.27	1.40	1.33
5	B	614	FAD	C9-C9A	3.26	1.44	1.39
5	A	611	FAD	C9A-C5X	3.09	1.46	1.41
5	B	614	FAD	C9A-N10	2.99	1.46	1.41
5	B	614	FAD	C8-C7	2.98	1.48	1.40
6	A	612	UQ5	O3-C3M	-2.97	1.38	1.45
6	A	612	UQ5	C20-C19	-2.97	1.43	1.50
6	B	615	UQ5	O3-C3	2.96	1.43	1.36
6	B	615	UQ5	C21-C19	2.92	1.57	1.51
6	B	615	UQ5	C20-C19	-2.88	1.43	1.50
2	A	617	BHG	O5-C1	2.85	1.49	1.41
5	A	611	FAD	C4-N3	2.75	1.44	1.38
5	A	611	FAD	C10-N1	2.75	1.38	1.33
6	B	615	UQ5	O4-C4	2.75	1.43	1.36
2	A	617	BHG	O1-C1'	2.72	1.50	1.43
5	A	611	FAD	O4B-C1B	2.69	1.48	1.42
5	A	611	FAD	O4B-C4B	-2.56	1.39	1.45
5	B	614	FAD	C1'-N10	-2.51	1.41	1.47
6	A	612	UQ5	C11-C9	-2.42	1.46	1.51
6	A	612	UQ5	C6-C5	2.42	1.53	1.46
2	A	617	BHG	O5-C5	2.41	1.50	1.44
5	B	614	FAD	C2-N1	-2.40	1.31	1.36
2	A	616	BHG	O1-C1	-2.40	1.36	1.40
5	B	614	FAD	P-O5'	-2.39	1.50	1.59
6	B	615	UQ5	C11-C9	-2.37	1.46	1.51
6	B	615	UQ5	C23-C24	2.30	1.38	1.33
5	A	611	FAD	C4A-N3A	2.30	1.38	1.34
2	B	618	BHG	O5-C1	2.26	1.47	1.41
6	B	615	UQ5	C7-C6	2.26	1.55	1.51
6	A	612	UQ5	C4-C3	2.24	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	615	UQ5	O3-C3M	-2.20	1.40	1.45
6	A	612	UQ5	C25-C24	2.17	1.56	1.50
6	B	615	UQ5	C30-C29	2.15	1.56	1.50
2	A	617	BHG	O1-C1	-2.09	1.36	1.40
5	A	611	FAD	PA-O2A	-2.05	1.45	1.55
6	A	612	UQ5	C12-C13	-2.01	1.44	1.50
2	A	616	BHG	C1-C2	2.01	1.58	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	BHG	O1-C1'-C2'	12.19	150.73	109.37
2	A	616	BHG	C1'-O1-C1	11.18	132.78	113.68
2	A	616	BHG	O1-C1'-C2'	10.43	144.74	109.37
2	A	617	BHG	O1-C1'-C2'	9.85	142.78	109.37
6	A	612	UQ5	C8-C7-C6	7.63	130.88	112.08
5	B	614	FAD	O3'-C3'-C2'	7.32	125.55	108.93
2	A	616	BHG	O1-C1-C2	7.08	119.03	108.27
2	B	618	BHG	C1'-O1-C1	5.87	123.71	113.68
6	A	612	UQ5	C12-C11-C9	-5.27	95.72	113.19
5	B	614	FAD	P-O5'-C5'	5.03	150.18	121.35
6	B	615	UQ5	C12-C11-C9	-4.96	96.73	113.19
5	B	614	FAD	O4B-C1B-C2B	-4.49	97.02	106.62
5	B	614	FAD	O4'-C4'-C3'	4.22	119.12	109.25
5	A	611	FAD	O3'-C3'-C2'	4.21	118.50	108.93
5	B	614	FAD	C9A-C5X-N5	4.12	126.83	122.45
5	B	614	FAD	O2-C2-N1	-3.94	115.25	121.80
6	A	612	UQ5	C15-C14-C16	3.88	121.97	115.23
6	B	615	UQ5	C8-C7-C6	3.84	121.54	112.08
6	A	612	UQ5	C1M-C1-C6	-3.83	118.16	124.45
5	B	614	FAD	O2-C2-N3	3.80	125.87	118.58
5	A	611	FAD	O2-C2-N3	3.77	125.82	118.58
6	B	615	UQ5	C1-C6-C5	-3.77	115.96	119.62
5	A	611	FAD	O4B-C1B-C2B	-3.76	98.58	106.62
6	B	615	UQ5	C20-C19-C21	3.66	121.58	115.23
6	A	612	UQ5	O2-C2-C3	-3.64	113.31	121.03
6	A	612	UQ5	C6-C1-C2	3.63	122.03	119.17
5	A	611	FAD	P-O5'-C5'	3.62	142.10	121.35
6	B	615	UQ5	C6-C1-C2	3.56	121.98	119.17
6	B	615	UQ5	C1M-C1-C6	-3.53	118.65	124.45
6	B	615	UQ5	O2-C2-C3	-3.52	113.57	121.03
2	A	616	BHG	O5-C1-O1	-3.50	101.78	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	612	UQ5	C20-C19-C21	3.49	121.29	115.23
6	A	612	UQ5	C10-C9-C11	3.33	121.01	115.23
6	B	615	UQ5	C11-C12-C13	3.33	128.50	112.02
6	B	615	UQ5	C15-C14-C16	3.18	120.74	115.23
6	B	615	UQ5	C10-C9-C11	3.16	120.72	115.23
2	A	617	BHG	O1-C1-C2	3.07	112.94	108.27
5	A	611	FAD	O2-C2-N1	-3.02	116.78	121.80
6	B	615	UQ5	O4-C4-C5	3.00	126.75	116.64
6	A	612	UQ5	O5-C5-C6	-2.97	116.04	121.79
5	B	614	FAD	C2'-C1'-N10	2.92	123.98	110.20
6	A	612	UQ5	C17-C18-C19	2.87	134.19	127.62
6	B	615	UQ5	C10-C9-C8	-2.74	116.60	123.63
6	B	615	UQ5	C25-C24-C26	2.71	119.92	115.23
5	A	611	FAD	C5X-C9A-N10	-2.70	115.53	117.97
5	A	611	FAD	O4'-C4'-C3'	2.67	115.51	109.25
6	A	612	UQ5	C31-C29-C30	-2.67	108.44	114.59
6	A	612	UQ5	C16-C17-C18	2.59	124.82	112.02
5	B	614	FAD	C5X-N5-C4X	-2.55	113.96	118.09
6	A	612	UQ5	C1-C6-C5	-2.55	117.14	119.62
2	A	617	BHG	C1'-O1-C1	-2.54	109.33	113.68
5	A	611	FAD	C3B-C2B-C1B	2.50	106.20	101.46
2	B	618	BHG	C4'-C3'-C2'	2.50	127.01	114.37
5	A	611	FAD	C9A-C5X-N5	2.49	125.10	122.45
5	A	611	FAD	C2'-C1'-N10	2.43	121.71	110.20
6	A	612	UQ5	O4-C4-C5	2.36	124.59	116.64
6	A	612	UQ5	C11-C12-C13	2.32	123.52	112.02
2	A	617	BHG	O5-C1-O1	2.31	115.51	110.04
5	B	614	FAD	O3P-PA-O1A	2.30	117.61	110.70
6	B	615	UQ5	O5-C5-C6	-2.29	117.35	121.79
6	B	615	UQ5	C26-C27-C28	2.29	123.34	112.02
6	B	615	UQ5	C31-C29-C30	-2.26	109.38	114.59
5	B	614	FAD	C4-C4X-N5	-2.24	115.11	118.21
5	A	611	FAD	O3B-C3B-C4B	-2.21	104.73	111.08
6	A	612	UQ5	C3-C2-C1	2.20	122.45	118.10
2	A	617	BHG	C4'-C3'-C2'	2.20	125.46	114.37
6	B	615	UQ5	O4-C4-C3	-2.17	115.44	123.64
6	A	612	UQ5	C26-C27-C28	2.15	122.63	112.02
6	B	615	UQ5	C16-C17-C18	2.14	122.61	112.02
6	B	615	UQ5	C4M-O4-C4	2.12	123.94	116.47
6	B	615	UQ5	C25-C24-C23	-2.07	118.31	123.63
6	B	615	UQ5	C7-C6-C5	2.05	120.90	118.52
5	B	614	FAD	C3B-C2B-C1B	2.02	105.29	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	615	UQ5	C3-C2-C1	2.01	122.07	118.10
5	A	611	FAD	C5X-N5-C4X	-2.01	114.84	118.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	616	BHG	C4
2	A	617	BHG	C4
2	B	618	BHG	C4

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	616	BHG	C2-C1-O1-C1'
2	A	616	BHG	O5-C1-O1-C1'
2	A	617	BHG	C2-C1-O1-C1'
2	A	617	BHG	O5-C1-O1-C1'
2	A	617	BHG	C2'-C1'-O1-C1
5	B	614	FAD	C5'-O5'-P-O2P
6	A	612	UQ5	C1-C6-C7-C8
6	A	612	UQ5	C5-C6-C7-C8
6	A	612	UQ5	C6-C7-C8-C9
6	A	612	UQ5	C16-C17-C18-C19
6	A	612	UQ5	C25-C24-C26-C27
6	A	612	UQ5	C26-C27-C28-C29
6	A	612	UQ5	C27-C28-C29-C30
6	B	615	UQ5	C1-C6-C7-C8
6	B	615	UQ5	C5-C6-C7-C8
6	B	615	UQ5	C16-C17-C18-C19
6	B	615	UQ5	C26-C27-C28-C29
6	B	615	UQ5	C27-C28-C29-C31
6	A	612	UQ5	C27-C28-C29-C31
6	B	615	UQ5	C27-C28-C29-C30
6	B	615	UQ5	C20-C19-C21-C22
6	A	612	UQ5	C23-C24-C26-C27
6	B	615	UQ5	C18-C19-C21-C22
6	A	612	UQ5	C20-C19-C21-C22
6	B	615	UQ5	C25-C24-C26-C27
6	B	615	UQ5	C23-C24-C26-C27
6	A	612	UQ5	C9-C11-C12-C13
6	A	612	UQ5	C14-C16-C17-C18
6	B	615	UQ5	C14-C16-C17-C18

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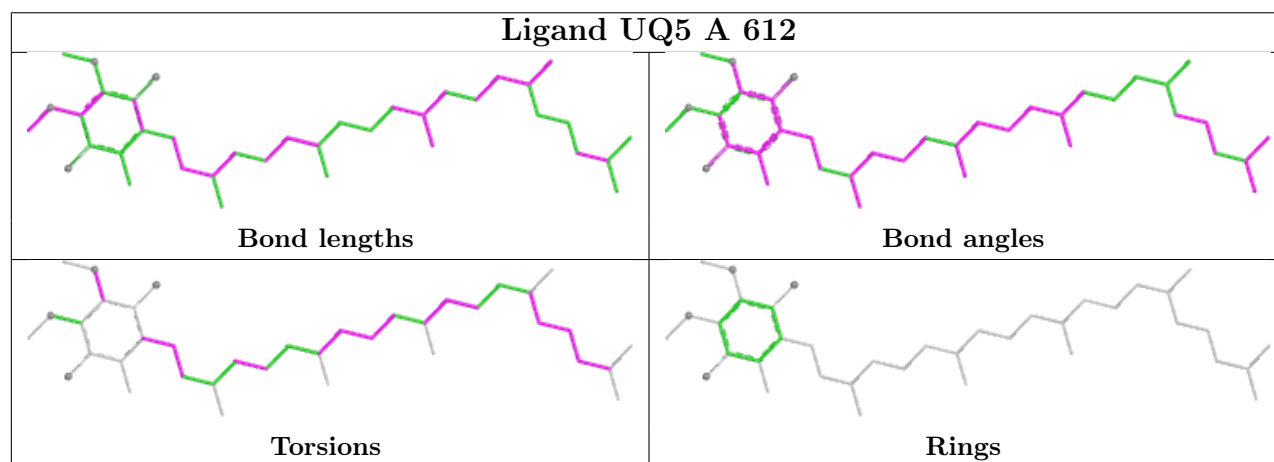
Mol	Chain	Res	Type	Atoms
6	B	615	UQ5	C19-C21-C22-C23
6	A	612	UQ5	C18-C19-C21-C22
2	A	617	BHG	C4-C5-C6-O6
2	B	618	BHG	C1'-C2'-C3'-C4'
6	B	615	UQ5	C15-C14-C16-C17
2	A	616	BHG	C2'-C3'-C4'-C5'
2	A	616	BHG	C3'-C4'-C5'-C6'
6	A	612	UQ5	C13-C14-C16-C17
6	B	615	UQ5	C13-C14-C16-C17
2	B	618	BHG	C2'-C3'-C4'-C5'
2	B	618	BHG	C3'-C4'-C5'-C6'
6	A	612	UQ5	C15-C14-C16-C17
2	A	616	BHG	O1-C1'-C2'-C3'
6	A	612	UQ5	C19-C21-C22-C23
2	B	618	BHG	O1-C1'-C2'-C3'
7	A	624	EDO	O1-C1-C2-O2
2	A	617	BHG	O5-C5-C6-O6
2	A	616	BHG	C1'-C2'-C3'-C4'
6	B	615	UQ5	C3-C4-O4-C4M
5	B	614	FAD	PA-O3P-P-O5'
7	A	621	EDO	O1-C1-C2-O2
7	A	623	EDO	O1-C1-C2-O2
6	A	612	UQ5	C5-C4-O4-C4M
5	B	614	FAD	C5'-O5'-P-O1P
5	B	614	FAD	C5'-O5'-P-O3P
6	A	612	UQ5	C24-C26-C27-C28
2	B	618	BHG	O5-C1-O1-C1'
6	B	615	UQ5	C9-C11-C12-C13
5	A	611	FAD	PA-O3P-P-O5'
2	A	616	BHG	C2'-C1'-O1-C1
7	A	622	EDO	O1-C1-C2-O2
6	B	615	UQ5	C24-C26-C27-C28
7	A	625	EDO	O1-C1-C2-O2
5	A	611	FAD	O4B-C4B-C5B-O5B
7	A	619	EDO	O1-C1-C2-O2
6	A	612	UQ5	C3-C4-O4-C4M
7	B	620	EDO	O1-C1-C2-O2
5	A	611	FAD	PA-O3P-P-O2P
5	B	614	FAD	PA-O3P-P-O2P
5	B	614	FAD	O4B-C4B-C5B-O5B

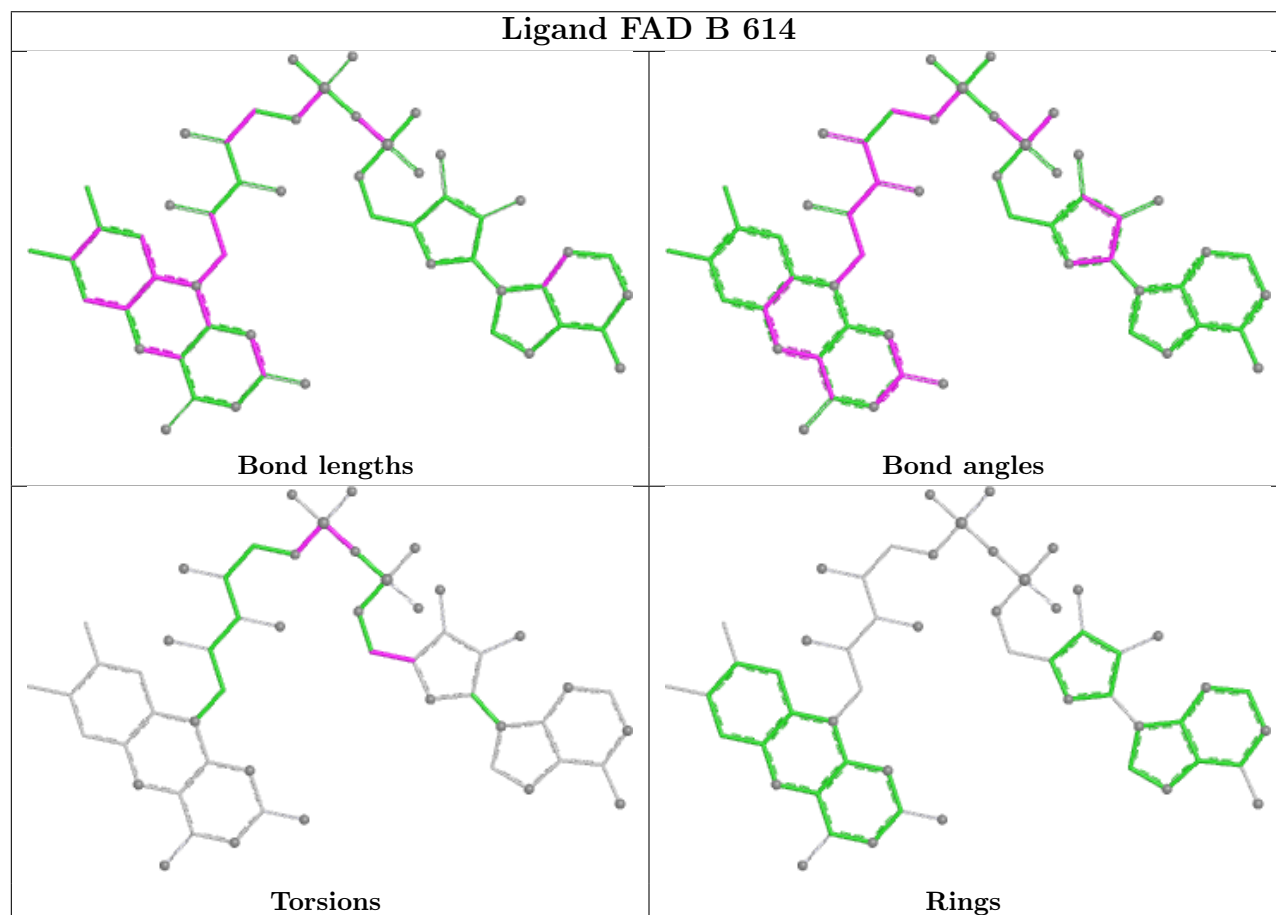
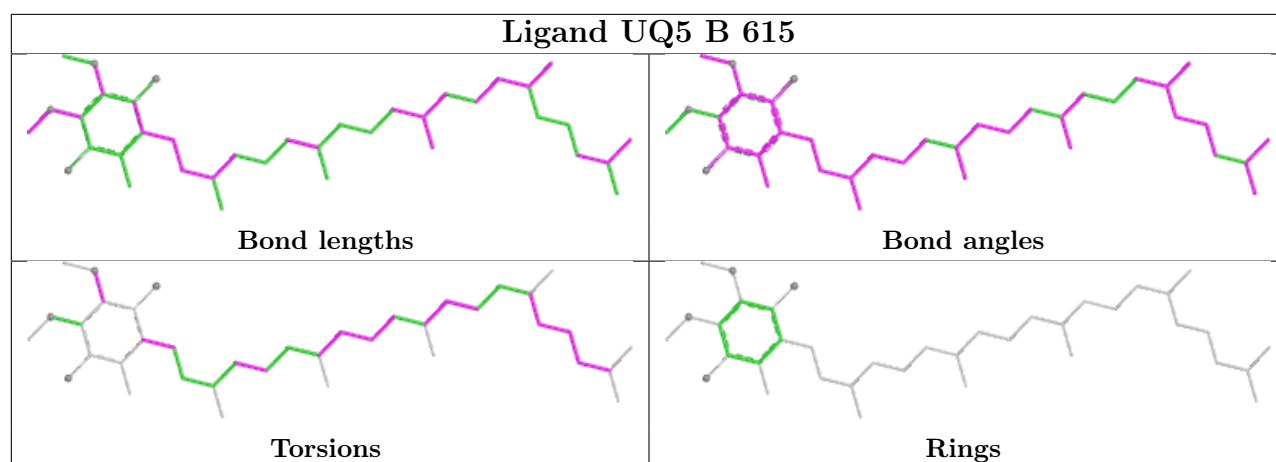
There are no ring outliers.

11 monomers are involved in 57 short contacts:

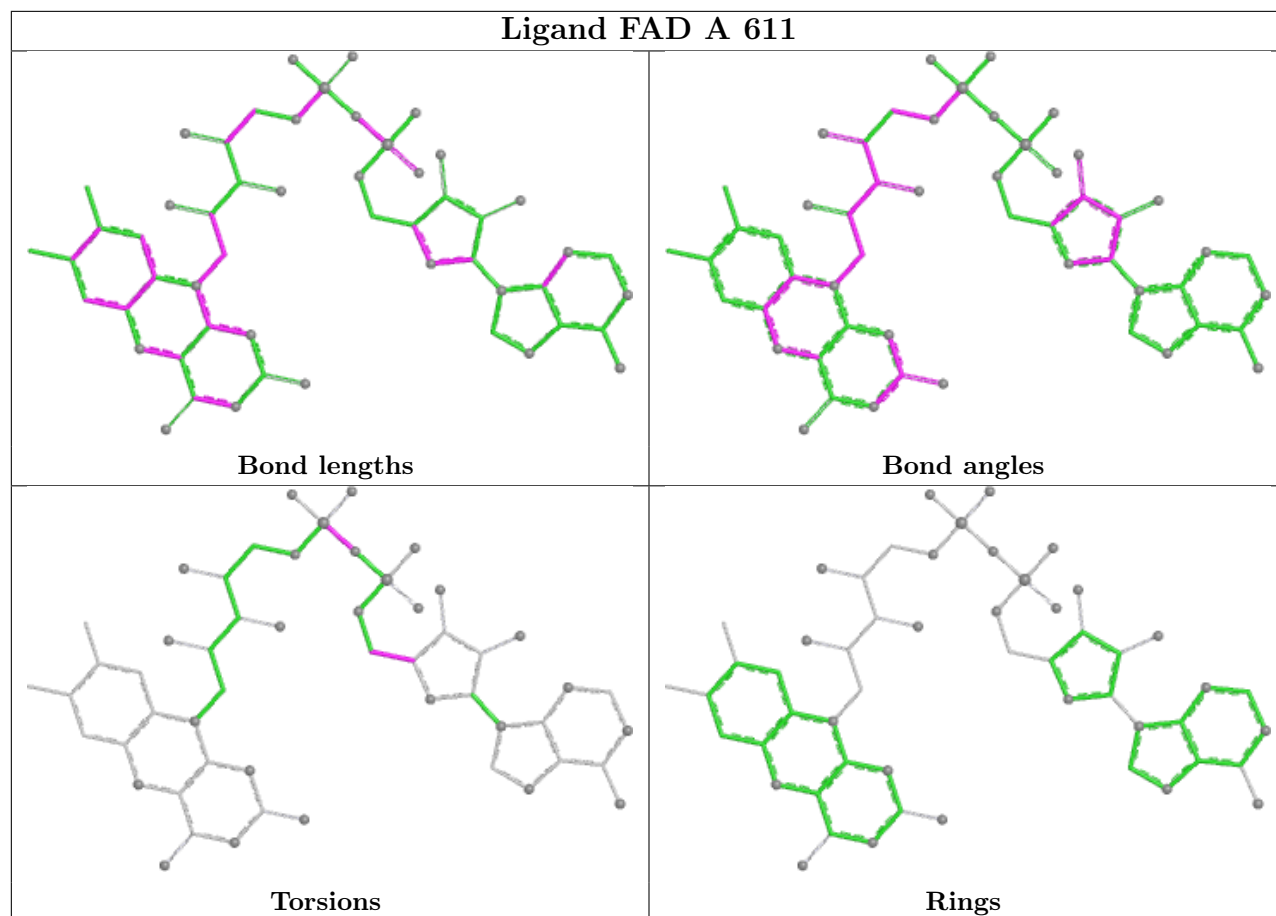
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	628	EDO	1	0
7	A	623	EDO	7	0
6	A	612	UQ5	16	0
6	B	615	UQ5	13	0
5	B	614	FAD	3	0
7	A	621	EDO	3	0
5	A	611	FAD	2	0
7	A	622	EDO	3	0
7	A	627	EDO	1	0
2	A	617	BHG	5	0
7	A	619	EDO	3	0

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.

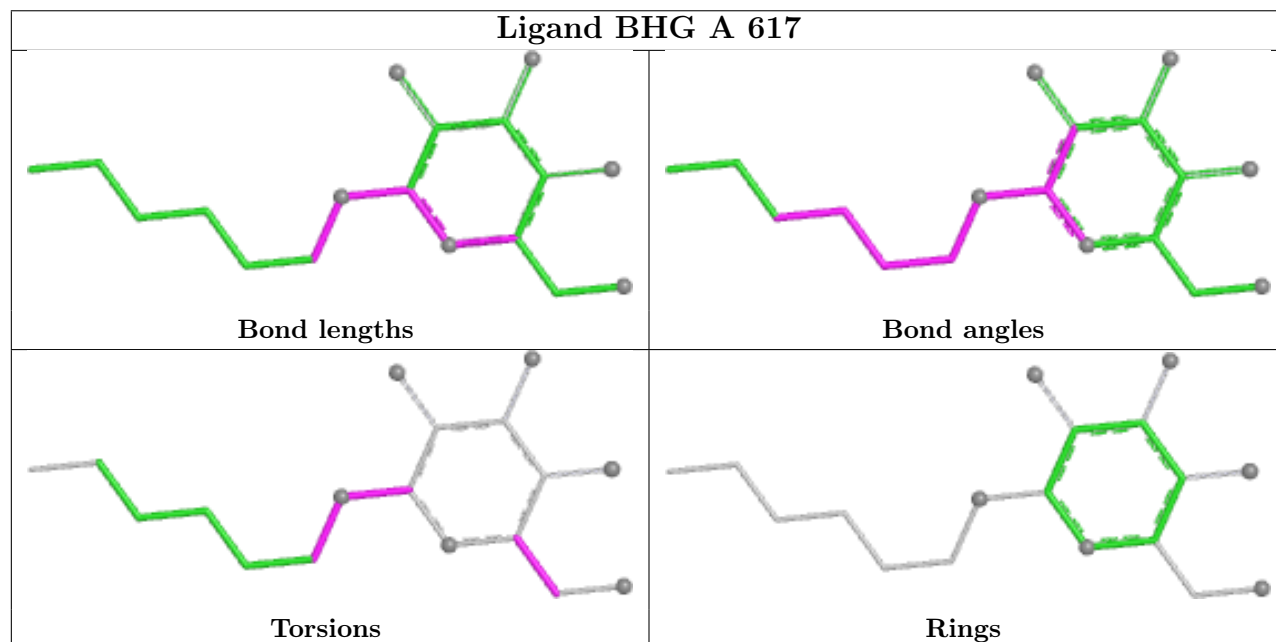


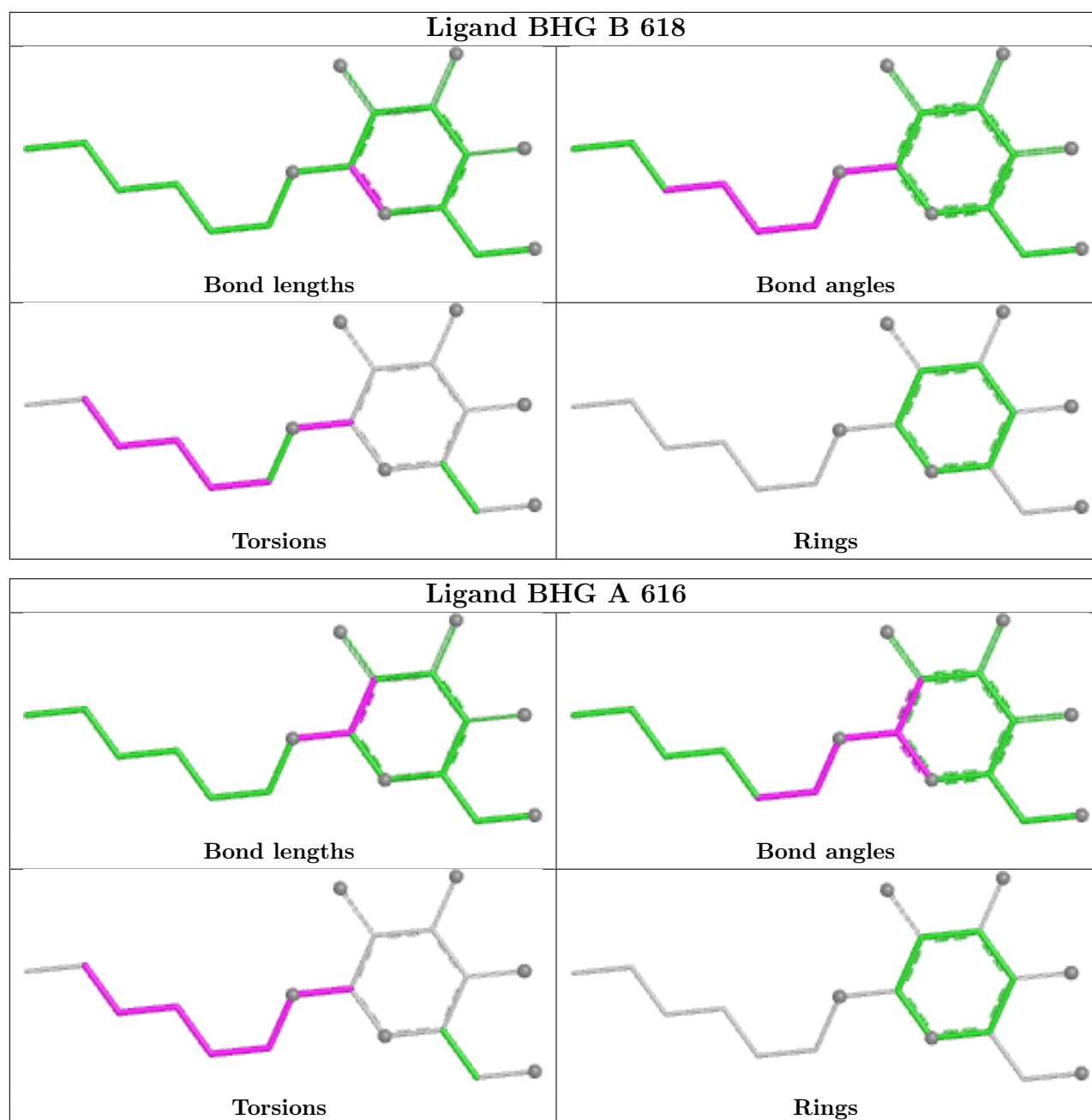


Ligand FAD A 611



Ligand BHG A 617





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	581/584 (99%)	-0.31	7 (1%) 76 73	13, 30, 57, 84	0
1	B	578/584 (98%)	0.76	38 (6%) 24 21	38, 64, 79, 86	0
All	All	1159/1168 (99%)	0.22	45 (3%) 43 38	13, 49, 77, 86	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502	ALA	4.8
1	A	7	PRO	4.3
1	B	176	GLY	4.2
1	B	188	ILE	3.8
1	B	181	ILE	3.6
1	A	6	VAL	3.5
1	B	43	ALA	3.4
1	B	41	VAL	2.9
1	B	165	TYR	2.9
1	B	7	PRO	2.9
1	B	24	TRP	2.8
1	B	390	LEU	2.8
1	B	27	VAL	2.8
1	A	390	LEU	2.7
1	A	133	MET	2.7
1	B	68	CYS	2.7
1	A	540	GLN	2.7
1	B	207	LYS	2.6
1	B	396	GLY	2.6
1	A	8	ARG	2.5
1	B	38	VAL	2.5
1	B	532	VAL	2.4
1	B	157	LEU	2.4
1	B	44	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	18	ARG	2.3
1	B	395	ILE	2.3
1	B	164	GLY	2.2
1	B	32	PHE	2.2
1	B	501	PRO	2.2
1	B	11	THR	2.2
1	B	133	MET	2.2
1	B	227	PHE	2.2
1	B	535	PHE	2.2
1	B	154	ALA	2.1
1	B	76	ILE	2.1
1	B	496	HIS	2.1
1	A	391	GLN	2.1
1	B	552	ASN	2.1
1	B	9	ILE	2.1
1	B	15	ILE	2.1
1	B	162	TYR	2.1
1	B	538	LEU	2.0
1	B	22	LYS	2.0
1	B	392	SER	2.0
1	B	208	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	BHG	B	618	18/18	0.42	0.17	61,76,78,78	0
2	BHG	A	617	18/18	0.51	0.24	55,75,78,79	0

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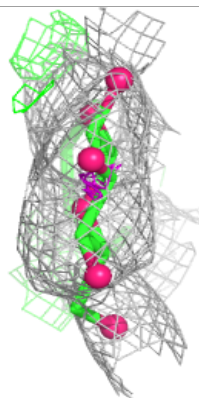
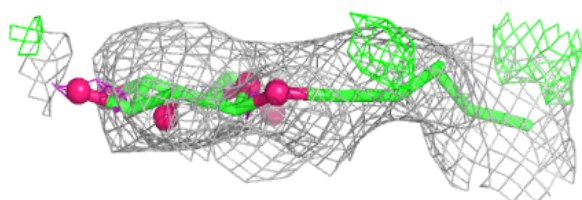
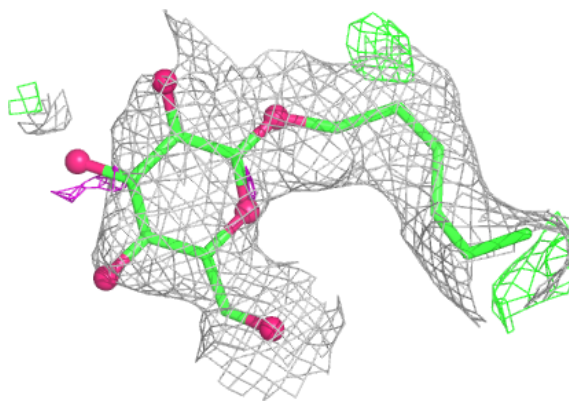
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BHG	A	616	18/18	0.69	0.22	52,76,78,79	0
7	EDO	A	627	4/4	0.70	0.19	57,58,58,58	0
7	EDO	A	628	4/4	0.76	0.14	53,54,55,55	0
6	UQ5	B	615	38/38	0.78	0.21	51,56,68,71	0
6	UQ5	A	612	38/38	0.82	0.21	39,48,62,63	0
7	EDO	B	620	4/4	0.82	0.14	49,53,54,56	0
7	EDO	A	622	4/4	0.85	0.30	51,55,55,57	0
7	EDO	A	625	4/4	0.86	0.14	49,55,55,57	0
7	EDO	A	626	4/4	0.88	0.10	43,45,45,46	0
7	EDO	A	621	4/4	0.88	0.17	45,47,48,49	0
7	EDO	A	619	4/4	0.90	0.12	37,37,38,43	0
5	FAD	B	614	53/53	0.90	0.11	44,60,68,69	0
7	EDO	A	624	4/4	0.91	0.19	35,41,42,42	0
7	EDO	A	623	4/4	0.91	0.26	48,49,49,53	0
3	NA	A	1070	1/1	0.96	0.03	37,37,37,37	0
4	SF4	B	613	8/8	0.97	0.05	55,58,59,59	0
5	FAD	A	611	53/53	0.98	0.05	16,20,24,26	0
4	SF4	A	610	8/8	0.99	0.04	16,19,22,22	0

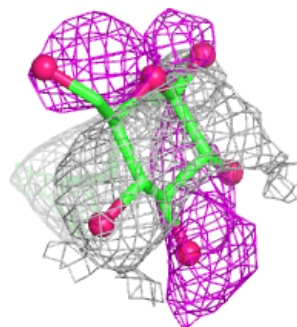
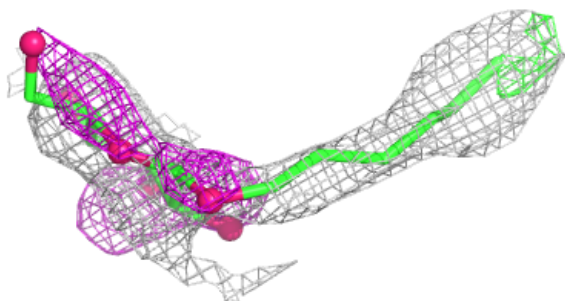
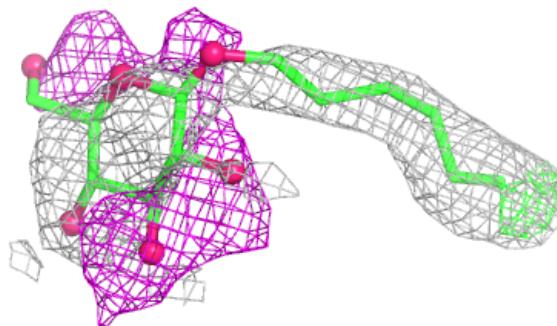
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BHG B 618:

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

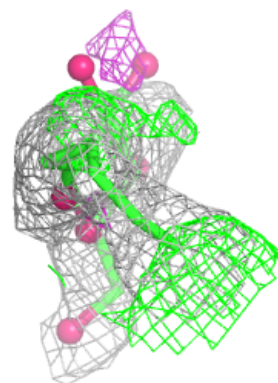
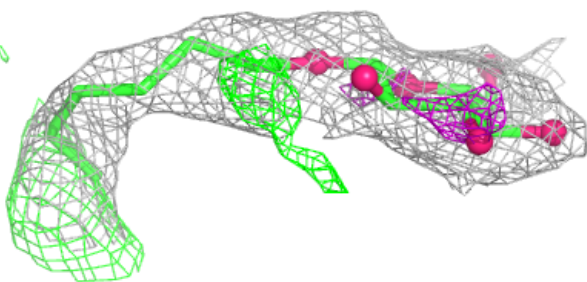
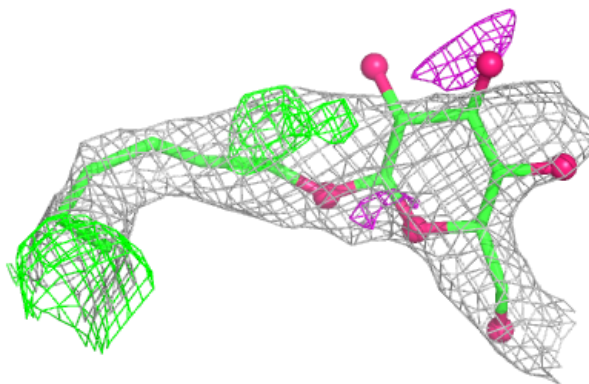
**Electron density around BHG A 617:**

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

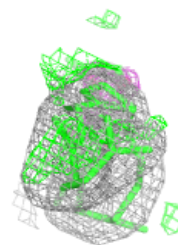
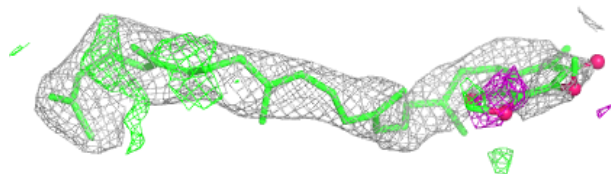
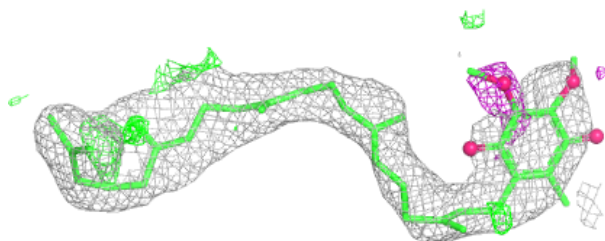


Electron density around BHG A 616:

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

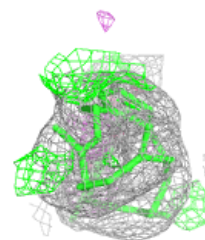
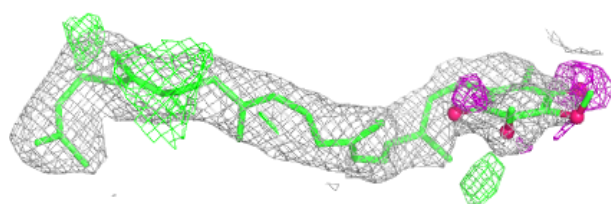
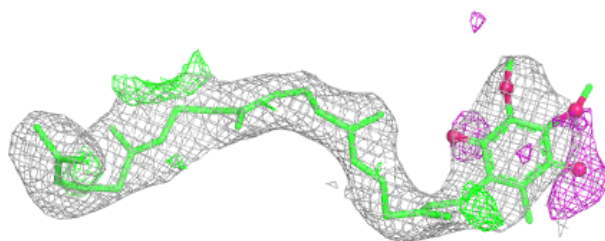
**Electron density around UQ5 B 615:**

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

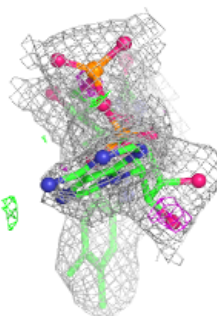
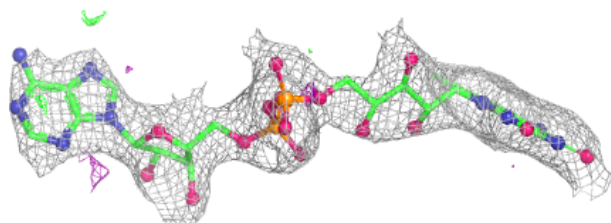
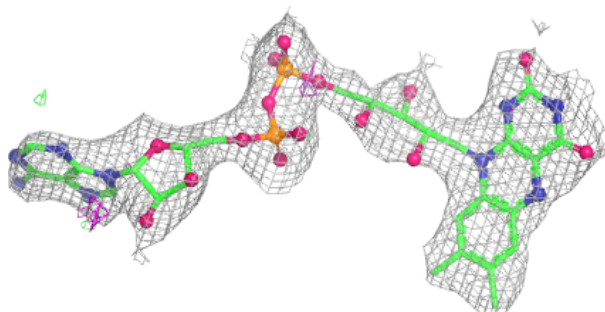


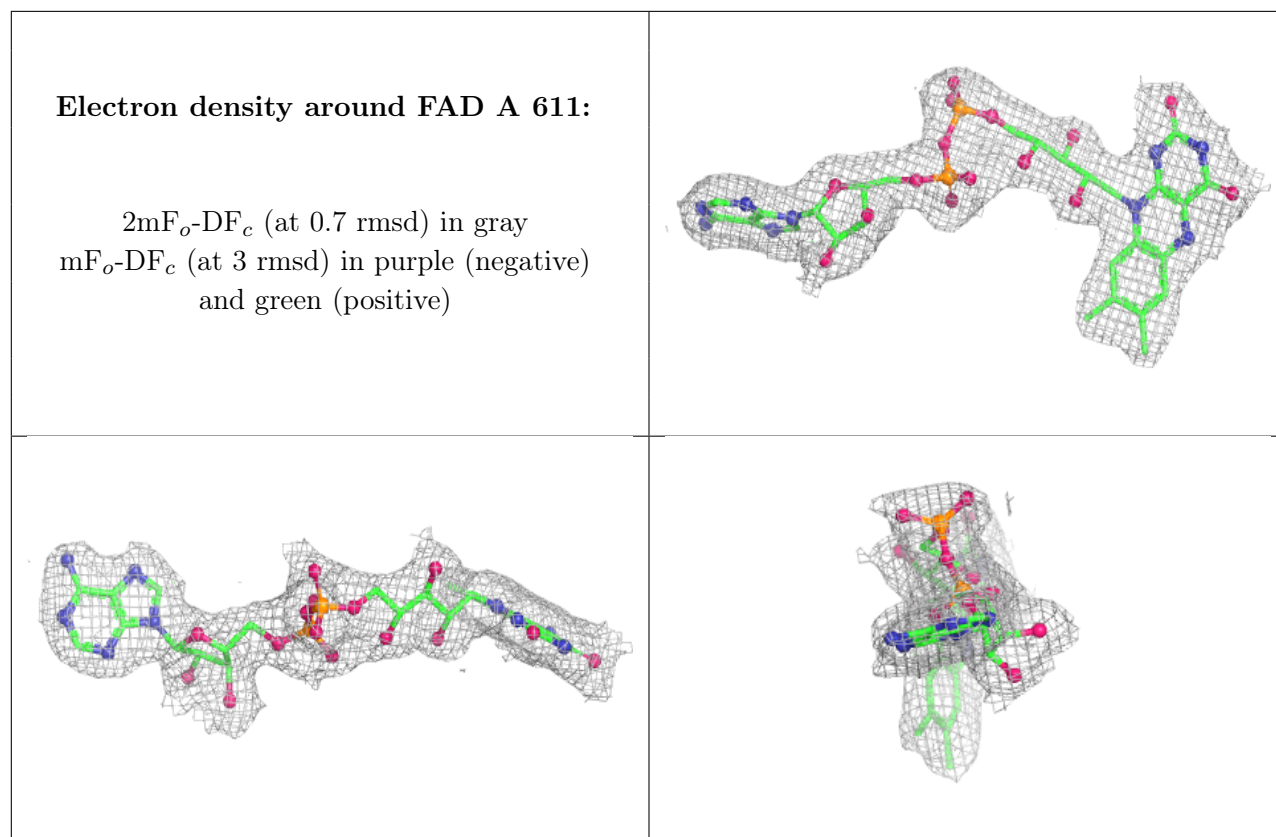
Electron density around UQ5 A 612:

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

**Electron density around FAD B 614:**

$2mF_o-DF_c$ (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.