



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:59 PM UTC

PDB ID : 2ACZ / pdb_00002acz
Title : Complex II (Succinate Dehydrogenase) From E. Coli with Atpenin A5 inhibitor
co-crystallized at the ubiquinone binding site
Authors : Horsefield, R.; Yankovskaya, V.; Sexton, G.; Whittingham, W.; Shiomi, K.;
Omura, S.; Byrne, B.; Cecchini, G.; Iwata, S.
Deposited on : 2005-07-19
Resolution : 3.10 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

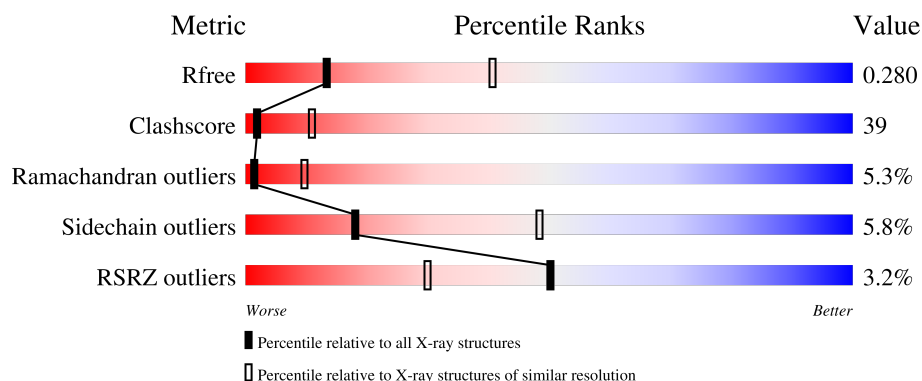
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	588	4% 38% 52% 9%
2	B	238	% 45% 47% 7%
3	C	129	3% 51% 41% 7%
4	D	115	2% 52% 40% 6%

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
10	HEB	C	130	X	-	-	-
12	CDN	C	132	X	-	-	-
5	OAA	A	589	-	-	X	-
9	F3S	B	304	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8521 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	91	0	0
			4522	2812	821	861	28			

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			

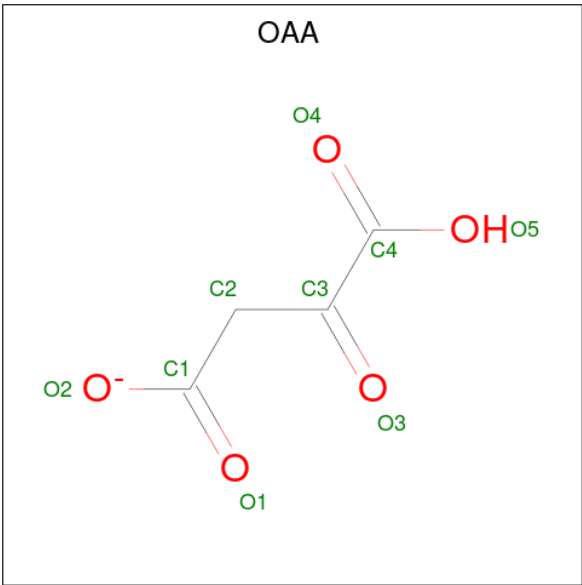
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b556 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			1008	668	166	168	6			

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor protein.

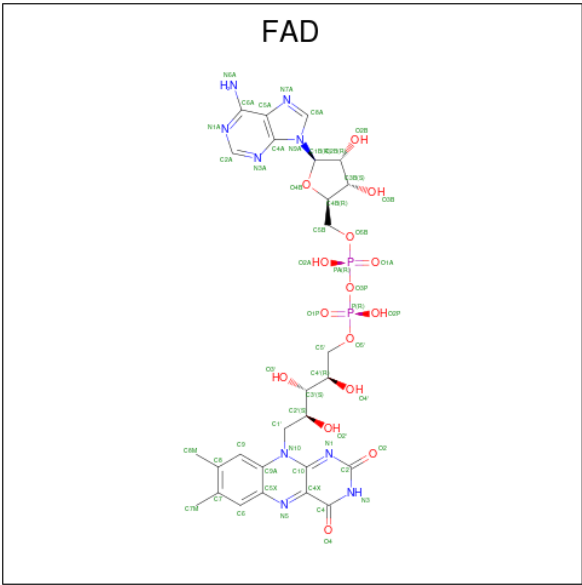
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	113	Total	C	N	O	S	0	0	0
			898	615	136	144	3			

- Molecule 5 is OXALOACETATE ION (CCD ID: OAA) (formula: C₄H₃O₅).



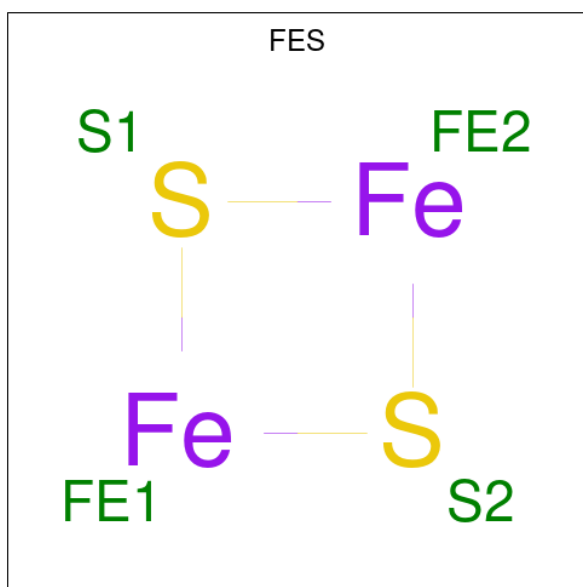
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



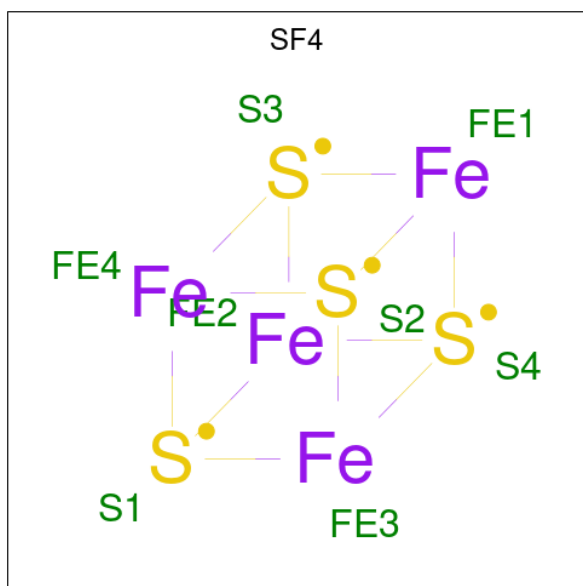
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



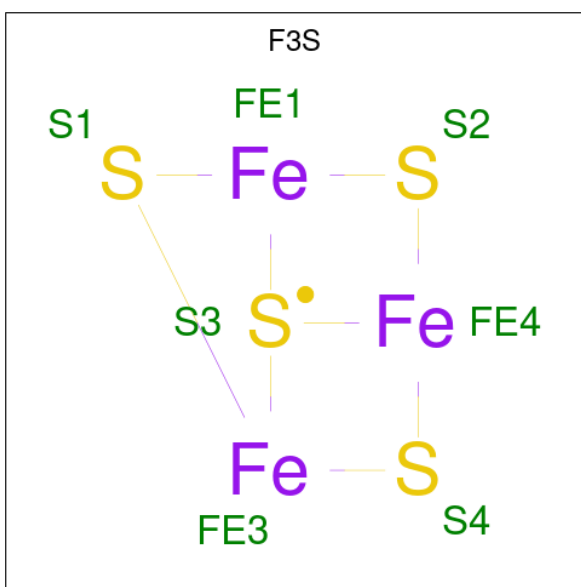
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



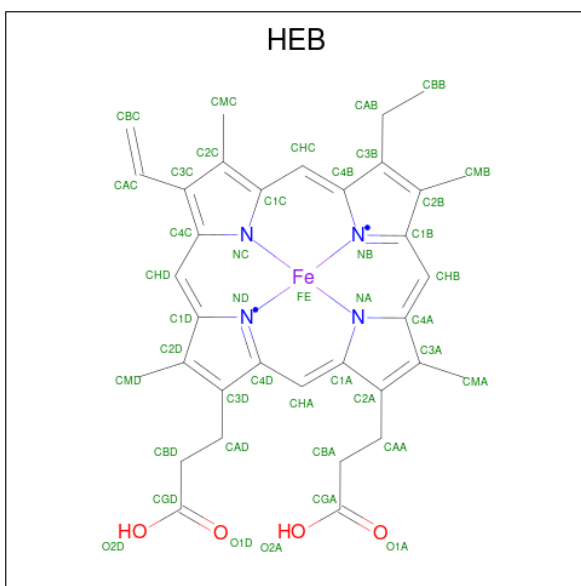
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



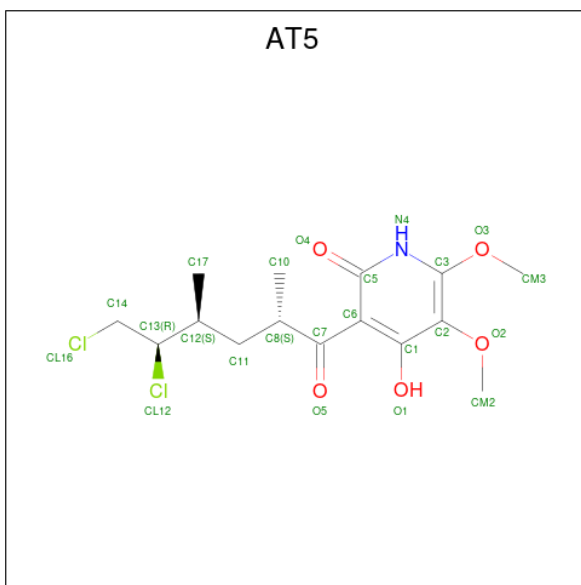
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is HEME B/C (CCD ID: HEB) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



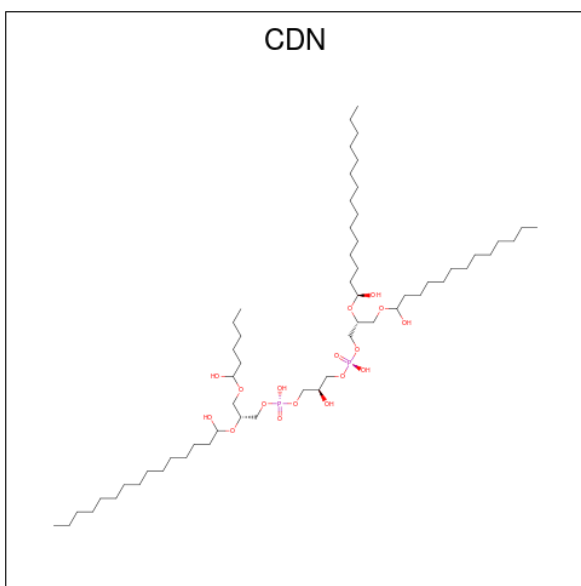
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 3-[(2S,4S,5R)-5,6-DICHLORO-2,4-DIMETHYL-1-OXOHXYL]-4-HYDROXY-5,6-DIMETHOXY-2(1H)-PYRIDINONE (CCD ID: AT5) (formula: C₁₅H₂₁Cl₂NO₅).



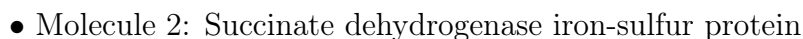
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Cl	N	O	0	0
			23	15	2	1	5		

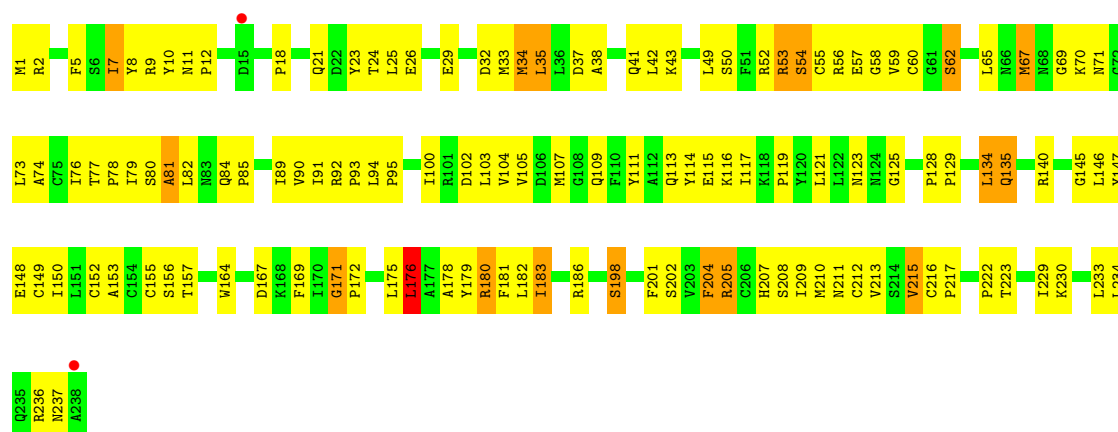
- Molecule 12 is CARDIOLIPIN (CCD ID: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).



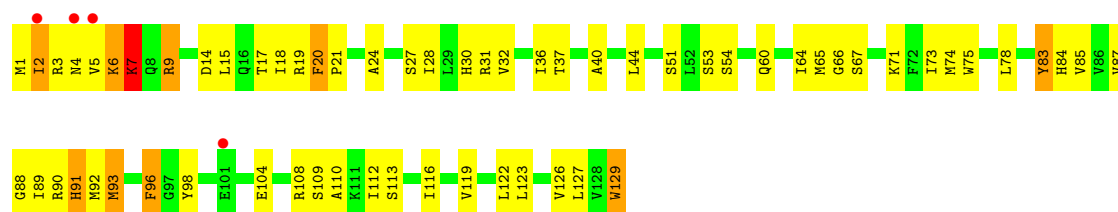
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O	P	0	0
			77	58	17	2		

- Molecule 1: Succinate dehydrogenase flavoprotein subunit

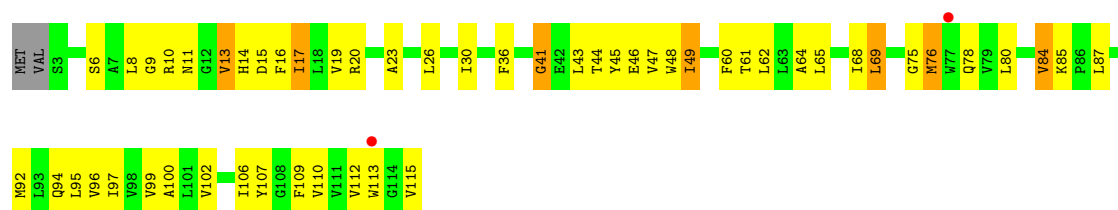




• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



• Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.76 Å 138.76 Å 521.87 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 40.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.10) 97.8 (40.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.12 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.308 (Not available) , 0.280	Depositor DCC
R_{free} test set	966 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8521	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: SF4, F3S, CDN, OAA, AT5, HEB, FAD, FES

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	0.56	1/4611 (0.0%)	1.07	32/6237 (0.5%)
2	B	0.57	0/1908	1.12	15/2578 (0.6%)
3	C	0.56	0/1030	1.08	6/1394 (0.4%)
4	D	0.67	1/923 (0.1%)	1.09	5/1262 (0.4%)
All	All	0.58	2/8472 (0.0%)	1.08	58/11471 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	SER	C-N	18.37	1.58	1.34
4	D	76	MET	SD-CE	5.09	1.92	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	84	VAL	N-CA-C	9.30	116.16	106.21
2	B	171	GLY	CA-C-N	8.92	128.25	118.97
2	B	171	GLY	C-N-CA	8.92	128.25	118.97
2	B	62	SER	N-CA-C	7.26	118.84	111.07
3	C	6	LYS	N-CA-C	7.22	121.62	110.42
4	D	112	VAL	N-CA-C	7.01	117.15	110.42
1	A	545	PHE	CA-C-N	6.91	128.47	119.84
1	A	545	PHE	C-N-CA	6.91	128.47	119.84
2	B	84	GLN	CA-C-N	6.87	128.43	119.84
2	B	84	GLN	C-N-CA	6.87	128.43	119.84
2	B	7	ILE	N-CA-C	6.86	119.31	108.89
3	C	20	PHE	N-CA-C	6.81	120.27	109.64
1	A	409	VAL	N-CA-C	6.80	116.90	110.30
1	A	277	ALA	CA-C-N	6.78	128.32	119.84
1	A	277	ALA	C-N-CA	6.78	128.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASP	N-CA-C	-6.67	104.62	112.89
1	A	244	THR	N-CA-C	6.65	120.84	107.41
1	A	231	VAL	N-CA-C	6.59	114.30	108.63
1	A	392	VAL	N-CA-C	-6.39	104.99	112.98
1	A	553	TRP	N-CA-C	6.35	120.38	111.30
2	B	11	ASN	CA-C-N	6.21	126.67	119.47
2	B	11	ASN	C-N-CA	6.21	126.67	119.47
1	A	252	LEU	N-CA-C	6.20	119.25	110.50
1	A	102	MET	N-CA-C	-6.17	105.75	113.28
2	B	183	ILE	CB-CA-C	-6.15	105.12	112.19
1	A	274	GLU	N-CA-C	-6.14	105.28	112.89
1	A	107	SER	N-CA-C	-6.08	101.52	110.52
1	A	574	GLU	N-CA-C	6.05	123.19	109.81
3	C	9	ARG	CA-C-N	6.05	126.24	120.31
3	C	9	ARG	C-N-CA	6.05	126.24	120.31
2	B	215	VAL	N-CA-C	6.03	120.00	113.43
3	C	7	LYS	N-CA-C	5.89	123.35	110.80
1	A	310	HIS	N-CA-C	5.87	116.18	108.07
1	A	412	GLY	N-CA-C	-5.87	105.70	112.50
1	A	199	VAL	N-CA-C	5.86	116.24	107.51
1	A	455	ASP	CA-C-N	5.84	125.52	119.56
1	A	455	ASP	C-N-CA	5.84	125.52	119.56
2	B	198	SER	N-CA-C	5.82	119.90	113.21
2	B	176	LEU	N-CA-C	-5.77	105.07	111.36
1	A	389	ILE	N-CA-C	-5.76	103.97	112.04
2	B	216	CYS	N-CA-C	5.76	122.54	109.81
1	A	157	HIS	N-CA-C	5.74	119.10	111.30
1	A	419	LEU	N-CA-C	5.60	117.86	111.02
1	A	155	LYS	N-CA-C	5.58	117.17	111.14
3	C	53	SER	N-CA-C	5.51	118.80	111.75
4	D	87	LEU	N-CA-C	5.50	117.71	111.11
1	A	255	GLU	N-CA-C	-5.48	106.30	112.87
1	A	33	CYS	N-CA-C	5.42	117.21	108.32
2	B	205	ARG	N-CA-C	-5.42	106.67	113.28
2	B	204	PHE	N-CA-C	5.41	122.32	110.80
4	D	107	TYR	N-CA-C	-5.33	105.58	111.71
1	A	513	CYS	N-CA-C	-5.30	105.19	110.97
1	A	258	ARG	N-CA-C	-5.28	105.69	111.82
1	A	32	THR	N-CA-C	-5.17	102.62	110.28
1	A	213	THR	N-CA-C	-5.15	106.50	112.89
1	A	265	LEU	N-CA-C	5.06	116.98	109.69
1	A	201	ALA	N-CA-C	-5.05	102.00	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	17	ILE	N-CA-C	5.05	115.28	110.53

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	4522	0	4426	410	0
2	B	1869	0	1850	149	0
3	C	1008	0	1066	80	0
4	D	898	0	936	48	0
5	A	9	0	2	5	0
6	A	53	0	29	9	0
7	B	4	0	0	1	0
8	B	8	0	0	0	0
9	B	7	0	0	4	0
10	C	43	0	32	10	0
11	C	23	0	20	4	0
12	C	77	0	112	19	0
All	All	8521	0	8473	660	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 39.

All (660) 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)
10:C:130:HEB:HBB1	12:C:132:CDN:C24	1.84	1.07
3:C:6:LYS:HE3	3:C:7:LYS:HG3	1.33	1.06
1:A:577:LEU:HD21	1:A:580:ALA:HA	1.38	1.04
2:B:180:ARG:HG2	2:B:180:ARG:HH11	1.23	1.02
2:B:35:LEU:HD23	2:B:67:MET:HE2	1.37	1.01
1:A:578:ARG:HB3	1:A:579:PRO:HD3	1.39	1.00
1:A:577:LEU:HD23	1:A:577:LEU:H	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CD2	2:B:134:LEU:HA	2.01	0.96
1:A:119:PHE:HB2	2:B:135:GLN:H	1.28	0.96
4:D:9:GLY:HA2	4:D:14:HIS:HD2	1.31	0.94
1:A:205:ALA:HB2	1:A:220:GLY:H	1.31	0.93
1:A:362:THR:HG22	1:A:368:ALA:HA	1.49	0.92
3:C:2:ILE:HG12	3:C:5:VAL:HB	1.51	0.92
10:C:130:HEB:HAC	4:D:23:ALA:HB1	1.51	0.92
1:A:577:LEU:H	1:A:577:LEU:CD2	1.83	0.90
2:B:34:MET:HE3	2:B:34:MET:HA	1.50	0.90
1:A:240:GLN:HB2	1:A:357:MET:HE1	1.53	0.89
1:A:128:GLY:HA3	1:A:400:LEU:HD11	1.51	0.88
2:B:94:LEU:HB3	2:B:157:THR:HG21	1.55	0.88
1:A:205:ALA:CB	1:A:220:GLY:H	1.87	0.88
12:C:132:CDN:OA3	4:D:41:GLY:O	1.91	0.87
1:A:82:GLN:HB2	1:A:577:LEU:HB3	1.57	0.85
2:B:180:ARG:HG2	2:B:180:ARG:NH1	1.89	0.83
2:B:172:PRO:HG3	9:B:304:F3S:S3	2.18	0.83
1:A:54:THR:HG22	1:A:134:THR:OG1	1.78	0.83
3:C:78:LEU:HD21	12:C:132:CDN:H162	1.61	0.83
1:A:9:ASP:H	1:A:32:THR:CG2	1.91	0.82
1:A:324:GLU:O	1:A:328:PRO:HG3	1.79	0.81
1:A:562:GLU:HB2	1:A:568:ARG:HH12	1.45	0.81
1:A:234:GLN:HG3	1:A:361:PRO:HG3	1.62	0.81
1:A:117:ARG:HG3	1:A:118:PRO:HD2	1.63	0.81
1:A:257:CYS:HB3	1:A:315:LEU:HD21	1.63	0.81
2:B:9:ARG:HH12	2:B:49:LEU:HA	1.46	0.81
1:A:559:TYR:HB2	1:A:569:ARG:HH21	1.45	0.80
2:B:35:LEU:HD21	2:B:91:ILE:HD11	1.64	0.80
4:D:9:GLY:HA2	4:D:14:HIS:CD2	2.17	0.79
1:A:263:TYR:HB3	1:A:265:LEU:HD21	1.63	0.79
3:C:89:ILE:HG22	3:C:93:MET:HE3	1.64	0.79
3:C:60:GLN:O	3:C:64:ILE:HG13	1.83	0.79
3:C:32:VAL:O	3:C:36:ILE:HD13	1.82	0.78
2:B:35:LEU:HD12	2:B:35:LEU:O	1.84	0.78
2:B:81:ALA:C	2:B:82:LEU:HD12	2.09	0.78
3:C:1:MET:HG3	3:C:6:LYS:HA	1.65	0.78
1:A:273:MET:HE1	1:A:292:SER:HB2	1.65	0.78
1:A:331:LEU:O	1:A:335:ARG:HG3	1.83	0.77
3:C:92:MET:HE3	4:D:20:ARG:HG3	1.65	0.77
2:B:140:ARG:O	2:B:140:ARG:HD3	1.84	0.77
1:A:9:ASP:H	1:A:32:THR:HG23	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:LEU:HD23	4:D:65:LEU:HD12	1.66	0.77
1:A:263:TYR:HB2	1:A:314:LYS:HB3	1.67	0.76
1:A:82:GLN:CB	1:A:577:LEU:HB3	2.14	0.76
1:A:237:GLU:OE1	1:A:529:SER:HB3	1.85	0.76
3:C:93:MET:HG2	3:C:98:TYR:HB2	1.67	0.76
2:B:77:THR:CG2	2:B:82:LEU:HD11	2.16	0.76
1:A:559:TYR:CA	1:A:569:ARG:HH21	1.99	0.76
1:A:242:HIS:O	1:A:351:PRO:HA	1.86	0.76
3:C:119:VAL:O	3:C:123:LEU:HD12	1.86	0.75
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.67	0.75
3:C:104:GLU:CD	3:C:104:GLU:H	1.94	0.75
1:A:560:LEU:HB3	1:A:568:ARG:HB2	1.66	0.75
3:C:6:LYS:HG2	3:C:7:LYS:N	2.02	0.75
1:A:356:MET:HE3	1:A:358:GLY:O	1.87	0.75
10:C:130:HEB:HBB1	12:C:132:CDN:H241	1.65	0.75
2:B:43:LYS:HE2	2:B:49:LEU:O	1.87	0.75
1:A:232:PRO:HB3	1:A:558:LEU:HD11	1.68	0.74
1:A:232:PRO:CB	1:A:558:LEU:HD11	2.17	0.74
1:A:392:VAL:HG13	1:A:394:VAL:HG13	1.68	0.74
1:A:577:LEU:HD23	1:A:577:LEU:N	2.00	0.74
1:A:544:ASP:HB2	1:A:545:PHE:CE1	2.23	0.74
12:C:132:CDN:HA21	4:D:41:GLY:O	1.87	0.74
1:A:47:VAL:HG13	1:A:146:LEU:HD23	1.68	0.73
1:A:475:ARG:O	1:A:542:ARG:HA	1.88	0.73
3:C:2:ILE:CG1	3:C:5:VAL:HB	2.18	0.73
1:A:254:THR:HG22	1:A:330:ILE:HD11	1.69	0.73
1:A:567:THR:O	1:A:568:ARG:HD2	1.88	0.73
1:A:273:MET:HE1	1:A:292:SER:CB	2.17	0.73
2:B:77:THR:HG22	2:B:82:LEU:HD11	1.70	0.73
2:B:9:ARG:HH12	2:B:49:LEU:CA	2.01	0.73
3:C:28:ILE:HD11	11:C:131:AT5:H172	1.70	0.73
1:A:47:VAL:HG13	1:A:146:LEU:CD2	2.18	0.72
1:A:584:LYS:HG2	1:A:585:ILE:H	1.54	0.72
1:A:559:TYR:CB	1:A:569:ARG:HH21	2.02	0.72
1:A:117:ARG:HG3	1:A:118:PRO:CD	2.19	0.72
1:A:434:GLU:O	1:A:438:GLU:HB2	1.89	0.72
1:A:555:CYS:HB2	1:A:571:VAL:HG13	1.71	0.72
2:B:146:LEU:CD1	2:B:183:ILE:HD11	2.20	0.71
1:A:12:VAL:HB	1:A:35:LEU:HD12	1.72	0.71
4:D:92:MET:O	4:D:96:VAL:HG23	1.89	0.71
1:A:17:GLY:HA3	1:A:408:LEU:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CE2	1:A:480:MET:HG3	2.25	0.71
1:A:9:ASP:CG	1:A:32:THR:HG22	2.15	0.71
1:A:82:GLN:HB3	1:A:577:LEU:HD13	1.73	0.71
1:A:108:ARG:HD2	1:A:119:PHE:O	1.91	0.71
3:C:51:SER:HB3	4:D:48:TRP:HE1	1.56	0.71
4:D:16:PHE:O	4:D:20:ARG:HD3	1.91	0.70
1:A:256:GLY:O	1:A:260:GLU:HG2	1.91	0.70
1:A:537:ARG:HH12	1:A:554:LEU:HD12	1.56	0.70
1:A:545:PHE:N	1:A:546:PRO:HD3	2.07	0.70
2:B:1:MET:H1	2:B:29:GLU:HB2	1.57	0.70
1:A:568:ARG:O	1:A:569:ARG:HG2	1.92	0.69
3:C:126:VAL:HG11	12:C:132:CDN:OB9	1.92	0.69
1:A:222:GLY:HA3	1:A:389:ILE:HD12	1.74	0.69
1:A:523:ALA:O	1:A:526:THR:HB	1.93	0.69
1:A:370:THR:HG23	1:A:380:VAL:HG22	1.73	0.69
1:A:577:LEU:HG	1:A:578:ARG:N	2.08	0.69
1:A:467:MET:SD	1:A:523:ALA:HB1	2.33	0.68
1:A:44:SER:O	1:A:47:VAL:HG22	1.93	0.68
1:A:578:ARG:HB3	1:A:579:PRO:CD	2.20	0.68
1:A:218:ASN:N	1:A:218:ASN:HD22	1.91	0.68
1:A:327:LEU:N	1:A:328:PRO:HD3	2.08	0.68
1:A:355:TYR:CE2	1:A:399:ARG:HD3	2.29	0.68
2:B:92:ARG:HD3	3:C:17:THR:HG21	1.76	0.68
4:D:6:SER:HB2	4:D:94:GLN:NE2	2.08	0.68
1:A:234:GLN:HG3	1:A:361:PRO:CG	2.24	0.68
1:A:242:HIS:HB2	1:A:354:HIS:HB2	1.76	0.67
1:A:453:GLY:HA3	1:A:496:ASN:O	1.93	0.67
2:B:9:ARG:NH1	2:B:49:LEU:HA	2.09	0.67
2:B:76:ILE:O	2:B:78:PRO:HD3	1.94	0.67
1:A:287:ASP:OD1	1:A:538:GLY:HA2	1.94	0.67
1:A:75:GLY:O	1:A:398:ASN:HB3	1.93	0.67
2:B:107:MET:HE1	2:B:153:ALA:HB2	1.76	0.67
4:D:9:GLY:CA	4:D:14:HIS:HD2	2.08	0.67
10:C:130:HEB:HBB1	12:C:132:CDN:H243	1.76	0.67
1:A:357:MET:CE	1:A:357:MET:H	2.08	0.67
2:B:82:LEU:O	2:B:89:ILE:HG12	1.95	0.67
1:A:69:MET:O	1:A:73:VAL:HG23	1.95	0.67
2:B:92:ARG:HH11	3:C:17:THR:HG21	1.58	0.67
1:A:562:GLU:HB2	1:A:568:ARG:NH1	2.09	0.67
1:A:24:LEU:O	1:A:28:GLN:HG2	1.95	0.66
1:A:61:HIS:NE2	1:A:131:ALA:HB3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CB	2:B:135:GLN:H	2.04	0.66
1:A:46:THR:HB	1:A:146:LEU:HD13	1.78	0.66
1:A:54:THR:HA	1:A:134:THR:HA	1.78	0.66
1:A:23:ALA:HB2	1:A:35:LEU:HD13	1.78	0.66
1:A:117:ARG:CG	1:A:118:PRO:HD2	2.26	0.66
1:A:578:ARG:CB	1:A:579:PRO:HD3	2.21	0.65
2:B:34:MET:HA	2:B:34:MET:CE	2.25	0.65
3:C:90:ARG:HE	3:C:109:SER:HB2	1.61	0.65
1:A:320:LYS:HE2	1:A:324:GLU:OE1	1.96	0.65
2:B:10:TYR:CE2	2:B:12:PRO:HG3	2.30	0.65
1:A:105:PRO:HD2	1:A:144:ALA:HB1	1.78	0.65
1:A:167:LEU:HB2	1:A:181:THR:OG1	1.95	0.65
1:A:567:THR:C	1:A:568:ARG:HD2	2.22	0.65
2:B:95:PRO:HD2	2:B:157:THR:CG2	2.27	0.65
2:B:230:LYS:HA	2:B:233:LEU:HD12	1.78	0.65
1:A:559:TYR:HB2	1:A:569:ARG:NH2	2.11	0.64
1:A:298:ARG:NH1	1:A:543:PHE:HZ	1.95	0.64
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.80	0.64
10:C:130:HEB:HBD1	10:C:130:HEB:HHA	1.79	0.64
1:A:240:GLN:NE2	1:A:399:ARG:HB3	2.12	0.64
1:A:245:GLY:O	1:A:349:VAL:HA	1.96	0.64
1:A:291:ARG:NH2	1:A:538:GLY:O	2.31	0.64
1:A:208:ILE:HG13	1:A:209:TYR:CD1	2.32	0.63
1:A:239:TRP:CZ3	1:A:356:MET:HB2	2.32	0.63
1:A:298:ARG:HH11	1:A:543:PHE:HZ	1.44	0.63
1:A:123:SER:HA	1:A:134:THR:O	1.99	0.63
2:B:179:TYR:HA	2:B:182:LEU:HD12	1.79	0.63
3:C:112:ILE:O	3:C:116:ILE:HG13	1.98	0.63
1:A:205:ALA:HB2	1:A:220:GLY:N	2.09	0.63
1:A:357:MET:HE2	1:A:357:MET:N	2.13	0.63
2:B:71:ASN:OD1	2:B:94:LEU:HD23	1.98	0.63
1:A:49:ALA:HA	6:A:601:FAD:N5	2.14	0.62
1:A:286:ARG:HH21	5:A:589:OAA:H22	1.63	0.62
2:B:211:ASN:ND2	3:C:21:PRO:HD2	2.15	0.62
1:A:508:THR:OG1	2:B:50:SER:HB2	1.99	0.62
1:A:583:PRO:O	1:A:584:LYS:HB2	1.98	0.62
1:A:125:ASN:OD1	1:A:132:ALA:HB2	1.99	0.62
1:A:9:ASP:OD2	1:A:32:THR:HG22	2.00	0.62
1:A:236:MET:HE3	1:A:236:MET:HA	1.82	0.62
1:A:286:ARG:NH2	5:A:589:OAA:H22	2.14	0.62
1:A:6:ARG:HB3	1:A:8:PHE:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:O	1:A:225:MET:HG3	2.00	0.62
1:A:532:PHE:CD1	1:A:569:ARG:HD3	2.35	0.62
3:C:83:TYR:C	3:C:83:TYR:CD2	2.77	0.62
2:B:211:ASN:HD21	3:C:21:PRO:HD2	1.65	0.61
3:C:1:MET:HG3	3:C:6:LYS:CA	2.29	0.61
3:C:83:TYR:CE2	3:C:87:VAL:HG21	2.35	0.61
1:A:54:THR:HG23	1:A:402:GLY:HA3	1.81	0.61
1:A:562:GLU:CB	1:A:568:ARG:HH12	2.12	0.61
1:A:126:PHE:HE2	5:A:589:OAA:H21	1.63	0.61
2:B:35:LEU:HD21	2:B:91:ILE:CD1	2.29	0.61
1:A:370:THR:HG23	1:A:380:VAL:CG2	2.31	0.61
2:B:94:LEU:HB3	2:B:157:THR:CG2	2.27	0.61
1:A:234:GLN:O	1:A:236:MET:N	2.33	0.61
1:A:454:GLU:OE2	1:A:493:ARG:NE	2.30	0.61
2:B:223:THR:HG22	9:B:304:F3S:S1	2.41	0.60
1:A:298:ARG:NH1	1:A:543:PHE:CZ	2.69	0.60
1:A:38:LYS:NZ	1:A:217:ILE:HG23	2.16	0.60
4:D:95:LEU:O	4:D:99:VAL:HG23	2.01	0.60
1:A:49:ALA:HA	6:A:601:FAD:C5X	2.31	0.60
1:A:104:LEU:HD12	1:A:105:PRO:HD2	1.84	0.60
1:A:177:VAL:HG21	1:A:383:LEU:HB2	1.82	0.60
1:A:571:VAL:HG12	1:A:572:ASN:N	2.17	0.59
1:A:532:PHE:HD1	1:A:569:ARG:HH11	1.49	0.59
2:B:69:GLY:O	3:C:19:ARG:HB3	2.02	0.59
1:A:199:VAL:HG22	1:A:384:PHE:HB2	1.83	0.59
1:A:119:PHE:CG	2:B:134:LEU:HA	2.36	0.59
1:A:287:ASP:H	1:A:398:ASN:ND2	2.01	0.59
2:B:209:ILE:HG23	3:C:24:ALA:HA	1.84	0.59
1:A:463:LEU:HD13	1:A:520:MET:CE	2.32	0.59
2:B:67:MET:HE1	2:B:74:ALA:HA	1.84	0.59
1:A:63:ASP:OD1	1:A:64:ASN:N	2.33	0.59
1:A:164:TRP:CZ2	1:A:184:CYS:HB2	2.37	0.59
1:A:205:ALA:HA	1:A:218:ASN:HB3	1.84	0.59
1:A:371:VAL:HA	1:A:376:GLU:O	2.03	0.59
3:C:6:LYS:HG2	3:C:7:LYS:H	1.67	0.59
1:A:571:VAL:CG1	1:A:572:ASN:N	2.66	0.59
1:A:577:LEU:HG	1:A:578:ARG:H	1.67	0.59
2:B:201:PHE:O	2:B:205:ARG:HG2	2.03	0.59
2:B:114:TYR:O	2:B:119:PRO:HG3	2.03	0.59
1:A:72:THR:HA	1:A:400:LEU:HD22	1.84	0.58
1:A:287:ASP:H	1:A:398:ASN:HD21	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:O	1:A:221:ASP:N	2.36	0.58
1:A:216:HIS:HB2	2:B:53:ARG:HE	1.69	0.58
1:A:208:ILE:HG13	1:A:209:TYR:HD1	1.67	0.58
2:B:60:CYS:SG	2:B:62:SER:HB2	2.43	0.58
1:A:59:ASN:ND2	1:A:120:GLY:HA3	2.19	0.58
1:A:295:ILE:C	1:A:297:ILE:H	2.09	0.58
3:C:2:ILE:HG13	3:C:3:ARG:N	2.19	0.58
1:A:161:PHE:HB3	1:A:164:TRP:CD1	2.39	0.58
3:C:71:LYS:HD3	3:C:129:TRP:CD1	2.39	0.58
2:B:56:ARG:O	2:B:56:ARG:HG2	2.04	0.57
2:B:94:LEU:CB	2:B:157:THR:HG21	2.32	0.57
1:A:244:THR:HG22	1:A:349:VAL:HG21	1.86	0.57
1:A:338:ALA:O	1:A:340:VAL:HG23	2.03	0.57
1:A:386:VAL:HG11	1:A:415:ALA:HB2	1.86	0.57
1:A:556:HIS:HB2	1:A:572:ASN:HB3	1.85	0.57
4:D:102:VAL:HG12	4:D:106:ILE:HD12	1.85	0.57
1:A:511:VAL:O	1:A:515:GLU:HG3	2.05	0.57
1:A:369:LEU:HD23	1:A:379:VAL:HA	1.86	0.57
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.40	0.57
1:A:76:SER:O	1:A:79:ILE:HG22	2.04	0.57
3:C:85:VAL:O	3:C:89:ILE:HG13	2.05	0.57
1:A:252:LEU:HD13	1:A:354:HIS:CE1	2.40	0.57
1:A:205:ALA:CB	1:A:220:GLY:N	2.64	0.57
3:C:6:LYS:HE3	3:C:7:LYS:CG	2.22	0.56
4:D:10:ARG:H	4:D:14:HIS:CD2	2.23	0.56
1:A:126:PHE:CE2	5:A:589:OAA:H21	2.40	0.56
3:C:83:TYR:C	3:C:83:TYR:HD2	2.11	0.56
1:A:324:GLU:C	1:A:328:PRO:HG3	2.30	0.56
1:A:172:ASN:HD22	1:A:173:GLN:H	1.54	0.56
1:A:368:ALA:O	1:A:380:VAL:HG23	2.05	0.56
1:A:38:LYS:HE2	6:A:601:FAD:C8A	2.35	0.56
4:D:44:THR:HG22	4:D:46:GLU:HG2	1.86	0.56
1:A:272:PHE:CE1	1:A:273:MET:HE2	2.41	0.56
1:A:357:MET:H	1:A:357:MET:HE2	1.70	0.56
3:C:1:MET:CG	3:C:6:LYS:HA	2.36	0.56
1:A:139:ASP:OD2	1:A:330:ILE:HG12	2.06	0.55
2:B:9:ARG:HH11	2:B:49:LEU:HD13	1.71	0.55
2:B:117:ILE:HD13	2:B:178:ALA:HA	1.86	0.55
3:C:71:LYS:HD3	3:C:129:TRP:HD1	1.70	0.55
3:C:88:GLY:O	3:C:91:HIS:HB2	2.07	0.55
1:A:64:ASN:HD21	1:A:66:GLU:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:130:HEB:CBB	12:C:132:CDN:C24	2.74	0.55
1:A:270:GLU:HG2	1:A:271:ARG:N	2.21	0.55
1:A:476:GLU:HB2	1:A:544:ASP:OD1	2.05	0.55
2:B:92:ARG:CD	3:C:17:THR:HG21	2.35	0.55
1:A:54:THR:OG1	1:A:403:ASN:ND2	2.39	0.55
2:B:117:ILE:O	2:B:117:ILE:HD12	2.06	0.55
2:B:116:LYS:NZ	2:B:167:ASP:O	2.40	0.55
1:A:216:HIS:CB	2:B:53:ARG:HE	2.20	0.55
1:A:45:HIS:HB2	1:A:218:ASN:HD21	1.72	0.54
1:A:455:ASP:HB2	1:A:498:ARG:HH21	1.72	0.54
3:C:28:ILE:HD11	11:C:131:AT5:C17	2.38	0.54
1:A:320:LYS:HG2	1:A:320:LYS:O	2.07	0.54
3:C:14:ASP:O	3:C:17:THR:HB	2.07	0.54
1:A:232:PRO:HB2	1:A:558:LEU:HD11	1.89	0.54
1:A:485:GLU:O	1:A:489:VAL:HG23	2.07	0.54
2:B:95:PRO:HD2	2:B:157:THR:HG22	1.88	0.54
3:C:78:LEU:HD21	12:C:132:CDN:C16	2.35	0.54
1:A:264:LEU:C	1:A:265:LEU:HD23	2.32	0.54
2:B:1:MET:N	2:B:29:GLU:HB2	2.22	0.54
2:B:95:PRO:CG	3:C:18:ILE:HD11	2.38	0.54
4:D:15:ASP:O	4:D:19:VAL:HG23	2.08	0.54
2:B:25:LEU:HD13	2:B:42:LEU:HD23	1.89	0.54
1:A:147:HIS:O	1:A:151:GLN:HG3	2.07	0.54
1:A:172:ASN:HD21	1:A:430:ARG:HG3	1.73	0.54
1:A:205:ALA:C	1:A:207:ARG:H	2.16	0.54
1:A:446:ARG:HH22	1:A:497:ALA:HB3	1.71	0.54
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.43	0.54
1:A:557:SER:HB2	1:A:569:ARG:HH12	1.73	0.54
2:B:59:VAL:HG12	2:B:59:VAL:O	2.07	0.54
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.43	0.53
1:A:573:MET:O	1:A:574:GLU:CB	2.56	0.53
2:B:229:ILE:O	2:B:233:LEU:HG	2.08	0.53
1:A:235:ASP:OD1	1:A:235:ASP:N	2.41	0.53
2:B:150:ILE:HD11	2:B:152:CYS:HB3	1.90	0.53
2:B:77:THR:HG22	2:B:82:LEU:CD1	2.37	0.53
1:A:126:PHE:O	1:A:129:GLU:HG2	2.09	0.53
1:A:151:GLN:HB3	2:B:119:PRO:O	2.08	0.53
1:A:528:VAL:HG12	1:A:569:ARG:HD2	1.90	0.53
1:A:573:MET:O	1:A:574:GLU:HB2	2.08	0.53
2:B:9:ARG:HH12	2:B:49:LEU:CB	2.22	0.53
2:B:58:GLY:HA2	7:B:302:FES:S2	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:LEU:HD13	11:C:131:AT5:H101	1.90	0.53
12:C:132:CDN:OB3	4:D:41:GLY:HA2	2.08	0.53
2:B:223:THR:CG2	9:B:304:F3S:S1	2.96	0.53
3:C:96:PHE:N	3:C:96:PHE:CD2	2.76	0.53
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.89	0.53
1:A:210:GLN:CD	1:A:465:GLU:HA	2.33	0.53
1:A:263:TYR:HB3	1:A:265:LEU:CD2	2.36	0.53
1:A:254:THR:HG22	1:A:330:ILE:CD1	2.38	0.53
1:A:404:SER:O	1:A:407:ASP:HB3	2.09	0.53
2:B:35:LEU:HD11	2:B:91:ILE:CD1	2.39	0.53
2:B:117:ILE:HD13	2:B:178:ALA:CA	2.37	0.53
1:A:86:GLU:OE1	1:A:578:ARG:HB3	2.09	0.52
1:A:254:THR:HA	5:A:589:OAA:O5	2.09	0.52
1:A:357:MET:CE	1:A:357:MET:N	2.72	0.52
1:A:265:LEU:HD22	1:A:271:ARG:HG2	1.90	0.52
1:A:214:ASN:HD22	1:A:214:ASN:N	2.07	0.52
1:A:215:ALA:C	1:A:217:ILE:H	2.15	0.52
2:B:2:ARG:HE	2:B:24:THR:HG21	1.75	0.52
3:C:78:LEU:HD11	12:C:132:CDN:H142	1.91	0.52
12:C:132:CDN:HA21	4:D:41:GLY:C	2.35	0.52
1:A:295:ILE:C	1:A:297:ILE:N	2.64	0.52
1:A:38:LYS:HG2	1:A:165:TYR:HD1	1.75	0.52
1:A:165:TYR:OH	1:A:221:ASP:OD1	2.24	0.52
1:A:357:MET:H	1:A:357:MET:HE3	1.73	0.52
3:C:30:HIS:CD2	3:C:84:HIS:ND1	2.77	0.52
2:B:198:SER:O	4:D:11:ASN:HB2	2.10	0.52
1:A:531:ASN:O	1:A:542:ARG:NH1	2.43	0.52
2:B:156:SER:OG	2:B:172:PRO:HD2	2.10	0.52
1:A:172:ASN:O	1:A:175:GLY:N	2.40	0.52
1:A:369:LEU:HD21	1:A:379:VAL:HG22	1.92	0.52
2:B:52:ARG:NH2	2:B:105:VAL:O	2.43	0.51
2:B:111:TYR:O	2:B:114:TYR:HB3	2.11	0.51
10:C:130:HEB:CAC	4:D:23:ALA:HB1	2.34	0.51
1:A:202:THR:OG1	1:A:222:GLY:HA3	2.10	0.51
1:A:14:GLY:HA2	6:A:601:FAD:C1B	2.40	0.51
1:A:14:GLY:HA2	6:A:601:FAD:H1B	1.90	0.51
2:B:209:ILE:HG12	3:C:27:SER:OG	2.11	0.51
1:A:276:TYR:CE2	1:A:292:SER:HA	2.46	0.51
4:D:26:LEU:O	4:D:30:ILE:HG13	2.11	0.51
1:A:76:SER:O	1:A:79:ILE:CG2	2.58	0.51
3:C:30:HIS:CD2	3:C:84:HIS:HD1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:VAL:HG13	10:C:130:HEB:HBC1	1.93	0.51
3:C:108:ARG:O	3:C:112:ILE:HG13	2.11	0.51
1:A:532:PHE:CG	1:A:569:ARG:HD3	2.46	0.50
2:B:79:ILE:O	2:B:80:SER:C	2.54	0.50
1:A:22:ALA:O	1:A:26:ILE:HG13	2.10	0.50
1:A:255:GLU:CD	1:A:286:ARG:HH12	2.19	0.50
1:A:459:ILE:HG23	1:A:490:ILE:CG2	2.41	0.50
1:A:475:ARG:HE	1:A:540:HIS:HD2	1.59	0.50
1:A:556:HIS:O	1:A:571:VAL:HA	2.11	0.50
1:A:139:ASP:HB2	1:A:327:LEU:HA	1.93	0.50
1:A:459:ILE:HD13	1:A:494:LEU:HA	1.93	0.50
1:A:119:PHE:CE2	2:B:134:LEU:HA	2.47	0.50
1:A:145:LEU:C	1:A:145:LEU:HD23	2.36	0.50
1:A:361:PRO:HA	1:A:391:CYS:O	2.12	0.50
2:B:207:HIS:HE1	3:C:31:ARG:NH2	2.09	0.50
1:A:78:TYR:CD2	1:A:583:PRO:HA	2.46	0.50
1:A:47:VAL:HG13	1:A:146:LEU:HD22	1.94	0.50
1:A:54:THR:O	1:A:406:LEU:HD22	2.12	0.50
1:A:295:ILE:HG23	1:A:298:ARG:HH21	1.76	0.50
1:A:82:GLN:HG2	1:A:575:PRO:HA	1.94	0.49
1:A:355:TYR:CD2	1:A:399:ARG:HD3	2.47	0.49
1:A:577:LEU:CG	1:A:578:ARG:H	2.25	0.49
1:A:232:PRO:CD	1:A:370:THR:HG22	2.42	0.49
1:A:252:LEU:HG	1:A:253:VAL:N	2.26	0.49
1:A:463:LEU:O	1:A:467:MET:HG2	2.12	0.49
2:B:123:ASN:ND2	2:B:125:GLY:H	2.10	0.49
1:A:549:ASP:OD1	1:A:552:ASN:HB2	2.12	0.49
4:D:44:THR:HB	4:D:47:VAL:HG23	1.95	0.49
1:A:9:ASP:N	1:A:32:THR:CG2	2.70	0.49
1:A:232:PRO:HD2	1:A:370:THR:HG22	1.94	0.49
1:A:533:ARG:HB3	1:A:540:HIS:CE1	2.47	0.49
2:B:35:LEU:CD2	2:B:91:ILE:HD11	2.40	0.49
2:B:148:GLU:O	2:B:149:CYS:C	2.53	0.49
2:B:212:CYS:SG	2:B:223:THR:HG23	2.52	0.49
1:A:218:ASN:N	1:A:218:ASN:ND2	2.57	0.49
1:A:286:ARG:HB2	1:A:398:ASN:HD21	1.77	0.49
1:A:404:SER:HB3	6:A:601:FAD:O2	2.11	0.49
4:D:44:THR:HG22	4:D:46:GLU:H	1.77	0.49
1:A:125:ASN:CG	1:A:132:ALA:HB2	2.37	0.49
1:A:412:GLY:O	1:A:415:ALA:HB3	2.12	0.49
2:B:146:LEU:HD11	2:B:183:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:VAL:O	3:C:122:LEU:HB3	2.12	0.49
1:A:119:PHE:HB2	2:B:135:GLN:N	2.12	0.49
1:A:307:TRP:CD1	1:A:348:PRO:HG2	2.47	0.49
1:A:405:LEU:HG	6:A:601:FAD:C2	2.43	0.49
1:A:174:ASP:HB2	1:A:430:ARG:NH2	2.27	0.48
1:A:197:ALA:HB1	1:A:384:PHE:CE1	2.48	0.48
1:A:559:TYR:HA	1:A:569:ARG:HH21	1.78	0.48
2:B:155:CYS:SG	2:B:156:SER:N	2.85	0.48
4:D:109:PHE:HB3	4:D:113:TRP:CZ3	2.47	0.48
1:A:81:ASP:HB3	1:A:83:ASP:OD1	2.13	0.48
1:A:40:PHE:O	1:A:43:ARG:HG2	2.14	0.48
1:A:43:ARG:O	1:A:44:SER:C	2.57	0.48
1:A:128:GLY:CA	1:A:400:LEU:HD11	2.33	0.48
1:A:263:TYR:O	1:A:313:LEU:HA	2.13	0.48
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.94	0.48
1:A:272:PHE:CZ	1:A:293:ILE:HG23	2.48	0.48
1:A:359:GLY:N	1:A:391:CYS:HB2	2.28	0.48
1:A:490:ILE:HA	1:A:493:ARG:HB3	1.96	0.48
2:B:201:PHE:HA	2:B:205:ARG:HD3	1.96	0.48
3:C:1:MET:CB	3:C:6:LYS:HA	2.44	0.48
1:A:341:ASP:OD1	1:A:343:VAL:HG23	2.14	0.48
1:A:534:THR:HB	1:A:553:TRP:HE1	1.78	0.48
1:A:78:TYR:O	1:A:554:LEU:HD11	2.13	0.48
1:A:242:HIS:HE1	1:A:286:ARG:HH21	1.62	0.48
2:B:9:ARG:NH1	2:B:49:LEU:CD1	2.77	0.48
2:B:107:MET:HE1	2:B:153:ALA:CB	2.40	0.48
3:C:37:THR:O	3:C:40:ALA:HB3	2.13	0.48
1:A:143:HIS:HE1	2:B:147:TYR:O	1.97	0.48
1:A:234:GLN:HB3	1:A:235:ASP:OD1	2.13	0.48
1:A:368:ALA:CB	1:A:383:LEU:HD23	2.44	0.48
1:A:545:PHE:N	1:A:546:PRO:CD	2.76	0.48
1:A:172:ASN:HD22	1:A:173:GLN:N	2.11	0.47
1:A:172:ASN:HB3	1:A:176:ALA:H	1.78	0.47
2:B:95:PRO:HB3	3:C:18:ILE:HD11	1.96	0.47
2:B:150:ILE:CD1	2:B:152:CYS:HB3	2.43	0.47
3:C:20:PHE:N	3:C:20:PHE:CD1	2.82	0.47
1:A:125:ASN:O	1:A:259:GLY:HA3	2.15	0.47
1:A:254:THR:C	1:A:256:GLY:N	2.70	0.47
1:A:307:TRP:HD1	1:A:348:PRO:HG2	1.79	0.47
1:A:444:LEU:HG	1:A:448:ASN:ND2	2.29	0.47
2:B:95:PRO:CB	3:C:18:ILE:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ARG:C	2:B:237:ASN:HD22	2.23	0.47
1:A:9:ASP:CB	1:A:32:THR:HG22	2.44	0.47
1:A:323:LEU:HB3	1:A:331:LEU:HD21	1.96	0.47
1:A:459:ILE:HG21	1:A:494:LEU:HD13	1.97	0.47
1:A:463:LEU:HD13	1:A:520:MET:HE1	1.96	0.47
1:A:240:GLN:HE22	1:A:399:ARG:HB3	1.78	0.47
1:A:252:LEU:HG	1:A:253:VAL:H	1.78	0.47
2:B:150:ILE:HG13	2:B:152:CYS:HB3	1.97	0.47
3:C:110:ALA:O	3:C:113:SER:HB2	2.14	0.47
1:A:11:VAL:HG23	1:A:195:ALA:CB	2.43	0.47
2:B:215:VAL:O	2:B:217:PRO:HD3	2.14	0.47
1:A:65:TRP:O	1:A:68:HIS:HB3	2.15	0.47
1:A:215:ALA:C	1:A:217:ILE:N	2.71	0.47
1:A:240:GLN:NE2	1:A:399:ARG:O	2.47	0.47
1:A:292:SER:O	1:A:296:GLU:HG2	2.14	0.47
2:B:55:CYS:O	2:B:56:ARG:HB3	2.13	0.47
1:A:137:ALA:O	1:A:138:ALA:HB3	2.15	0.47
1:A:421:GLU:O	1:A:424:ALA:HB3	2.15	0.47
1:A:537:ARG:NH1	1:A:554:LEU:HD12	2.25	0.47
1:A:1:MET:O	1:A:1:MET:HG3	2.15	0.47
1:A:322:VAL:O	1:A:326:ARG:HB2	2.15	0.47
1:A:549:ASP:HB3	1:A:553:TRP:HB2	1.96	0.47
1:A:220:GLY:O	1:A:221:ASP:C	2.56	0.47
3:C:127:LEU:HB2	12:C:132:CDN:H512	1.97	0.47
4:D:64:ALA:O	4:D:68:ILE:HG13	2.14	0.47
1:A:263:TYR:CD1	1:A:314:LYS:HD3	2.50	0.46
1:A:436:ASP:OD2	1:A:436:ASP:N	2.48	0.46
1:A:567:THR:O	1:A:568:ARG:CD	2.61	0.46
2:B:164:TRP:O	4:D:85:LYS:NZ	2.46	0.46
1:A:4:PRO:HB2	1:A:191:VAL:HG22	1.96	0.46
1:A:365:THR:OG1	1:A:367:GLN:HG3	2.15	0.46
2:B:34:MET:HE3	2:B:34:MET:CA	2.34	0.46
2:B:70:LYS:HB2	3:C:19:ARG:HD3	1.98	0.46
1:A:242:HIS:CE1	1:A:286:ARG:HH21	2.34	0.46
1:A:532:PHE:HD1	1:A:569:ARG:NH1	2.12	0.46
4:D:43:LEU:HD21	4:D:48:TRP:CE3	2.50	0.46
4:D:75:GLY:O	4:D:78:GLN:HB2	2.15	0.46
1:A:104:LEU:HD12	1:A:105:PRO:CD	2.45	0.46
1:A:240:GLN:CB	1:A:357:MET:HE1	2.36	0.46
2:B:21:GLN:NE2	2:B:23:TYR:OH	2.48	0.46
1:A:255:GLU:CD	1:A:286:ARG:HH22	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:N	1:A:328:PRO:CD	2.76	0.46
1:A:520:MET:O	1:A:522:THR:N	2.48	0.46
1:A:69:MET:HE1	1:A:577:LEU:HD12	1.98	0.46
1:A:468:GLN:O	1:A:472:SER:HB2	2.16	0.46
2:B:128:PRO:HA	2:B:129:PRO:HD3	1.80	0.46
3:C:92:MET:HE3	4:D:20:ARG:CG	2.43	0.46
1:A:69:MET:HG2	1:A:85:ILE:HG22	1.97	0.46
1:A:207:ARG:C	1:A:209:TYR:H	2.23	0.46
1:A:254:THR:C	1:A:256:GLY:H	2.23	0.46
3:C:2:ILE:HG13	3:C:3:ARG:H	1.81	0.46
1:A:276:TYR:CE2	1:A:295:ILE:HD12	2.51	0.46
3:C:18:ILE:HG22	3:C:20:PHE:CE1	2.51	0.46
1:A:242:HIS:CE1	1:A:286:ARG:NH2	2.85	0.45
2:B:54:SER:O	2:B:55:CYS:C	2.56	0.45
2:B:208:SER:HA	9:B:304:F3S:S1	2.56	0.45
1:A:81:ASP:OD2	1:A:81:ASP:N	2.49	0.45
1:A:499:LEU:HG	1:A:501:ASP:O	2.15	0.45
4:D:113:TRP:CD1	4:D:113:TRP:C	2.94	0.45
1:A:200:LEU:HD12	1:A:360:ILE:CD1	2.46	0.45
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.46	0.45
1:A:38:LYS:HZ2	1:A:217:ILE:HG23	1.79	0.45
1:A:267:LYS:HZ1	1:A:301:ARG:HD3	1.81	0.45
1:A:314:LYS:NZ	1:A:317:HIS:HB3	2.32	0.45
2:B:157:THR:HG22	2:B:157:THR:O	2.16	0.45
3:C:44:LEU:HB3	12:C:132:CDN:H381	1.98	0.45
3:C:66:GLY:O	3:C:67:SER:C	2.58	0.45
1:A:276:TYR:CZ	1:A:292:SER:HA	2.52	0.45
2:B:209:ILE:HD11	11:C:131:AT5:N4	2.32	0.45
2:B:89:ILE:O	2:B:89:ILE:HG22	2.15	0.45
1:A:471:PHE:CE2	1:A:527:ALA:HA	2.52	0.45
1:A:486:GLN:O	1:A:490:ILE:HG13	2.16	0.45
1:A:491:ARG:NH1	1:A:524:TYR:HE1	2.15	0.45
2:B:94:LEU:HD22	2:B:157:THR:HG21	1.98	0.45
1:A:165:TYR:CE1	6:A:601:FAD:N6A	2.85	0.45
1:A:307:TRP:HE3	1:A:307:TRP:HA	1.82	0.45
1:A:513:CYS:O	1:A:516:LEU:HB3	2.16	0.45
4:D:45:TYR:O	4:D:49:ILE:HG22	2.17	0.45
1:A:520:MET:C	1:A:522:THR:N	2.75	0.45
2:B:180:ARG:HD3	2:B:181:PHE:CE1	2.52	0.45
4:D:110:VAL:HA	4:D:113:TRP:CE2	2.52	0.45
1:A:579:PRO:O	1:A:580:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLN:HB3	1:A:577:LEU:HB3	1.96	0.44
2:B:100:ILE:HB	2:B:104:VAL:O	2.17	0.44
2:B:121:LEU:HD11	2:B:186:ARG:HB2	1.98	0.44
1:A:100:GLU:OE2	1:A:101:HIS:HD2	1.99	0.44
1:A:307:TRP:HA	1:A:307:TRP:CE3	2.52	0.44
2:B:157:THR:CG2	2:B:157:THR:O	2.63	0.44
2:B:234:LEU:HD23	4:D:13:VAL:HG13	1.99	0.44
1:A:104:LEU:HA	1:A:105:PRO:HD3	1.80	0.44
1:A:220:GLY:O	1:A:223:VAL:N	2.51	0.44
1:A:359:GLY:HA3	1:A:389:ILE:O	2.17	0.44
2:B:176:LEU:HD12	2:B:222:PRO:HA	1.99	0.44
1:A:240:GLN:N	1:A:357:MET:HE1	2.31	0.44
1:A:433:SER:C	1:A:435:SER:N	2.76	0.44
1:A:545:PHE:O	1:A:547:ASP:N	2.49	0.44
1:A:571:VAL:CG1	1:A:572:ASN:H	2.30	0.44
4:D:6:SER:HB2	4:D:94:GLN:HE22	1.82	0.44
1:A:172:ASN:ND2	1:A:430:ARG:HG3	2.32	0.44
2:B:23:TYR:CD2	2:B:42:LEU:HD13	2.52	0.44
2:B:53:ARG:CG	2:B:53:ARG:HH11	2.31	0.44
2:B:109:GLN:O	2:B:113:GLN:HG2	2.18	0.44
1:A:151:GLN:O	1:A:154:LEU:HB2	2.17	0.44
1:A:169:LEU:N	1:A:169:LEU:HD23	2.33	0.44
1:A:274:GLU:O	1:A:278:PRO:HA	2.17	0.44
2:B:37:ASP:O	2:B:41:GLN:HG2	2.16	0.44
1:A:267:LYS:HZ1	1:A:301:ARG:HH11	1.66	0.44
2:B:60:CYS:SG	2:B:62:SER:CB	3.06	0.44
1:A:13:ILE:HD12	1:A:200:LEU:HD23	2.00	0.44
1:A:81:ASP:O	1:A:85:ILE:HG13	2.18	0.44
1:A:213:THR:HG21	1:A:252:LEU:HD12	2.00	0.44
1:A:559:TYR:CA	1:A:569:ARG:NH2	2.75	0.44
2:B:9:ARG:HH12	2:B:49:LEU:HB2	1.83	0.44
2:B:33:MET:HE3	2:B:38:ALA:HB2	1.99	0.44
2:B:236:ARG:HH11	2:B:236:ARG:HG3	1.83	0.44
3:C:93:MET:HG2	3:C:98:TYR:CB	2.45	0.44
1:A:326:ARG:O	1:A:327:LEU:HD23	2.18	0.43
2:B:7:ILE:HG12	2:B:91:ILE:HB	2.00	0.43
2:B:65:LEU:CD1	2:B:74:ALA:HB2	2.48	0.43
1:A:43:ARG:O	1:A:44:SER:O	2.36	0.43
3:C:73:ILE:C	3:C:75:TRP:N	2.74	0.43
1:A:84:ALA:CB	1:A:394:VAL:HG12	2.49	0.43
1:A:529:SER:HA	1:A:569:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ILE:HG22	3:C:93:MET:CE	2.43	0.43
1:A:236:MET:HA	1:A:236:MET:CE	2.48	0.43
1:A:243:PRO:HD3	1:A:286:ARG:HD3	1.99	0.43
1:A:84:ALA:HB1	1:A:394:VAL:HG12	2.00	0.43
1:A:298:ARG:HE	1:A:298:ARG:HB2	1.63	0.43
3:C:96:PHE:N	3:C:96:PHE:HD2	2.16	0.43
4:D:80:LEU:CD2	4:D:84:VAL:HG21	2.48	0.43
1:A:433:SER:O	1:A:435:SER:N	2.51	0.43
1:A:559:TYR:N	1:A:569:ARG:NH2	2.67	0.43
2:B:207:HIS:CE1	3:C:31:ARG:NH2	2.86	0.43
1:A:482:LYS:HD3	1:A:482:LYS:HA	1.85	0.43
2:B:35:LEU:HD12	2:B:35:LEU:C	2.42	0.43
1:A:205:ALA:HB1	1:A:220:GLY:H	1.75	0.43
1:A:270:GLU:HG2	1:A:271:ARG:H	1.83	0.43
1:A:287:ASP:OD2	1:A:288:VAL:N	2.50	0.43
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.54	0.43
10:C:130:HEB:CBB	12:C:132:CDN:H241	2.42	0.43
4:D:44:THR:CG2	4:D:46:GLU:HG2	2.49	0.43
1:A:61:HIS:NE2	1:A:131:ALA:CB	2.80	0.43
1:A:253:VAL:HG13	1:A:330:ILE:HD12	2.00	0.43
1:A:407:ASP:O	1:A:408:LEU:C	2.61	0.43
2:B:100:ILE:HG12	3:C:9:ARG:NH2	2.34	0.43
1:A:293:ILE:HG22	1:A:311:ALA:HB2	2.00	0.43
1:A:320:LYS:HG3	1:A:343:VAL:HG11	1.99	0.43
1:A:560:LEU:HD12	1:A:561:PRO:CD	2.48	0.43
2:B:171:GLY:O	2:B:175:LEU:HG	2.19	0.43
2:B:211:ASN:O	2:B:215:VAL:HG22	2.19	0.43
3:C:123:LEU:HB3	12:C:132:CDN:H521	2.01	0.43
1:A:255:GLU:CB	1:A:286:ARG:HH22	2.32	0.42
2:B:33:MET:O	2:B:79:ILE:HG12	2.19	0.42
3:C:73:ILE:O	3:C:75:TRP:N	2.52	0.42
4:D:68:ILE:O	4:D:69:LEU:C	2.62	0.42
2:B:209:ILE:O	2:B:210:MET:HB2	2.20	0.42
1:A:39:VAL:CG2	1:A:43:ARG:HB2	2.49	0.42
2:B:67:MET:CE	2:B:74:ALA:HA	2.49	0.42
3:C:122:LEU:O	3:C:126:VAL:HG23	2.18	0.42
4:D:76:MET:HB3	4:D:97:ILE:HD13	1.99	0.42
1:A:242:HIS:CD2	1:A:252:LEU:HD11	2.54	0.42
1:A:285:GLY:O	1:A:289:VAL:HG23	2.19	0.42
4:D:115:VAL:OXT	4:D:115:VAL:HG12	2.20	0.42
1:A:39:VAL:HG21	1:A:43:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD11	2:B:91:ILE:HD11	2.02	0.42
2:B:55:CYS:O	2:B:57:GLU:HG2	2.20	0.42
2:B:65:LEU:HD22	2:B:103:LEU:HD13	2.02	0.42
1:A:242:HIS:CG	1:A:252:LEU:HD11	2.55	0.42
1:A:324:GLU:HG2	1:A:331:LEU:CD1	2.49	0.42
4:D:62:LEU:HD23	4:D:65:LEU:CD1	2.45	0.42
1:A:60:THR:HG21	1:A:123:SER:O	2.18	0.42
1:A:129:GLU:HG3	1:A:131:ALA:O	2.20	0.42
1:A:222:GLY:HA3	1:A:389:ILE:CD1	2.45	0.42
1:A:508:THR:HG22	1:A:512:GLU:OE2	2.20	0.42
1:A:516:LEU:O	1:A:517:ASP:C	2.63	0.42
1:A:6:ARG:HD2	1:A:191:VAL:HG11	2.02	0.42
1:A:174:ASP:HB2	1:A:430:ARG:CZ	2.50	0.42
1:A:178:VAL:HG23	1:A:178:VAL:O	2.20	0.42
1:A:240:GLN:H	1:A:357:MET:HE1	1.85	0.42
2:B:150:ILE:CG1	2:B:152:CYS:HB3	2.50	0.42
10:C:130:HEB:HBB1	12:C:132:CDN:H242	1.89	0.42
1:A:108:ARG:CD	1:A:119:PHE:O	2.65	0.41
2:B:211:ASN:HD21	3:C:24:ALA:HB2	1.86	0.41
4:D:6:SER:CB	4:D:94:GLN:HE22	2.33	0.41
1:A:50:GLN:O	1:A:51:GLY:C	2.63	0.41
2:B:5:PHE:HB2	2:B:23:TYR:HB2	2.02	0.41
6:A:601:FAD:H9	6:A:601:FAD:H1'1	1.80	0.41
3:C:20:PHE:HA	3:C:21:PRO:HD3	1.93	0.41
1:A:305:GLY:C	1:A:307:TRP:N	2.77	0.41
1:A:576:LYS:O	1:A:576:LYS:HG3	2.20	0.41
1:A:577:LEU:CD2	1:A:577:LEU:N	2.61	0.41
4:D:61:THR:O	4:D:64:ALA:HB3	2.21	0.41
1:A:460:ARG:HG2	1:A:464:GLN:OE1	2.19	0.41
3:C:2:ILE:HD11	3:C:5:VAL:HG21	2.01	0.41
4:D:49:ILE:HG12	4:D:49:ILE:O	2.21	0.41
4:D:97:ILE:O	4:D:100:ALA:HB3	2.20	0.41
1:A:119:PHE:CD2	2:B:134:LEU:CA	2.90	0.41
1:A:483:GLY:C	1:A:485:GLU:N	2.78	0.41
4:D:13:VAL:H	4:D:13:VAL:HG23	1.64	0.41
1:A:79:ILE:O	1:A:79:ILE:HG12	2.19	0.41
1:A:108:ARG:HG3	2:B:135:GLN:HG2	2.03	0.41
1:A:276:TYR:HE2	1:A:295:ILE:HD12	1.86	0.41
1:A:522:THR:O	1:A:523:ALA:C	2.63	0.41
2:B:201:PHE:O	2:B:202:SER:C	2.61	0.41
1:A:122:GLN:HE21	1:A:122:GLN:HB3	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:C	1:A:389:ILE:HD11	2.45	0.41
1:A:544:ASP:C	1:A:546:PRO:HD3	2.46	0.41
4:D:36:PHE:CE2	4:D:48:TRP:HZ3	2.39	0.41
1:A:91:THR:O	1:A:91:THR:HG22	2.21	0.41
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.94	0.41
1:A:242:HIS:HB2	1:A:354:HIS:CB	2.46	0.41
1:A:246:ILE:HD13	1:A:338:ALA:HB2	2.03	0.41
1:A:276:TYR:OH	1:A:295:ILE:HB	2.21	0.41
1:A:443:ARG:HH22	1:A:518:ASN:HD21	1.69	0.41
1:A:483:GLY:O	1:A:487:LEU:HD13	2.21	0.41
1:A:554:LEU:HD12	1:A:554:LEU:HA	1.95	0.41
1:A:556:HIS:N	1:A:572:ASN:O	2.39	0.41
2:B:115:GLU:O	2:B:116:LYS:C	2.62	0.41
2:B:145:GLY:O	2:B:146:LEU:HD23	2.21	0.41
2:B:236:ARG:C	2:B:237:ASN:ND2	2.79	0.41
3:C:123:LEU:CB	12:C:132:CDN:H521	2.50	0.41
4:D:80:LEU:HD23	4:D:84:VAL:HG21	2.03	0.41
1:A:8:PHE:O	1:A:195:ALA:HA	2.21	0.41
1:A:185:ILE:H	1:A:185:ILE:HG13	1.62	0.41
1:A:479:ALA:O	1:A:480:MET:C	2.64	0.41
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.56	0.41
1:A:95:ALA:O	1:A:98:GLU:HB3	2.22	0.40
1:A:405:LEU:HA	1:A:408:LEU:HG	2.03	0.40
2:B:73:LEU:HG	2:B:217:PRO:CG	2.51	0.40
3:C:44:LEU:HA	3:C:44:LEU:HD23	1.88	0.40
3:C:65:MET:HG2	12:C:132:CDN:HA51	2.03	0.40
1:A:291:ARG:O	1:A:292:SER:C	2.63	0.40
2:B:35:LEU:CD2	2:B:67:MET:HE2	2.28	0.40
2:B:140:ARG:HD3	2:B:140:ARG:C	2.46	0.40
3:C:30:HIS:NE2	3:C:84:HIS:CE1	2.89	0.40
1:A:208:ILE:HG13	1:A:209:TYR:CE1	2.57	0.40
2:B:179:TYR:CE2	2:B:183:ILE:HD13	2.56	0.40
1:A:213:THR:HA	1:A:250:GLY:O	2.21	0.40
1:A:340:VAL:HG13	1:A:345:GLU:OE1	2.22	0.40
2:B:2:ARG:NE	2:B:24:THR:HG21	2.36	0.40
1:A:372:ASN:O	1:A:375:GLY:N	2.53	0.40
1:A:405:LEU:O	1:A:408:LEU:HB2	2.21	0.40
1:A:476:GLU:HG3	1:A:478:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/588 (100%)	461 (79%)	81 (14%)	44 (8%)	1	4
2	B	236/238 (99%)	205 (87%)	25 (11%)	6 (2%)	4	21
3	C	127/129 (98%)	111 (87%)	11 (9%)	5 (4%)	2	14
4	D	111/115 (96%)	100 (90%)	10 (9%)	1 (1%)	14	44
All	All	1060/1070 (99%)	877 (83%)	127 (12%)	56 (5%)	1	10

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	118	PRO
1	A	220	GLY
1	A	235	ASP
1	A	546	PRO
1	A	562	GLU
1	A	563	SER
1	A	575	PRO
3	C	2	ILE
1	A	51	GLY
1	A	120	GLY
1	A	205	ALA
1	A	218	ASN
1	A	236	MET
1	A	339	HIS
1	A	357	MET
1	A	358	GLY
1	A	453	GLY
1	A	472	SER
1	A	521	GLU
1	A	574	GLU
2	B	54	SER

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Mol	Chain	Res	Type
2	B	204	PHE
3	C	96	PHE
1	A	44	SER
1	A	272	PHE
1	A	434	GLU
1	A	467	MET
1	A	497	ALA
1	A	578	ARG
1	A	584	LYS
1	A	41	PRO
1	A	77	ASP
1	A	281	LYS
1	A	428	ALA
1	A	431	ASP
1	A	466	CYS
2	B	18	PRO
2	B	81	ALA
2	B	102	ASP
3	C	54	SER
3	C	74	MET
1	A	56	ALA
1	A	254	THR
1	A	303	CYS
1	A	477	GLY
2	B	85	PRO
3	C	7	LYS
4	D	41	GLY
1	A	105	PRO
1	A	565	SER
1	A	232	PRO
1	A	278	PRO
1	A	561	PRO
1	A	583	PRO
1	A	114	ILE

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	473/473 (100%)	445 (94%)	28 (6%)	18	48
2	B	208/208 (100%)	196 (94%)	12 (6%)	18	48
3	C	109/109 (100%)	104 (95%)	5 (5%)	24	55
4	D	94/96 (98%)	88 (94%)	6 (6%)	16	44
All	All	884/886 (100%)	833 (94%)	51 (6%)	18	48

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	CYS
1	A	47	VAL
1	A	60	THR
1	A	64	ASN
1	A	79	ILE
1	A	122	GLN
1	A	126	PHE
1	A	169	LEU
1	A	202	THR
1	A	218	ASN
1	A	235	ASP
1	A	252	LEU
1	A	265	LEU
1	A	278	PRO
1	A	293	ILE
1	A	303	CYS
1	A	352	THR
1	A	357	MET
1	A	371	VAL
1	A	389	ILE
1	A	436	ASP
1	A	478	ASP
1	A	504	SER
1	A	506	PHE
1	A	533	ARG
1	A	544	ASP
1	A	550	ASP
1	A	577	LEU
2	B	26	GLU
2	B	32	ASP
2	B	34	MET
2	B	35	LEU
2	B	53	ARG

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Mol	Chain	Res	Type
2	B	67	MET
2	B	90	VAL
2	B	134	LEU
2	B	135	GLN
2	B	176	LEU
2	B	180	ARG
2	B	213	VAL
3	C	4	ASN
3	C	83	TYR
3	C	91	HIS
3	C	93	MET
3	C	129	TRP
4	D	8	LEU
4	D	13	VAL
4	D	17	ILE
4	D	49	ILE
4	D	60	PHE
4	D	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	59	ASN
1	A	82	GLN
1	A	101	HIS
1	A	122	GLN
1	A	143	HIS
1	A	147	HIS
1	A	152	GLN
1	A	153	ASN
1	A	172	ASN
1	A	218	ASN
1	A	234	GLN
1	A	240	GLN
1	A	242	HIS
1	A	367	GLN
1	A	398	ASN
1	A	403	ASN
1	A	420	GLN
1	A	448	ASN
1	A	470	ASN

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	540	HIS
2	B	21	GLN
2	B	84	GLN
2	B	123	ASN
2	B	127	ASN
2	B	211	ASN
2	B	237	ASN
3	C	4	ASN
4	D	14	HIS
4	D	78	GLN
4	D	94	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	F3S	B	304	2	0,9,9	-	-	-		
10	HEB	C	130	3,4	50,50,50	1.50	8 (16%)	66,82,82	1.64	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CDN	C	132	-	76,76,76	2.05	11 (14%)	74,88,88	1.64	9 (12%)
8	SF4	B	303	2	0,12,12	-	-	-	-	-
5	OAA	A	589	-	8,8,8	3.88	4 (50%)	8,10,10	1.77	3 (37%)
7	FES	B	302	2	0,4,4	-	-	-	-	-
6	FAD	A	601	1	58,58,58	2.26	19 (32%)	85,89,89	2.52	15 (17%)
11	AT5	C	131	-	20,23,23	2.40	8 (40%)	21,32,32	2.15	5 (23%)

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
9	F3S	B	304	2	-	-	0/3/3/3
10	HEB	C	130	3,4	1/1/3/8	7/14/54/54	-
12	CDN	C	132	-	3/3/9/9	24/87/87/87	-
8	SF4	B	303	2	-	-	0/6/5/5
5	OAA	A	589	-	-	1/8/8/8	-
7	FES	B	302	2	-	-	0/1/1/1
6	FAD	A	601	1	-	3/34/50/50	0/6/6/6
11	AT5	C	131	-	-	10/20/22/22	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	589	OAA	C3-C4	-9.97	1.38	1.53
6	A	601	FAD	C4X-N5	7.54	1.47	1.30
12	C	132	CDN	OA8-CA7	7.44	1.53	1.40
12	C	132	CDN	OA6-CA5	-7.09	1.21	1.41
12	C	132	CDN	OB8-CB7	6.96	1.52	1.40
11	C	131	AT5	O4-C5	6.02	1.35	1.23
10	C	130	HEB	FE-ND	5.01	2.10	1.94
12	C	132	CDN	OB7-CB5	-4.99	1.21	1.39
12	C	132	CDN	OA7-CA5	4.98	1.56	1.39
12	C	132	CDN	OA9-CA7	-4.89	1.22	1.39
6	A	601	FAD	C5'-C4'	-4.88	1.45	1.51
6	A	601	FAD	C4A-N3A	4.83	1.43	1.34
12	C	132	CDN	OB9-CB7	-4.81	1.22	1.39
6	A	601	FAD	C9A-N10	4.68	1.49	1.41
11	C	131	AT5	C6-C1	4.68	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	FAD	PA-O3P	-4.28	1.54	1.59
6	A	601	FAD	C5A-C4A	-4.03	1.31	1.39
12	C	132	CDN	OB6-CB5	3.97	1.52	1.41
6	A	601	FAD	C8A-N9A	3.47	1.43	1.37
6	A	601	FAD	C9A-C5X	3.39	1.46	1.41
6	A	601	FAD	C6-C7	3.38	1.44	1.39
11	C	131	AT5	C8-C7	3.36	1.58	1.52
10	C	130	HEB	FE-NA	3.30	2.06	1.95
11	C	131	AT5	C6-C7	3.11	1.56	1.47
10	C	130	HEB	FE-NC	3.08	2.05	1.95
6	A	601	FAD	C2A-N3A	2.97	1.39	1.33
6	A	601	FAD	C10-N1	2.95	1.39	1.33
11	C	131	AT5	C11-C12	-2.85	1.49	1.54
10	C	130	HEB	C1A-NA	-2.72	1.34	1.39
11	C	131	AT5	O3-C3	2.67	1.39	1.33
5	A	589	OAA	O4-C4	2.60	1.29	1.22
10	C	130	HEB	C4B-NB	-2.60	1.35	1.40
12	C	132	CDN	OB6-CB4	-2.58	1.41	1.44
6	A	601	FAD	C2B-C3B	-2.57	1.46	1.53
10	C	130	HEB	FE-NB	2.46	2.02	1.94
6	A	601	FAD	C5X-N5	2.44	1.43	1.39
12	C	132	CDN	OA6-CA4	-2.42	1.41	1.44
6	A	601	FAD	O4-C4	2.41	1.28	1.23
6	A	601	FAD	C2'-C3'	-2.38	1.49	1.53
6	A	601	FAD	C6A-N1A	2.29	1.42	1.35
10	C	130	HEB	C1C-NC	-2.25	1.35	1.39
6	A	601	FAD	C1'-N10	-2.22	1.42	1.47
6	A	601	FAD	C9-C9A	2.22	1.43	1.39
5	A	589	OAA	O3-C3	2.15	1.27	1.23
10	C	130	HEB	CAC-C3C	2.14	1.53	1.47
5	A	589	OAA	O2-C1	-2.11	1.23	1.30
11	C	131	AT5	C17-C12	2.08	1.58	1.53
11	C	131	AT5	C11-C8	-2.08	1.48	1.54
6	A	601	FAD	P-O3P	-2.06	1.57	1.59
12	C	132	CDN	C11-CA5	2.00	1.54	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	FAD	O2A-PA-O5B	-9.50	64.50	107.57
6	A	601	FAD	O2A-PA-O3P	9.40	132.69	107.27
6	A	601	FAD	O3P-PA-O1A	-8.25	85.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	FAD	O5B-PA-O1A	6.64	135.24	108.94
6	A	601	FAD	N3A-C4A-N9A	-6.07	116.85	127.17
6	A	601	FAD	C5A-C4A-N9A	5.89	112.23	105.81
12	C	132	CDN	OB9-CB7-C71	5.81	125.23	109.37
11	C	131	AT5	C17-C12-C11	5.79	119.44	110.68
12	C	132	CDN	OA9-CA7-C31	5.65	124.80	109.37
12	C	132	CDN	OB7-CB5-C51	5.65	124.79	109.37
6	A	601	FAD	O2A-PA-O1A	-4.86	89.85	112.44
6	A	601	FAD	C4A-N9A-C8A	-4.53	100.98	105.74
11	C	131	AT5	C1-C6-C7	4.38	123.00	118.11
10	C	130	HEB	CHA-C1A-NA	3.98	128.79	124.45
12	C	132	CDN	C19-C18-C17	-3.82	95.04	114.37
6	A	601	FAD	C1'-N10-C9A	-3.82	113.22	120.63
10	C	130	HEB	C1D-ND-C4D	3.68	109.56	105.21
10	C	130	HEB	C4B-NB-C1B	3.66	109.54	105.21
12	C	132	CDN	C15-C14-C13	-3.61	96.13	114.37
11	C	131	AT5	O5-C7-C6	-3.43	115.30	119.67
6	A	601	FAD	N3A-C2A-N1A	-3.34	123.52	128.58
6	A	601	FAD	C5A-C4A-N3A	3.06	130.93	126.72
10	C	130	HEB	CHB-C4A-NA	3.04	127.77	124.45
6	A	601	FAD	C1'-C2'-C3'	2.89	117.51	109.66
5	A	589	OAA	O3-C3-C2	2.89	124.85	120.41
11	C	131	AT5	C6-C5-N4	2.87	123.00	115.10
10	C	130	HEB	C3C-C4C-NC	-2.86	107.39	109.80
10	C	130	HEB	CHC-C4B-NB	2.83	127.87	124.37
6	A	601	FAD	C5X-C9A-N10	-2.73	115.50	117.97
10	C	130	HEB	C4A-NA-C1A	2.59	110.04	105.82
10	C	130	HEB	CAD-C3D-C4D	2.51	129.07	124.70
10	C	130	HEB	CBD-CAD-C3D	2.48	119.38	112.53
12	C	132	CDN	C21-C20-C19	-2.47	101.86	114.37
10	C	130	HEB	CHC-C1C-NC	2.47	128.33	123.86
12	C	132	CDN	OA7-CA5-C11	2.44	116.03	109.37
5	A	589	OAA	O5-C4-C3	2.40	120.24	113.59
12	C	132	CDN	C22-C21-C20	-2.37	102.37	114.37
10	C	130	HEB	CHB-C1B-NB	2.37	126.97	124.42
10	C	130	HEB	CHA-C4D-ND	2.35	126.95	124.42
10	C	130	HEB	CHD-C1D-ND	2.34	127.27	124.37
6	A	601	FAD	C1B-N9A-C8A	2.28	132.15	127.09
6	A	601	FAD	C6-C5X-C9A	-2.25	115.96	119.05
12	C	132	CDN	C16-C15-C14	-2.11	103.73	114.37
5	A	589	OAA	O4-C4-C3	-2.09	119.22	121.81
10	C	130	HEB	CHD-C4C-NC	2.06	127.60	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	130	HEB	C3D-C4D-ND	-2.05	108.37	110.35
10	C	130	HEB	C4C-NC-C1C	2.05	109.16	105.82
11	C	131	AT5	O4-C5-C6	-2.01	119.65	125.69

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	130	HEB	NA
12	C	132	CDN	CA7
12	C	132	CDN	CB5
12	C	132	CDN	CB7

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	FAD	C5B-O5B-PA-O2A
11	C	131	AT5	C5-C6-C7-O5
11	C	131	AT5	C1-C6-C7-O5
11	C	131	AT5	C5-C6-C7-C8
11	C	131	AT5	C1-C6-C7-C8
11	C	131	AT5	C12-C13-C14-CL16
12	C	132	CDN	CB2-OB2-PB2-OB5
12	C	132	CDN	CB2-OB2-PB2-OB3
12	C	132	CDN	CB2-OB2-PB2-OB4
12	C	132	CDN	OB7-CB5-OB6-CB4
12	C	132	CDN	C52-C51-CB5-OB7
12	C	132	CDN	OA7-CA5-OA6-CA4
10	C	130	HEB	C4D-C3D-CAD-CBD
10	C	130	HEB	C2D-C3D-CAD-CBD
10	C	130	HEB	C4C-C3C-CAC-CBC
12	C	132	CDN	C60-C61-C62-C63
12	C	132	CDN	C58-C59-C60-C61
12	C	132	CDN	C55-C56-C57-C58
12	C	132	CDN	CB3-CB4-CB6-OB8
10	C	130	HEB	C2A-CAA-CBA-CGA
12	C	132	CDN	C54-C55-C56-C57
12	C	132	CDN	C14-C15-C16-C17
12	C	132	CDN	C72-C71-CB7-OB8
12	C	132	CDN	C61-C62-C63-C64
11	C	131	AT5	C12-C11-C8-C10
12	C	132	CDN	C31-CA7-OA8-CA6
12	C	132	CDN	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
10	C	130	HEB	C2C-C3C-CAC-CBC
12	C	132	CDN	C1-CB2-OB2-PB2
11	C	131	AT5	C12-C11-C8-C7
12	C	132	CDN	C32-C31-CA7-OA8
12	C	132	CDN	CB7-C71-C72-C73
10	C	130	HEB	CAA-CBA-CGA-O1A
10	C	130	HEB	CAA-CBA-CGA-O2A
11	C	131	AT5	O5-C7-C8-C10
12	C	132	CDN	CB2-C1-CA2-OA2
12	C	132	CDN	C35-C36-C37-C38
12	C	132	CDN	C56-C57-C58-C59
12	C	132	CDN	C52-C51-CB5-OB6
6	A	601	FAD	P-O3P-PA-O1A
5	A	589	OAA	O1-C1-C2-C3
6	A	601	FAD	O4B-C4B-C5B-O5B
11	C	131	AT5	C1-C2-O2-CM2
12	C	132	CDN	OA9-CA7-OA8-CA6
11	C	131	AT5	CL12-C13-C14-CL16

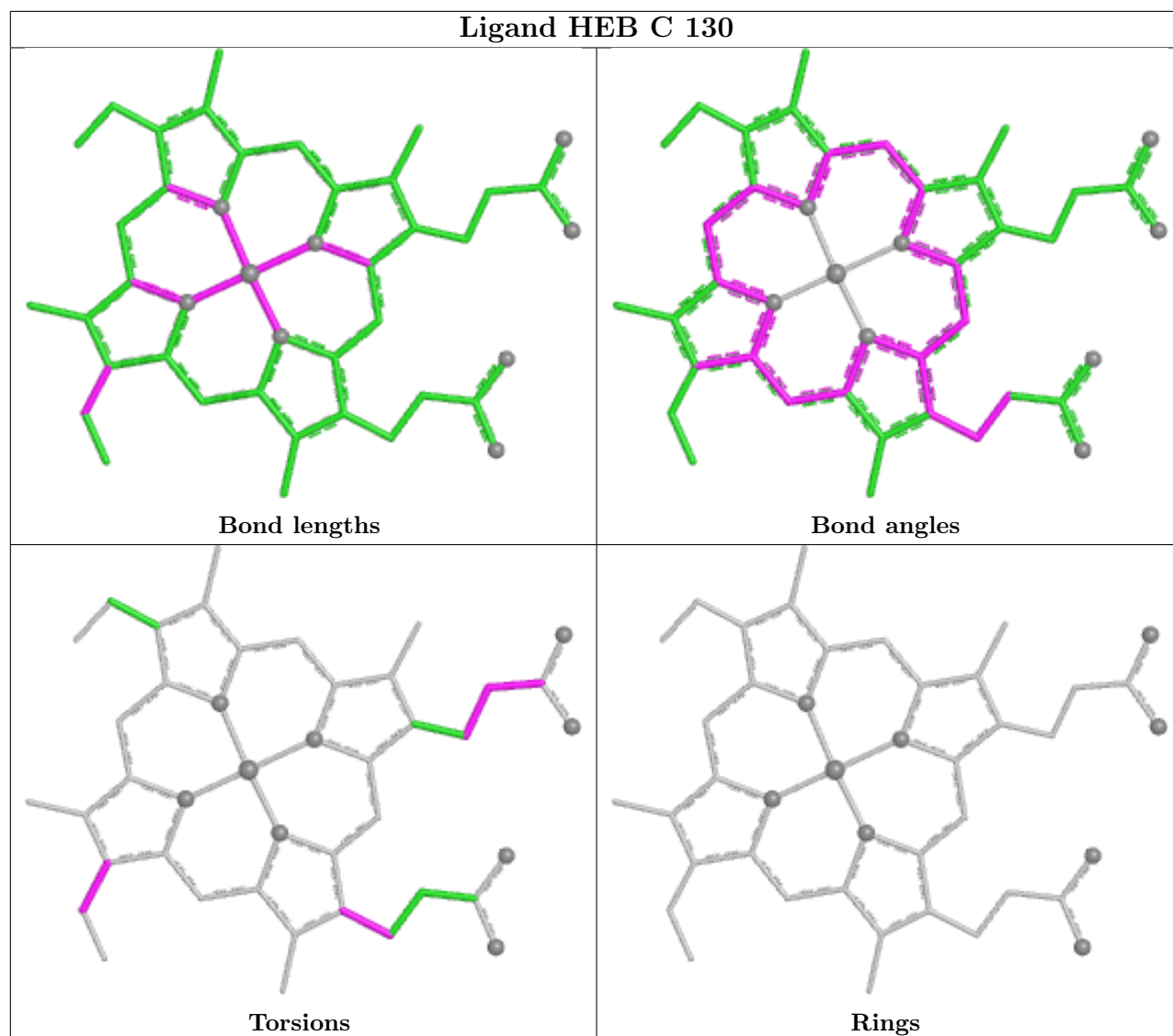
There are no ring outliers.

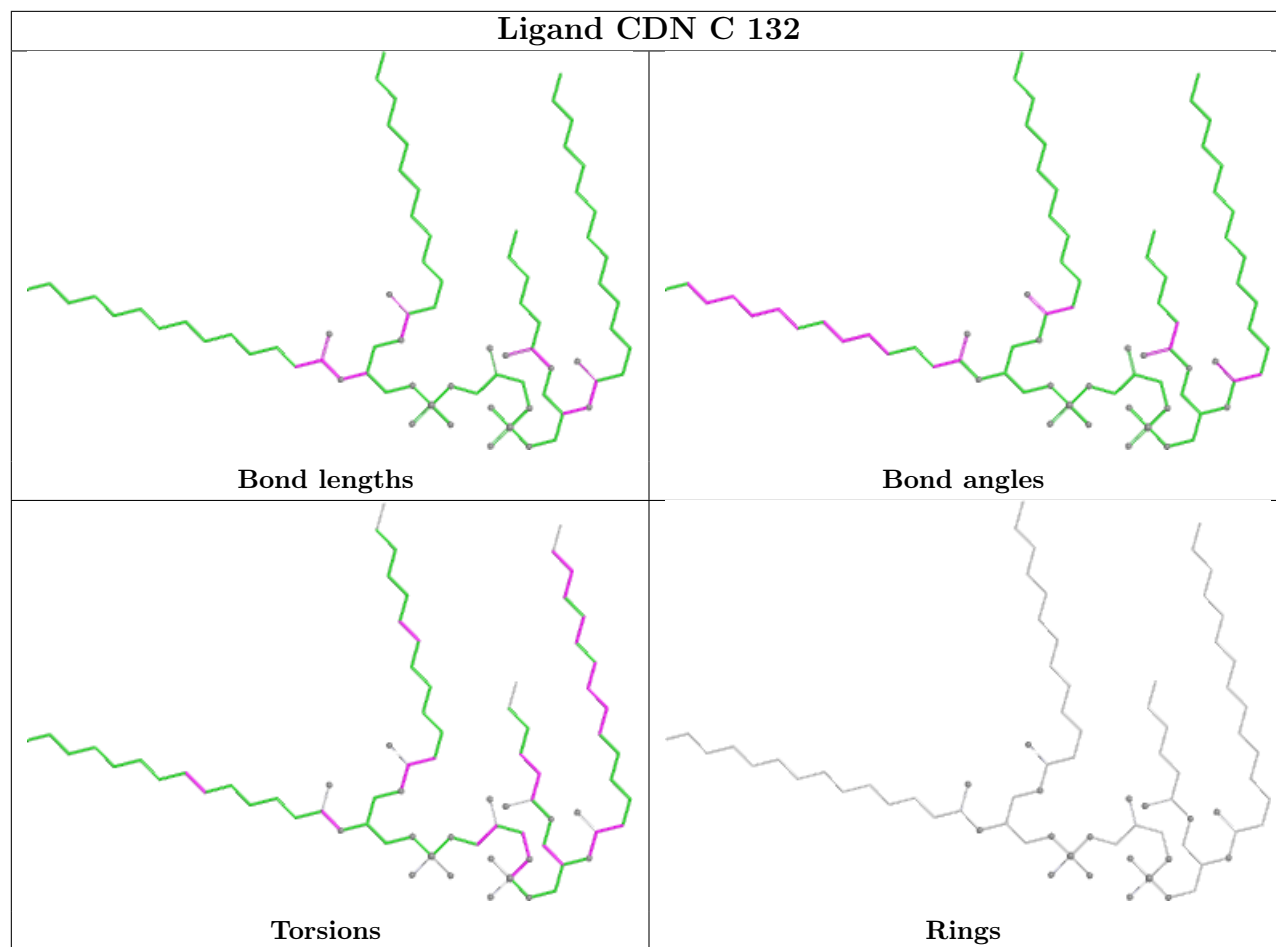
7 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	304	F3S	4	0
10	C	130	HEB	10	0
12	C	132	CDN	19	0
5	A	589	OAA	5	0
7	B	302	FES	1	0
6	A	601	FAD	9	0
11	C	131	AT5	4	0

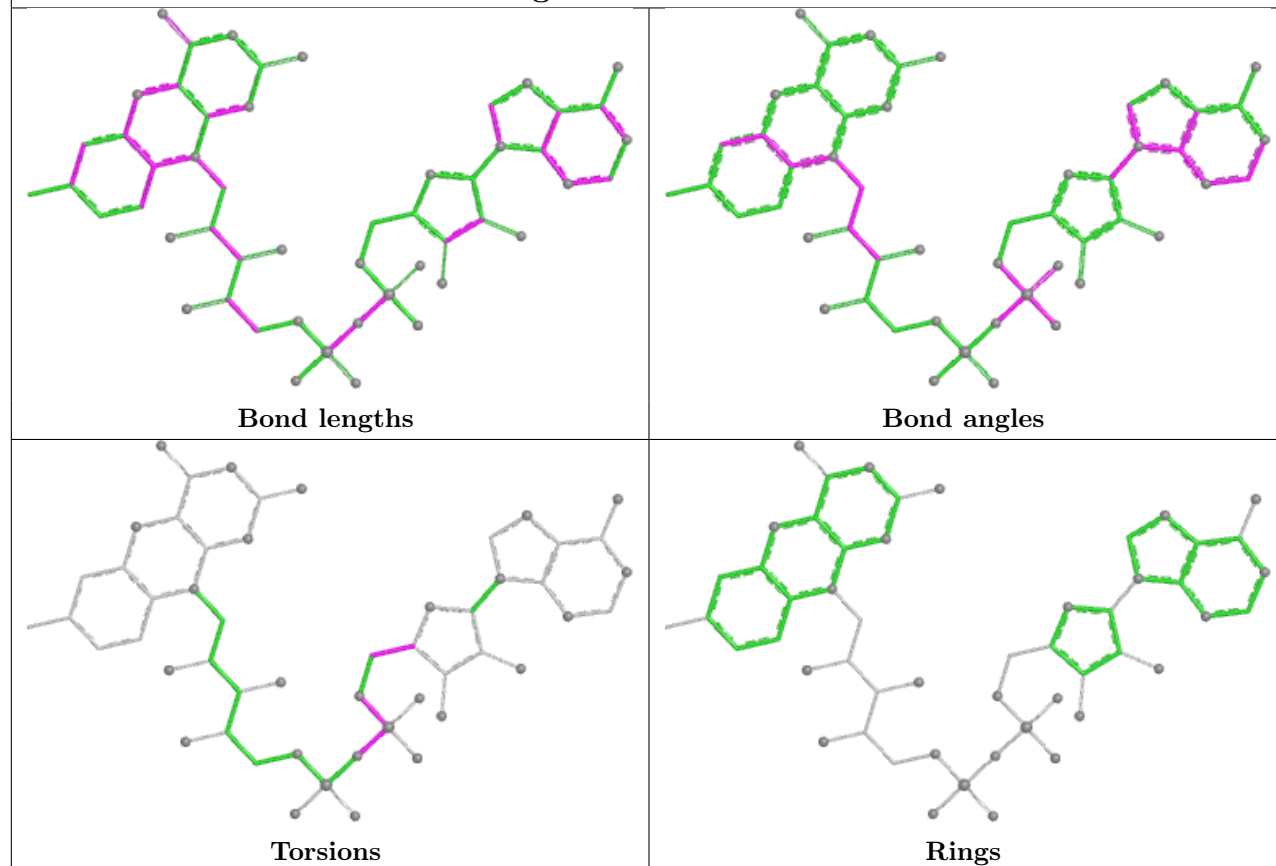
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

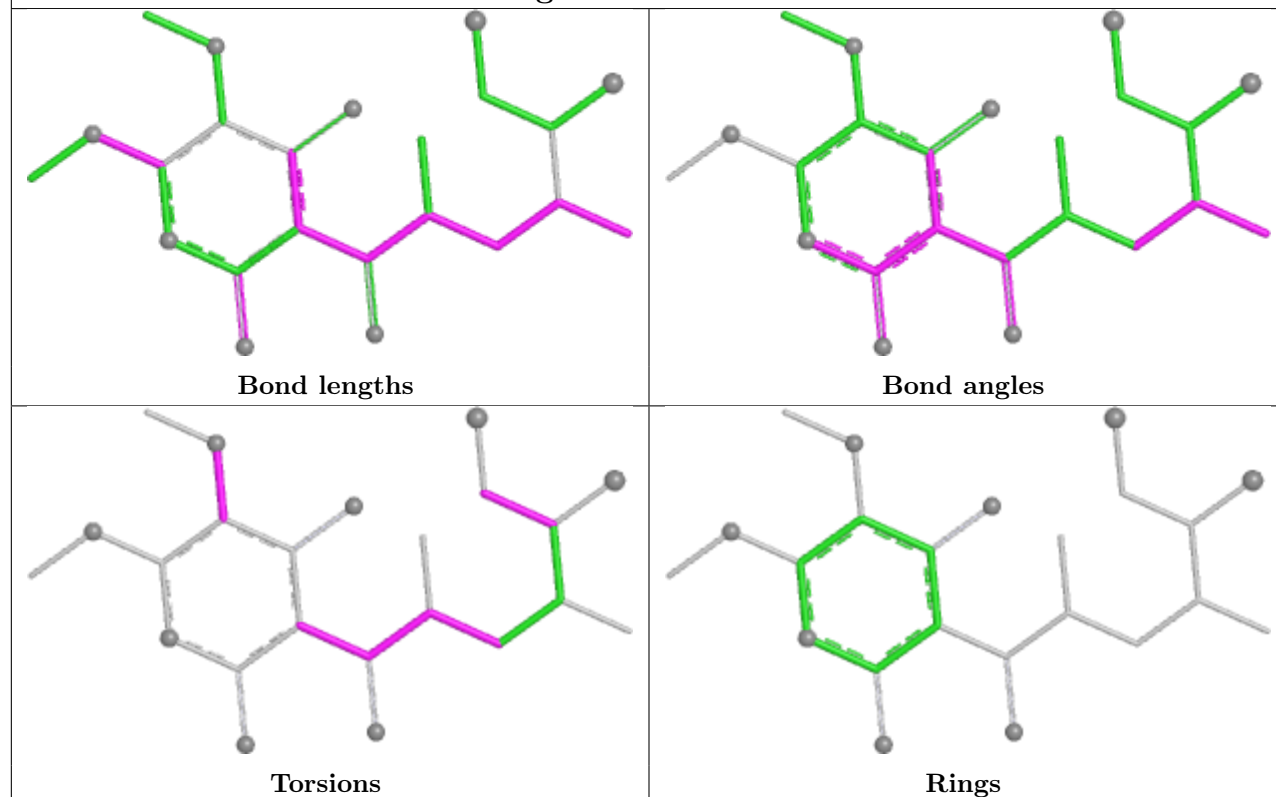




Ligand FAD A 601



Ligand AT5 C 131



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	577/588 (98%)	0.43	26 (4%)	38 20	41, 86, 112, 123	1 (0%)
2	B	238/238 (100%)	0.03	2 (0%)	82 65	37, 57, 99, 118	0
3	C	129/129 (100%)	0.02	4 (3%)	51 30	32, 60, 100, 132	0
4	D	113/115 (98%)	-0.13	2 (1%)	67 47	28, 44, 91, 100	0
All	All	1057/1070 (98%)	0.23	34 (3%)	50 30	28, 72, 109, 132	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	GLY	3.9
1	A	253	VAL	3.3
3	C	5	VAL	3.2
1	A	121	GLY	3.2
1	A	530	ALA	3.1
1	A	307	TRP	3.1
1	A	80	GLY	3.1
3	C	101	GLU	3.0
3	C	4	ASN	3.0
1	A	393	SER	3.0
4	D	113	TRP	2.9
3	C	2	ILE	2.9
1	A	78	TYR	2.9
1	A	355	TYR	2.8
1	A	131	ALA	2.7
1	A	585	ILE	2.7
1	A	567	THR	2.6
1	A	284	ALA	2.6
1	A	218	ASN	2.6
1	A	499	LEU	2.5
1	A	450	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	283	LEU	2.5
4	D	77	TRP	2.5
1	A	578	ARG	2.5
1	A	125	ASN	2.4
1	A	397	ALA	2.3
1	A	562	GLU	2.3
2	B	238	ALA	2.2
1	A	280	ALA	2.2
1	A	448	ASN	2.2
2	B	15	ASP	2.1
1	A	300	GLY	2.1
1	A	217	ILE	2.0
1	A	571	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.

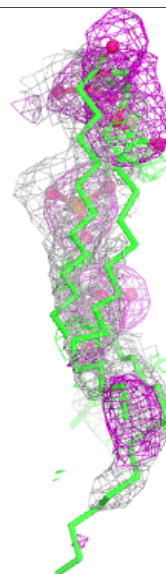
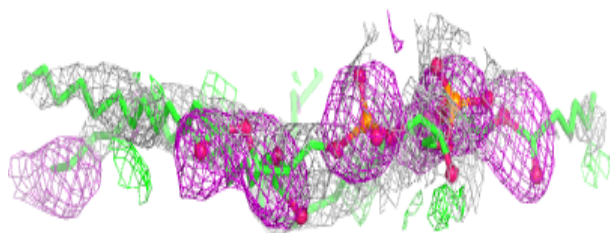
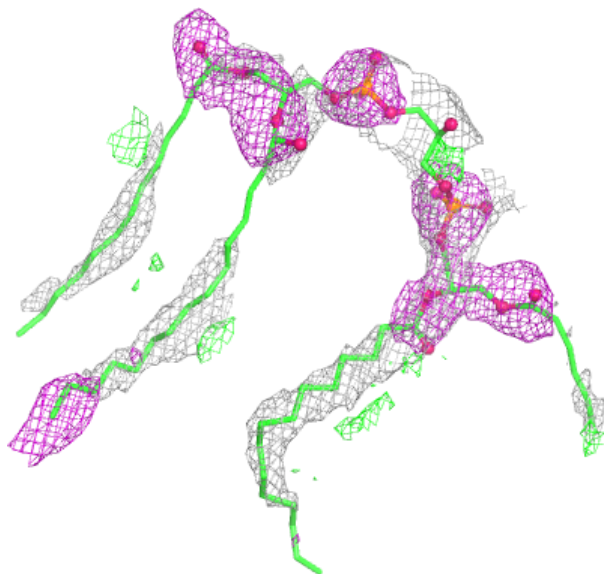
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	CDN	C	132	77/77	0.67	0.21	32,55,88,91	0
11	AT5	C	131	23/23	0.83	0.16	74,78,84,85	0
5	OAA	A	589	9/9	0.83	0.12	94,95,96,96	0
6	FAD	A	601	53/53	0.89	0.14	65,79,83,86	0
10	HEB	C	130	43/43	0.97	0.08	22,28,42,46	0
7	FES	B	302	4/4	0.99	0.04	53,57,58,60	0
8	SF4	B	303	8/8	0.99	0.04	42,46,49,49	0
9	F3S	B	304	7/7	0.99	0.03	33,39,41,42	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.

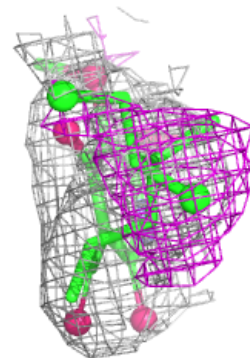
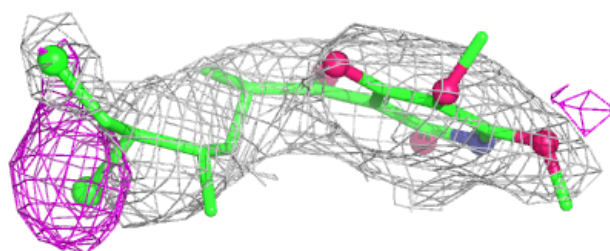
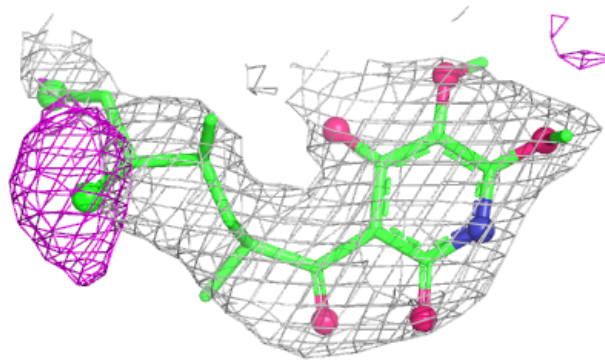
Electron density around CDN C 132:

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

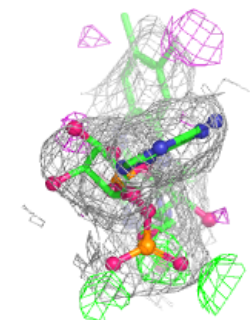
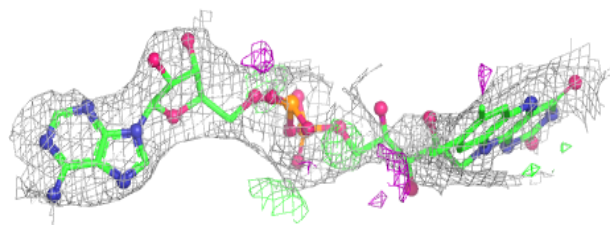
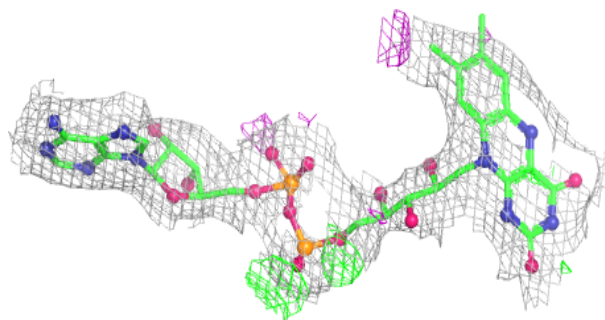


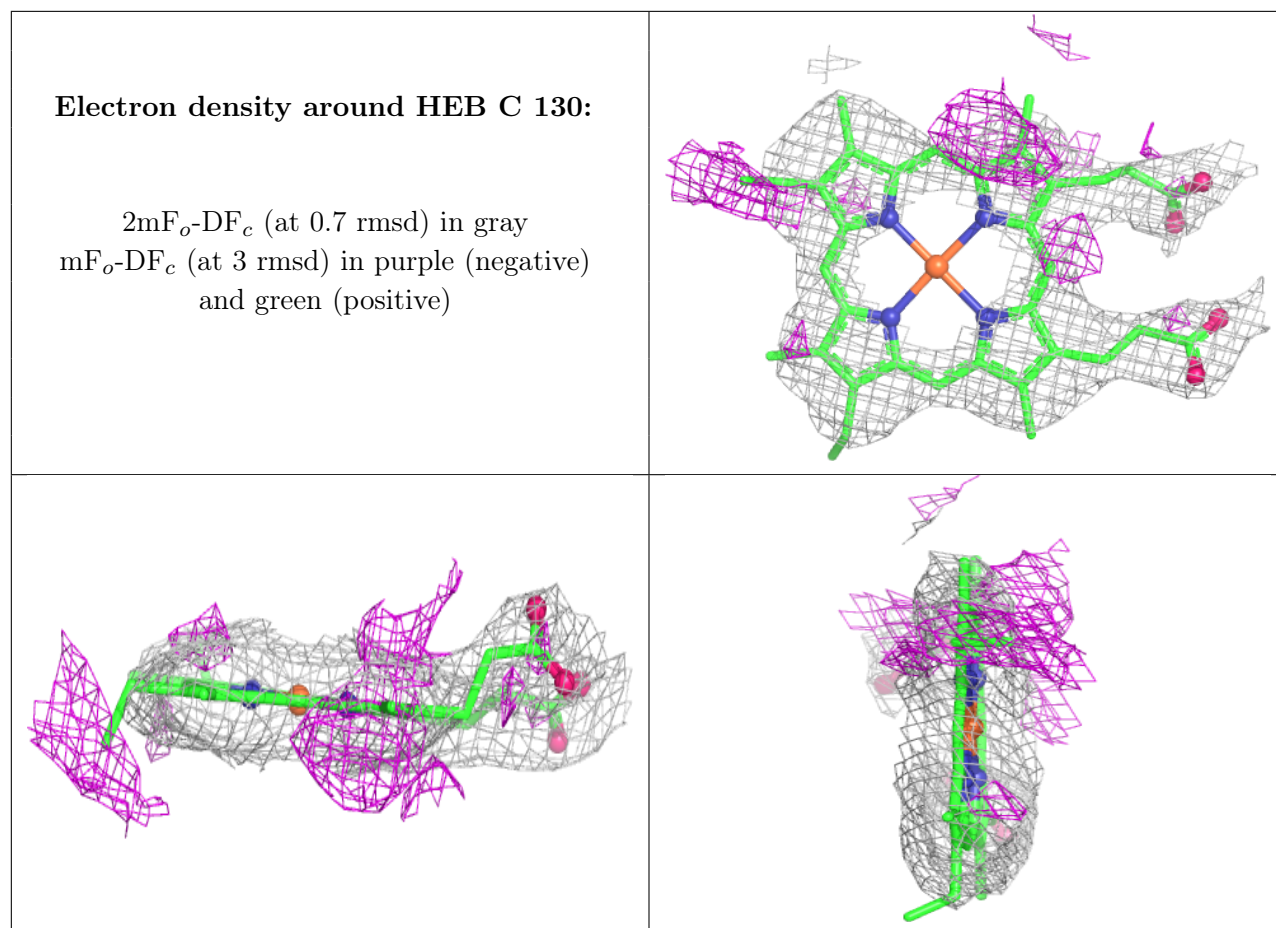
Electron density around AT5 C 131:

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

**Electron density around FAD A 601:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.