



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:07 AM UTC

PDB ID : 1YQ4 / pdb_00001yq4
Title : Avian respiratory complex ii with 3-nitropropionate and ubiquinone
Authors : Huang, L.; Sun, G.; Cobessi, D.; Wang, A.; Shen, J.T.; Tung, E.Y.; Anderson, V.E.; Berry, E.A.
Deposited on : 2005-02-01
Resolution : 2.33 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

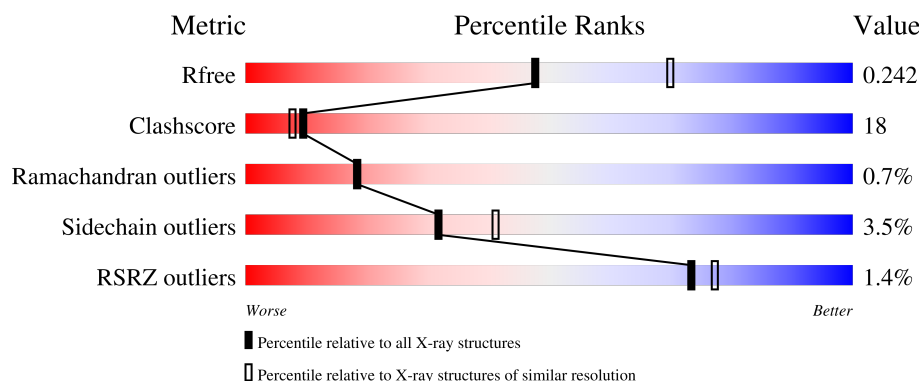
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	621	% 59% 36% ..
2	B	252	3% 56% 33% 7% .
3	C	141	% 60% 35% ..
4	D	103	% 62% 33% ..

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
6	3NP	A	1002	-	X	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 9291 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	614	Total	C	N	O	S	0	0	0
			4736	2962	845	900	29			

- Molecule 2 is a protein called succinate dehydrogenase Ip subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1934	1222	327	363	22			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	140	Total	C	N	O	S	0	0	1
			1074	706	179	185	4			

- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT.

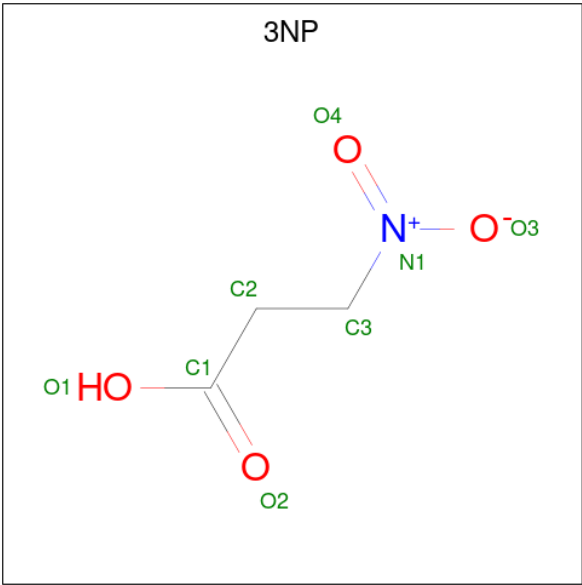
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			770	508	122	137	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is 3-NITROPROPANOIC ACID (CCD ID: 3NP) (formula: C₃H₅NO₄).



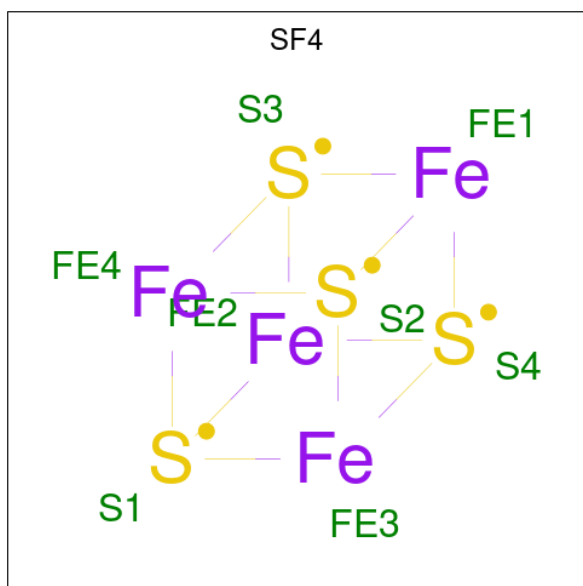
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O		0	0
			6	3	1	2			

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



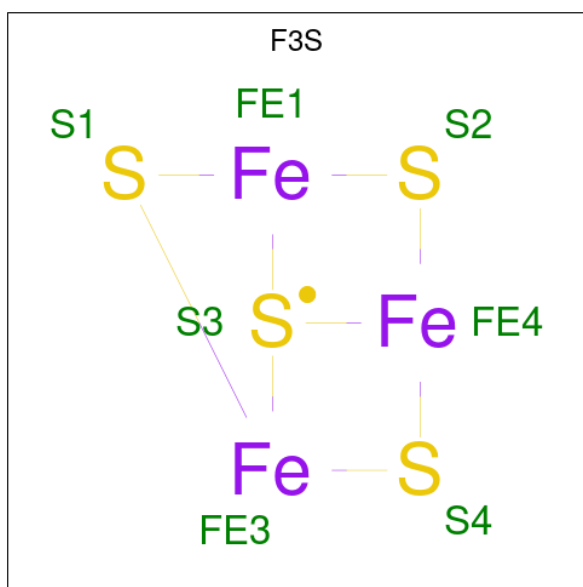
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

- 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).



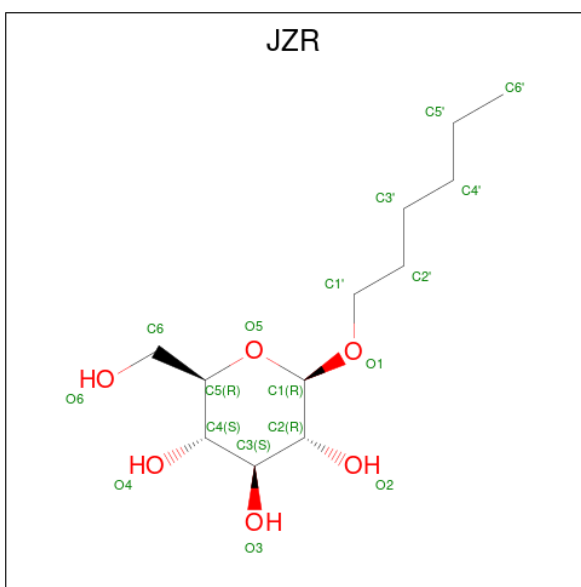
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



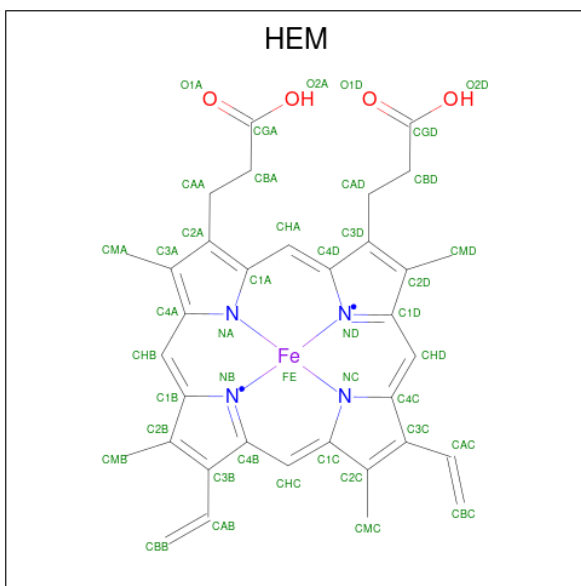
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: $C_{12}H_{24}O_6$).



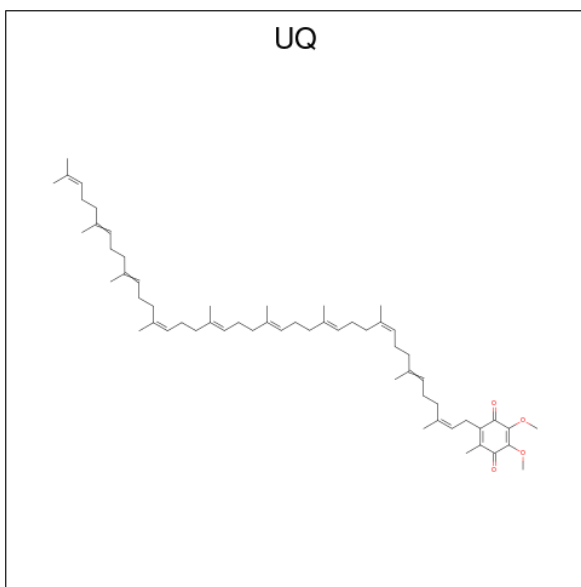
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	O		0	0
			18	12	6			

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



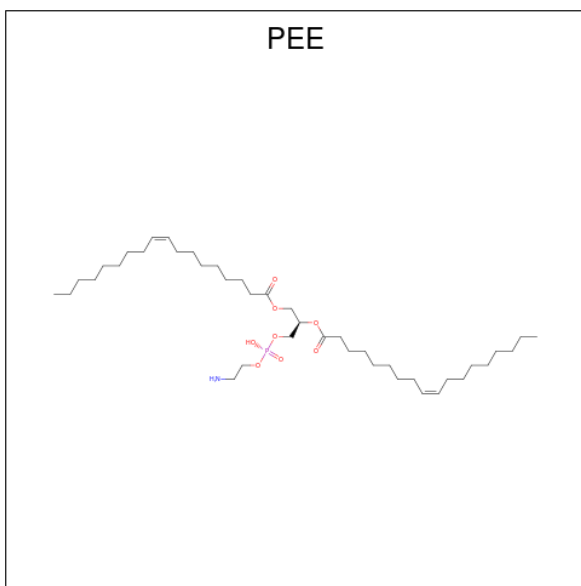
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		

- Molecule 13 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			14	10	4		

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			21	19	2		
14	D	1	Total	C		0	0
			24	24			

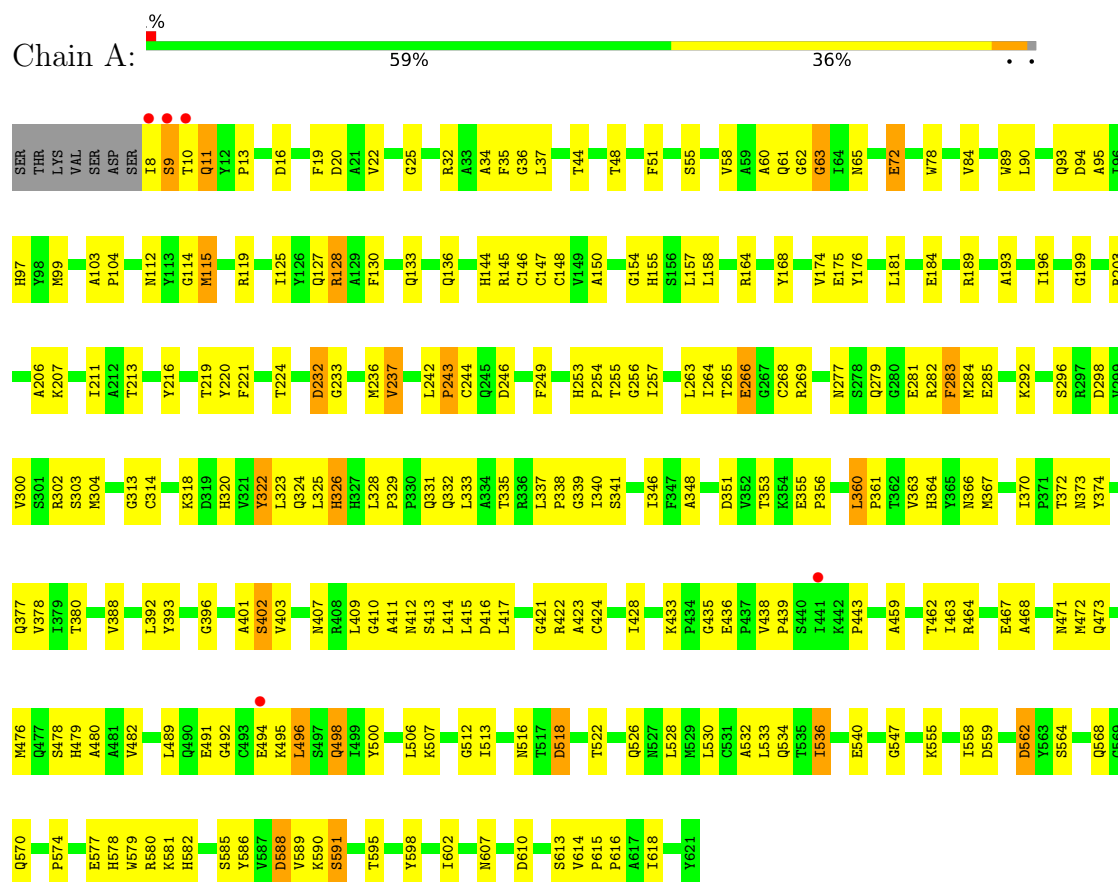
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	280	Total 280	O 280	0	0
15	B	159	Total 159	O 159	0	0
15	C	72	Total 72	O 72	0	0
15	D	64	Total 64	O 64	0	0

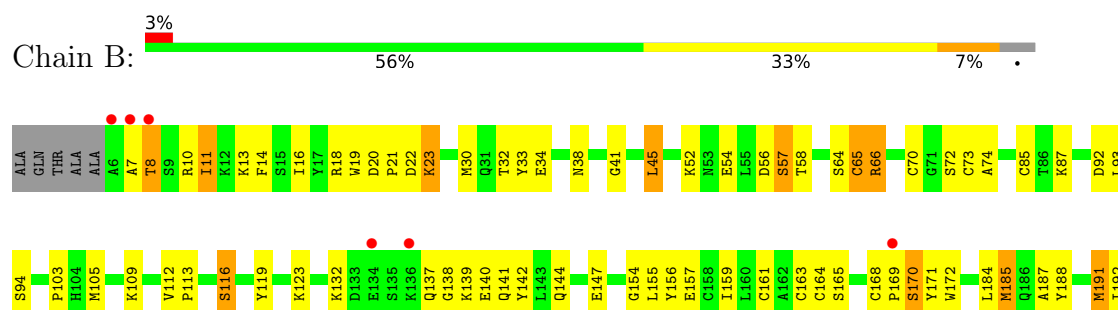
3 Residue-property plots

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

- Molecule 1: Succinate dehydrogenase flavoprotein subunit

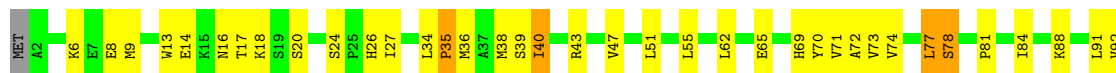


- Molecule 2: succinate dehydrogenase Ip subunit

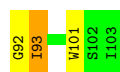
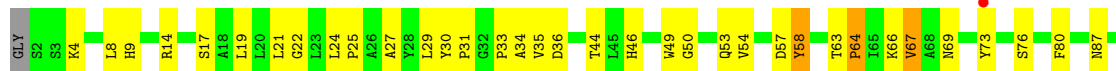




• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



• Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.59Å 83.49Å 288.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.38 – 2.33 56.38 – 2.33	Depositor EDS
% Data completeness (in resolution range)	79.4 (56.38-2.33) 94.4 (56.38-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.252 0.196 , 0.242	Depositor DCC
R_{free} test set	3830 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9291	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JZR, GOL, 3NP, FES, SF4, HEM, PEE, F3S, FAD, UQ

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	0.76	1/4837 (0.0%)	1.20	49/6550 (0.7%)
2	B	0.95	4/1976 (0.2%)	1.20	21/2666 (0.8%)
3	C	0.86	0/1103	1.13	9/1501 (0.6%)
4	D	0.87	0/793	1.14	4/1089 (0.4%)
All	All	0.83	5/8709 (0.1%)	1.19	83/11806 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	MET	SD-CE	12.76	2.11	1.79
2	B	30	MET	SD-CE	6.96	1.97	1.79
2	B	191	MET	SD-CE	-6.47	1.63	1.79
1	A	115	MET	SD-CE	5.84	1.94	1.79
2	B	105	MET	SD-CE	-5.66	1.65	1.79

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	THR	N-CA-C	-10.01	100.48	112.89
1	A	255	THR	N-CA-C	8.14	123.18	107.71
1	A	51	PHE	N-CA-C	-8.00	97.74	109.50
1	A	148	CYS	N-CA-C	7.88	120.84	108.79
4	D	93	ILE	N-CA-C	7.81	117.92	110.42
1	A	256	GLY	N-CA-C	-7.43	98.46	111.62
1	A	614	VAL	CA-C-N	7.38	124.97	119.66
1	A	614	VAL	C-N-CA	7.38	124.97	119.66
3	C	16	ASN	N-CA-C	7.31	120.18	111.33
1	A	61	GLN	N-CA-C	7.21	122.08	111.34
1	A	266	GLU	N-CA-C	-7.17	103.80	112.54
2	B	213	TYR	N-CA-C	7.02	121.55	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	GLU	N-CA-C	7.02	122.84	113.72
1	A	518	ASP	N-CA-C	-6.96	103.62	111.14
2	B	210	PHE	N-CA-C	6.96	122.18	112.93
1	A	579	TRP	N-CA-C	6.84	121.79	113.17
1	A	237	VAL	N-CA-C	-6.83	104.00	110.42
1	A	558	ILE	N-CA-C	6.81	116.52	106.85
1	A	555	LYS	N-CA-C	6.66	121.11	113.19
1	A	346	ILE	N-CA-C	6.57	117.25	110.36
1	A	613	SER	N-CA-C	-6.52	101.48	110.35
1	A	380	THR	N-CA-C	-6.51	100.04	110.14
2	B	234	ALA	N-CA-C	-6.39	104.39	111.36
2	B	23	LYS	N-CA-C	-6.37	96.93	109.10
2	B	225	CYS	CA-C-N	6.34	126.03	119.56
2	B	225	CYS	C-N-CA	6.34	126.03	119.56
2	B	214	ARG	N-CA-C	-6.34	105.53	113.20
1	A	94	ASP	N-CA-C	-6.24	104.40	111.14
2	B	73	CYS	N-CA-C	6.20	120.34	113.21
1	A	588	ASP	N-CA-C	-6.18	99.09	108.67
2	B	72	SER	N-CA-C	6.17	117.67	111.07
1	A	421	GLY	N-CA-C	-6.16	105.34	112.73
1	A	322	TYR	N-CA-C	6.14	118.96	109.07
1	A	36	GLY	N-CA-C	-6.12	105.39	112.73
1	A	526	GLN	N-CA-C	-6.04	104.61	111.07
1	A	244	CYS	N-CA-C	-6.01	100.82	110.14
3	C	62	LEU	N-CA-C	6.01	121.66	113.97
1	A	63	GLY	N-CA-C	5.99	118.04	110.38
1	A	44	THR	N-CA-C	5.95	119.17	109.59
1	A	373	ASN	N-CA-C	-5.92	101.23	110.17
2	B	171	TYR	N-CA-C	-5.90	105.57	112.89
1	A	150	ALA	CB-CA-C	-5.87	109.79	116.54
4	D	76	SER	N-CA-C	5.86	117.47	111.14
3	C	125	VAL	N-CA-C	-5.86	104.80	110.42
1	A	62	GLY	N-CA-C	5.82	119.93	112.83
1	A	355	GLU	CA-C-N	5.82	125.72	119.85
1	A	355	GLU	C-N-CA	5.82	125.72	119.85
1	A	224	THR	N-CA-C	-5.80	106.03	113.23
2	B	217	THR	N-CA-C	5.79	119.56	111.74
1	A	196	ILE	N-CA-C	5.76	116.50	110.62
2	B	65	CYS	N-CA-C	5.76	117.56	111.28
2	B	103	PRO	N-CA-C	5.68	120.00	111.14
1	A	283	PHE	N-CA-C	5.61	118.93	111.75
1	A	282	ARG	N-CA-C	-5.60	101.22	109.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ASP	N-CA-C	5.56	118.06	111.33
2	B	116	SER	N-CA-C	5.54	117.32	111.28
1	A	213	THR	N-CA-C	5.54	119.74	113.15
2	B	41	GLY	CA-C-N	5.53	125.14	119.56
2	B	41	GLY	C-N-CA	5.53	125.14	119.56
4	D	67	VAL	CB-CA-C	-5.48	104.96	111.81
3	C	20	SER	N-CA-C	-5.47	105.92	112.59
2	B	11	ILE	N-CA-C	5.47	116.23	107.98
3	C	24	SER	CA-C-N	-5.44	114.64	120.03
3	C	24	SER	C-N-CA	-5.44	114.64	120.03
1	A	498	GLN	N-CA-C	-5.43	105.01	111.03
3	C	71	VAL	N-CA-C	-5.40	105.23	110.42
1	A	522	THR	N-CA-C	-5.37	105.09	111.69
2	B	193	ASP	N-CA-C	-5.34	101.08	109.25
1	A	119	ARG	N-CA-C	5.34	118.26	109.72
1	A	176	TYR	N-CA-C	-5.32	100.22	108.90
3	C	115	LYS	N-CA-C	-5.31	102.53	110.23
4	D	58	TYR	N-CA-C	5.30	119.85	113.17
1	A	20	ASP	N-CA-C	-5.30	105.59	111.36
2	B	45	LEU	N-CA-C	-5.29	105.59	111.36
1	A	602	ILE	N-CA-C	5.26	115.17	108.12
1	A	11	GLN	N-CA-C	-5.21	106.18	112.54
1	A	346	ILE	CB-CA-C	-5.19	105.23	111.88
3	C	77	LEU	N-CA-C	-5.16	106.38	113.30
1	A	591	SER	N-CA-C	5.16	118.03	111.69
2	B	142	TYR	N-CA-C	-5.15	103.24	110.50
1	A	326	HIS	N-CA-C	5.06	118.55	112.38
1	A	193	ALA	N-CA-C	5.05	116.49	108.96
1	A	34	ALA	N-CA-C	5.00	116.42	111.07

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	4736	0	4614	164	0
2	B	1934	0	1920	78	0
3	C	1074	0	1115	51	0
4	D	770	0	763	32	0
5	A	53	0	29	6	0
6	A	6	0	0	0	0
7	B	4	0	0	0	0
8	B	8	0	0	0	0
9	B	7	0	0	0	0
10	B	6	0	8	0	0
11	C	18	0	24	0	0
12	C	41	0	24	0	0
13	C	14	0	9	10	0
14	C	21	0	35	1	0
14	D	24	0	40	0	0
15	A	280	0	0	3	0
15	B	159	0	0	4	0
15	C	72	0	0	6	0
15	D	64	0	0	4	0
All	All	9291	0	8581	310	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 18.

All (310) 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)
2:B:185:MET:SD	2:B:185:MET:CE	2.11	1.39
1:A:284:MET:HE1	1:A:303:SER:HB2	1.32	1.08
1:A:367:MET:HE3	1:A:407:ASN:HA	1.41	1.03
2:B:188:TYR:HA	2:B:191:MET:HE2	1.38	1.00
2:B:240:LYS:O	2:B:244:THR:HG23	1.71	0.88
1:A:277:ASN:HD21	1:A:281:GLU:HB3	1.39	0.85
1:A:401:ALA:N	1:A:402:SER:HA	1.91	0.85
2:B:220:ASN:HD21	3:C:36:MET:HE2	1.41	0.85
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.57	0.84
1:A:284:MET:HE1	1:A:303:SER:CB	2.10	0.82
1:A:32:ARG:NH2	1:A:422:ARG:HD2	1.95	0.82
2:B:214:ARG:HH22	4:D:53:GLN:HE22	1.26	0.80
1:A:112:ASN:HD22	2:B:138:GLY:H	1.28	0.79
2:B:214:ARG:HH12	4:D:53:GLN:NE2	1.80	0.79
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.31	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HH22	2:B:137:GLN:HE22	1.31	0.78
1:A:216:TYR:H	1:A:366:ASN:ND2	1.83	0.77
3:C:43:ARG:NH1	13:C:144:UQ:HM21	1.99	0.77
2:B:191:MET:HE1	2:B:238:ILE:HG12	1.66	0.76
13:C:144:UQ:HM23	4:D:58:TYR:OH	1.86	0.76
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.67	0.75
2:B:65:CYS:HB3	2:B:70:CYS:HB3	1.68	0.75
1:A:480:ALA:HB2	1:A:536:ILE:HD12	1.69	0.75
1:A:277:ASN:ND2	1:A:281:GLU:HB3	2.01	0.75
1:A:237:VAL:HG21	1:A:370:ILE:HG12	1.69	0.74
4:D:4:LYS:O	4:D:8:LEU:HG	1.88	0.73
1:A:103:ALA:HB3	1:A:104:PRO:HD3	1.71	0.73
3:C:101:ASN:ND2	3:C:104:ARG:HH11	1.88	0.72
3:C:140:ILE:HG22	3:C:141:SER:N	2.05	0.72
2:B:66:ARG:O	2:B:66:ARG:HG2	1.87	0.72
1:A:127:GLN:NE2	1:A:145:ARG:HA	2.04	0.72
2:B:216:HIS:HB2	15:C:1006:HOH:O	1.90	0.71
1:A:313:GLY:O	1:A:318:LYS:HD3	1.91	0.70
1:A:72:GLU:OE1	1:A:144:HIS:HD2	1.74	0.70
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.73	0.70
2:B:220:ASN:ND2	3:C:36:MET:HE2	2.07	0.69
1:A:257:ILE:HD11	1:A:348:ALA:HB2	1.75	0.69
1:A:58:VAL:HG23	1:A:155:HIS:HA	1.75	0.69
3:C:65:GLU:HB2	3:C:70:TYR:CZ	2.28	0.68
1:A:360:LEU:HD12	1:A:361:PRO:HD2	1.76	0.68
1:A:237:VAL:HG12	1:A:242:LEU:HB2	1.74	0.68
3:C:93:PHE:HB3	3:C:94:PRO:CD	2.24	0.68
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.76	0.67
3:C:65:GLU:HB2	3:C:70:TYR:CE1	2.29	0.67
3:C:96:SER:HG	3:C:133:SER:HG	1.40	0.67
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.10	0.66
3:C:26:HIS:CD2	3:C:27:ILE:H	2.14	0.66
3:C:101:ASN:HD21	3:C:104:ARG:NH1	1.94	0.66
1:A:417:LEU:HD21	5:A:1001:FAD:H5'2	1.78	0.65
2:B:214:ARG:HH12	4:D:53:GLN:HE21	1.44	0.65
3:C:69:HIS:O	3:C:73:VAL:HG23	1.96	0.65
1:A:283:PHE:CD1	1:A:284:MET:HE2	2.31	0.65
2:B:216:HIS:NE2	4:D:57:ASP:OD2	2.30	0.65
2:B:18:ARG:NH2	2:B:56:ASP:OD2	2.30	0.65
3:C:43:ARG:CZ	13:C:144:UQ:HM21	2.27	0.64
13:C:144:UQ:HM33	13:C:144:UQ:HM22	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:HB	1:A:158:LEU:HD23	1.80	0.64
1:A:331:GLN:NE2	1:A:335:THR:OG1	2.30	0.64
2:B:188:TYR:HD1	2:B:191:MET:CE	2.11	0.63
1:A:72:GLU:OE1	1:A:144:HIS:CD2	2.50	0.63
1:A:534:GLN:NE2	1:A:585:SER:OG	2.32	0.63
3:C:47:VAL:O	3:C:51:LEU:HG	1.98	0.62
3:C:105:HIS:ND1	15:C:1107:HOH:O	2.31	0.62
2:B:187:ALA:O	2:B:191:MET:HG3	2.00	0.62
1:A:65:ASN:CG	1:A:133:GLN:HE22	2.07	0.61
4:D:34:ALA:HB3	15:D:1470:HOH:O	2.01	0.61
1:A:479:HIS:O	1:A:489:LEU:HD23	2.01	0.60
2:B:147:GLU:CD	2:B:147:GLU:H	2.09	0.60
1:A:464:ARG:HB3	1:A:507:LYS:HE3	1.82	0.60
1:A:112:ASN:ND2	2:B:138:GLY:H	1.97	0.60
1:A:155:HIS:HD2	15:B:1007:HOH:O	1.84	0.60
1:A:396:GLY:HA2	1:A:417:LEU:HD23	1.83	0.60
3:C:43:ARG:NH1	13:C:144:UQ:CM2	2.64	0.60
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.37	0.60
2:B:154:GLY:H	2:B:157:GLU:CD	2.10	0.60
4:D:4:LYS:HE2	15:D:1217:HOH:O	2.02	0.59
3:C:77:LEU:O	3:C:78:SER:C	2.45	0.59
1:A:164:ARG:HH22	2:B:137:GLN:NE2	1.98	0.59
1:A:564:SER:HB3	1:A:618:ILE:HD11	1.85	0.59
4:D:53:GLN:HE21	4:D:53:GLN:HA	1.67	0.59
1:A:266:GLU:HG3	1:A:269:ARG:CZ	2.33	0.58
2:B:188:TYR:CA	2:B:191:MET:HE2	2.24	0.58
2:B:16:ILE:HD12	2:B:33:TYR:CD1	2.38	0.58
2:B:214:ARG:NH2	4:D:53:GLN:HE22	1.97	0.58
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.85	0.58
1:A:578:HIS:O	1:A:581:LYS:HE2	2.04	0.58
1:A:410:GLY:O	1:A:411:ALA:HB3	2.02	0.58
1:A:562:ASP:OD1	1:A:562:ASP:C	2.47	0.58
4:D:63:THR:HB	4:D:64:PRO:HD3	1.86	0.58
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.38	0.57
4:D:33:PRO:HG2	15:D:1079:HOH:O	2.03	0.57
1:A:435:GLY:O	1:A:436:GLU:C	2.47	0.57
4:D:53:GLN:NE2	4:D:53:GLN:HA	2.20	0.57
1:A:401:ALA:N	1:A:402:SER:CA	2.67	0.57
2:B:227:LYS:HB2	2:B:229:LEU:HD22	1.87	0.57
3:C:39:SER:OG	13:C:144:UQ:HM31	2.05	0.57
1:A:55:SER:O	1:A:58:VAL:HG12	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HB2	1:A:333:LEU:HD21	1.86	0.56
1:A:283:PHE:CE1	1:A:284:MET:HE2	2.40	0.56
2:B:10:ARG:HD3	2:B:38:ASN:HD21	1.71	0.56
2:B:21:PRO:HD2	2:B:109:LYS:HD2	1.86	0.56
1:A:396:GLY:HA2	1:A:417:LEU:CD2	2.36	0.56
1:A:324:GLN:HG3	1:A:326:HIS:CE1	2.41	0.56
3:C:6:LYS:HA	3:C:9:MET:HE3	1.88	0.56
1:A:89:TRP:CD2	1:A:616:PRO:HA	2.40	0.56
3:C:13:TRP:O	3:C:17:THR:HG23	2.05	0.55
2:B:19:TRP:CZ3	2:B:21:PRO:HB3	2.42	0.55
1:A:534:GLN:HG2	1:A:585:SER:HB2	1.87	0.55
2:B:52:LYS:HG2	2:B:57:SER:HA	1.88	0.55
1:A:438:VAL:HG23	1:A:439:PRO:HD2	1.88	0.55
4:D:63:THR:O	4:D:67:VAL:HG23	2.07	0.55
1:A:16:ASP:OD1	1:A:203:ARG:HB2	2.06	0.55
3:C:74:VAL:HA	3:C:77:LEU:HD12	1.89	0.55
1:A:559:ASP:OD2	1:A:580:ARG:HD3	2.08	0.54
1:A:409:LEU:O	1:A:412:ASN:HB2	2.08	0.54
1:A:60:ALA:HA	5:A:1001:FAD:N5	2.22	0.54
2:B:16:ILE:HD12	2:B:33:TYR:HD1	1.72	0.54
3:C:34:LEU:HD23	15:C:1160:HOH:O	2.07	0.54
3:C:40:ILE:HA	13:C:144:UQ:HM32	1.89	0.54
1:A:58:VAL:O	1:A:58:VAL:HG22	2.09	0.53
4:D:27:ALA:HA	4:D:35:VAL:HG11	1.89	0.53
1:A:339:GLY:HA3	15:A:1238:HOH:O	2.08	0.53
1:A:8:ILE:O	1:A:9:SER:HB3	2.09	0.53
1:A:60:ALA:HB3	1:A:154:GLY:CA	2.38	0.53
1:A:155:HIS:HE1	2:B:156:TYR:O	1.91	0.53
2:B:92:ASP:OD1	2:B:94:SER:OG	2.23	0.53
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.39	0.53
1:A:216:TYR:CD1	1:A:216:TYR:O	2.62	0.52
1:A:351:ASP:C	1:A:351:ASP:OD1	2.52	0.52
1:A:13:PRO:HA	15:A:1060:HOH:O	2.08	0.52
1:A:65:ASN:ND2	1:A:411:ALA:HB3	2.25	0.52
1:A:174:VAL:HG12	1:A:175:GLU:HG3	1.90	0.52
1:A:296:SER:OG	1:A:298:ASP:OD1	2.23	0.52
2:B:147:GLU:CD	2:B:147:GLU:N	2.67	0.52
4:D:22:GLY:O	4:D:25:PRO:HG2	2.10	0.52
1:A:237:VAL:HG21	1:A:370:ILE:CG1	2.39	0.52
4:D:36:ASP:OD1	4:D:93:ILE:HB	2.09	0.52
1:A:10:THR:HG23	1:A:10:THR:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:HA	1:A:473:GLN:HB3	1.93	0.51
13:C:144:UQ:HM33	13:C:144:UQ:CM2	2.40	0.51
3:C:72:ALA:O	3:C:73:VAL:C	2.51	0.51
4:D:87:ASN:HA	4:D:92:GLY:HA2	1.92	0.51
1:A:378:VAL:HG21	1:A:392:LEU:HG	1.92	0.51
1:A:581:LYS:HD2	1:A:598:TYR:CB	2.40	0.51
1:A:99:MET:HE2	1:A:403:VAL:HB	1.92	0.51
3:C:26:HIS:CG	3:C:27:ILE:H	2.28	0.51
1:A:476:MET:SD	1:A:532:ALA:HB1	2.51	0.51
1:A:233:GLY:O	1:A:237:VAL:HG23	2.11	0.51
1:A:246:ASP:HB3	1:A:249:PHE:HD1	1.75	0.51
1:A:25:GLY:HA2	5:A:1001:FAD:C1B	2.41	0.50
1:A:164:ARG:NH2	2:B:137:GLN:HE22	2.05	0.50
1:A:263:LEU:HD22	1:A:364:HIS:HE1	1.76	0.50
2:B:52:LYS:CG	2:B:57:SER:HA	2.40	0.50
1:A:413:SER:O	1:A:416:ASP:HB3	2.11	0.50
3:C:140:ILE:CG2	3:C:141:SER:N	2.73	0.50
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.94	0.50
2:B:119:TYR:O	2:B:123:LYS:HG3	2.11	0.50
1:A:189:ARG:HD2	1:A:439:PRO:HB2	1.94	0.50
2:B:168:CYS:SG	2:B:170:SER:HB2	2.51	0.50
1:A:464:ARG:O	1:A:467:GLU:N	2.45	0.50
2:B:198:TYR:O	2:B:202:ARG:HG3	2.11	0.50
3:C:14:GLU:O	3:C:18:LYS:HG2	2.10	0.50
2:B:56:ASP:C	2:B:58:THR:H	2.19	0.50
1:A:574:PRO:HD2	1:A:577:GLU:HB2	1.93	0.50
1:A:58:VAL:CG2	1:A:155:HIS:HA	2.42	0.49
1:A:103:ALA:HA	1:A:415:LEU:HD11	1.94	0.49
3:C:88:LYS:HB3	4:D:101:TRP:CZ2	2.47	0.49
2:B:45:LEU:HD22	2:B:85:CYS:HB3	1.94	0.49
1:A:97:HIS:C	1:A:97:HIS:CD2	2.90	0.49
3:C:93:PHE:HB3	3:C:94:PRO:HD2	1.93	0.49
3:C:6:LYS:HA	3:C:9:MET:CE	2.42	0.49
1:A:500:TYR:CD1	1:A:533:LEU:HD11	2.48	0.49
1:A:35:PHE:HB2	1:A:168:TYR:CD1	2.47	0.48
1:A:90:LEU:O	1:A:582:HIS:CE1	2.67	0.48
1:A:90:LEU:O	1:A:582:HIS:HE1	1.96	0.48
2:B:8:THR:HG22	2:B:8:THR:O	2.12	0.48
4:D:29:LEU:C	4:D:30:TYR:CD1	2.92	0.48
3:C:39:SER:HA	15:C:1200:HOH:O	2.13	0.48
3:C:95:LEU:HD21	14:C:145:PEE:H39	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:C	1:A:340:ILE:HD12	2.39	0.48
1:A:492:GLY:O	1:A:496:LEU:HB2	2.14	0.48
2:B:164:CYS:SG	2:B:165:SER:N	2.87	0.48
4:D:24:LEU:N	4:D:25:PRO:HD2	2.29	0.48
1:A:237:VAL:CG1	1:A:242:LEU:HB2	2.40	0.47
1:A:199:GLY:HA2	1:A:513:ILE:HG13	1.95	0.47
1:A:588:ASP:OD1	1:A:591:SER:OG	2.30	0.47
1:A:302:ARG:HA	1:A:482:VAL:HG11	1.97	0.47
2:B:14:PHE:O	2:B:32:THR:HA	2.14	0.47
3:C:97:TYR:HA	3:C:130:THR:OG1	2.15	0.47
1:A:472:MET:HE1	1:A:528:LEU:HD13	1.97	0.47
2:B:7:ALA:O	2:B:8:THR:HB	2.14	0.47
2:B:155:LEU:CD1	2:B:192:ILE:HD11	2.45	0.47
2:B:123:LYS:HB3	15:C:1143:HOH:O	2.15	0.47
2:B:169:PRO:HA	2:B:172:TRP:CD2	2.50	0.47
3:C:38:MET:HE1	3:C:123:GLY:O	2.14	0.47
1:A:37:LEU:HD21	1:A:428:ILE:HD12	1.97	0.47
1:A:125:ILE:HG21	1:A:147:CYS:HB3	1.96	0.46
2:B:10:ARG:HD3	2:B:38:ASN:ND2	2.31	0.46
2:B:221:CYS:O	2:B:224:THR:HG22	2.14	0.46
1:A:246:ASP:HB3	1:A:249:PHE:CD1	2.50	0.46
2:B:217:THR:HG22	2:B:217:THR:O	2.15	0.46
2:B:7:ALA:O	2:B:8:THR:CB	2.62	0.46
3:C:115:LYS:HB2	3:C:118:GLN:HG3	1.98	0.46
1:A:489:LEU:CD1	1:A:540:GLU:HA	2.45	0.46
1:A:494:GLU:O	1:A:495:LYS:C	2.59	0.46
1:A:65:ASN:OD1	1:A:133:GLN:NE2	2.41	0.46
1:A:157:LEU:HD23	1:A:157:LEU:C	2.40	0.46
2:B:23:LYS:HD2	15:B:1096:HOH:O	2.14	0.46
1:A:221:PHE:CA	1:A:473:GLN:HB3	2.46	0.46
4:D:21:LEU:O	4:D:25:PRO:HD2	2.16	0.46
2:B:139:LYS:O	2:B:140:GLU:HG2	2.16	0.46
1:A:253:HIS:O	1:A:361:PRO:HA	2.15	0.45
2:B:87:LYS:HE2	15:B:1063:HOH:O	2.15	0.45
2:B:123:LYS:HE3	3:C:8:GLU:OE1	2.16	0.45
1:A:463:ILE:O	1:A:506:LEU:HD23	2.17	0.45
2:B:225:CYS:SG	2:B:229:LEU:HB2	2.57	0.45
1:A:530:LEU:HD23	1:A:530:LEU:HA	1.75	0.45
2:B:11:ILE:CG2	2:B:34:GLU:HB3	2.47	0.45
4:D:50:GLY:O	4:D:54:VAL:HG23	2.17	0.45
1:A:254:PRO:O	1:A:304:MET:HE1	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:CYS:O	2:B:66:ARG:HB3	2.17	0.45
2:B:210:PHE:O	2:B:211:SER:C	2.58	0.45
1:A:263:LEU:HD22	1:A:364:HIS:CE1	2.52	0.45
2:B:74:ALA:HB1	2:B:163:CYS:SG	2.57	0.45
1:A:360:LEU:HD12	1:A:361:PRO:CD	2.47	0.45
4:D:69:ASN:HD22	4:D:69:ASN:HA	1.63	0.45
1:A:283:PHE:HD1	1:A:284:MET:HE2	1.76	0.45
1:A:322:TYR:HB3	1:A:356:PRO:HB2	1.99	0.45
1:A:377:GLN:HG2	1:A:393:TYR:CE1	2.51	0.45
1:A:468:ALA:O	1:A:471:ASN:HB2	2.16	0.45
1:A:516:ASN:OD1	1:A:518:ASP:HB3	2.17	0.45
1:A:263:LEU:HD23	5:A:1001:FAD:H6	2.00	0.44
1:A:329:PRO:HD2	1:A:332:GLN:OE1	2.17	0.44
1:A:340:ILE:HD12	1:A:341:SER:N	2.33	0.44
2:B:219:MET:HE3	2:B:222:THR:HB	2.00	0.44
1:A:207:LYS:HZ3	1:A:436:GLU:CD	2.25	0.44
4:D:9:HIS:HE1	4:D:49:TRP:CD1	2.35	0.44
4:D:24:LEU:HD23	4:D:24:LEU:HA	1.78	0.44
1:A:401:ALA:HB3	1:A:403:VAL:HG13	2.00	0.44
1:A:459:ALA:HB1	1:A:506:LEU:O	2.16	0.44
4:D:73:TYR:HB2	15:D:1528:HOH:O	2.17	0.44
1:A:84:VAL:HG22	1:A:93:GLN:HG2	1.99	0.44
1:A:401:ALA:H	1:A:402:SER:HA	1.78	0.44
1:A:422:ARG:O	1:A:423:ALA:C	2.57	0.44
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.89	0.44
2:B:159:ILE:HG13	2:B:161:CYS:HB3	1.99	0.43
2:B:225:CYS:HA	2:B:226:PRO:HD2	1.74	0.43
1:A:63:GLY:HA3	1:A:146:CYS:SG	2.58	0.43
1:A:581:LYS:HD2	1:A:598:TYR:HB3	1.99	0.43
3:C:123:GLY:O	3:C:126:VAL:HB	2.19	0.43
2:B:214:ARG:HD3	4:D:57:ASP:OD1	2.17	0.43
4:D:63:THR:CB	4:D:64:PRO:HD3	2.48	0.43
1:A:89:TRP:CE2	1:A:616:PRO:HA	2.54	0.43
1:A:512:GLY:HA2	15:B:1123:HOH:O	2.17	0.43
3:C:55:LEU:HD23	3:C:55:LEU:HA	1.77	0.43
1:A:114:GLY:O	1:A:115:MET:C	2.62	0.43
1:A:184:GLU:HB3	1:A:189:ARG:HE	1.83	0.43
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.91	0.43
1:A:424:CYS:O	1:A:428:ILE:HG13	2.19	0.43
1:A:22:VAL:HG23	1:A:206:ALA:HB2	2.01	0.42
1:A:372:THR:HA	1:A:377:GLN:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ASP:OD1	1:A:564:SER:OG	2.35	0.42
4:D:30:TYR:N	4:D:31:PRO:CD	2.83	0.42
1:A:257:ILE:HD11	1:A:348:ALA:CB	2.48	0.42
2:B:13:LYS:HA	2:B:33:TYR:O	2.20	0.42
3:C:27:ILE:HD12	3:C:27:ILE:HA	1.91	0.42
3:C:92:VAL:HG21	3:C:137:ILE:HG21	2.02	0.42
1:A:277:ASN:C	1:A:279:GLN:H	2.28	0.42
2:B:144:GLN:HG3	2:B:194:SER:OG	2.20	0.42
3:C:34:LEU:N	3:C:35:PRO:CD	2.83	0.42
1:A:128:ARG:HG2	1:A:146:CYS:HB3	2.01	0.42
1:A:264:ILE:HG21	1:A:323:LEU:HD23	2.02	0.42
1:A:351:ASP:OD1	1:A:353:THR:OG1	2.31	0.42
1:A:489:LEU:HD13	1:A:540:GLU:HA	2.02	0.42
1:A:337:LEU:N	1:A:338:PRO:CD	2.83	0.42
1:A:564:SER:CB	1:A:618:ILE:HD11	2.49	0.42
3:C:81:PRO:O	3:C:84:ILE:HB	2.20	0.42
4:D:17:SER:OG	4:D:46:HIS:CE1	2.73	0.42
1:A:491:GLU:HG2	1:A:495:LYS:HE3	2.01	0.41
3:C:122:SER:O	3:C:126:VAL:HG23	2.20	0.41
3:C:118:GLN:HG2	15:C:1337:HOH:O	2.20	0.41
2:B:220:ASN:HD21	3:C:36:MET:CE	2.22	0.41
3:C:38:MET:HE1	3:C:123:GLY:HA2	2.02	0.41
1:A:615:PRO:C	1:A:616:PRO:O	2.64	0.41
2:B:169:PRO:HA	2:B:172:TRP:CE3	2.55	0.41
1:A:90:LEU:O	1:A:90:LEU:HG	2.21	0.41
1:A:99:MET:CE	1:A:403:VAL:HB	2.51	0.41
1:A:314:CYS:N	1:A:320:HIS:O	2.44	0.41
3:C:125:VAL:O	3:C:126:VAL:C	2.64	0.41
2:B:20:ASP:OD1	2:B:22:ASP:HB2	2.21	0.41
1:A:95:ALA:HA	1:A:374:TYR:HB2	2.03	0.41
3:C:65:GLU:O	3:C:70:TYR:HE1	2.04	0.41
1:A:78:TRP:HB3	15:A:1028:HOH:O	2.21	0.41
1:A:232:ASP:O	1:A:236:MET:HG3	2.21	0.41
2:B:56:ASP:C	2:B:58:THR:N	2.79	0.41
1:A:607:ASN:ND2	1:A:610:ASP:HB2	2.36	0.41
2:B:191:MET:CE	2:B:238:ILE:HG12	2.43	0.41
2:B:238:ILE:O	2:B:242:MET:HG2	2.21	0.41
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.86	0.40
2:B:132:LYS:HG2	2:B:197:ASP:HB3	2.02	0.40
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.93	0.40
1:A:285:GLU:HG2	1:A:292:LYS:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:O	1:A:300:VAL:HG23	2.21	0.40
1:A:298:ASP:OD2	1:A:547:GLY:HA2	2.21	0.40
1:A:19:PHE:O	1:A:206:ALA:HA	2.22	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD2	1.87	0.40
1:A:586:TYR:HB2	1:A:595:THR:HB	2.03	0.40
3:C:39:SER:C	13:C:144:UQ:HM32	2.47	0.40
2:B:112:VAL:HA	2:B:113:PRO:HD2	1.89	0.40
2:B:218:ILE:HG12	13:C:144:UQ:O3	2.21	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	612/621 (99%)	569 (93%)	39 (6%)	4 (1%)	18	18
2	B	240/252 (95%)	227 (95%)	10 (4%)	3 (1%)	9	7
3	C	138/141 (98%)	130 (94%)	7 (5%)	1 (1%)	18	18
4	D	100/103 (97%)	94 (94%)	6 (6%)	0	100	100
All	All	1090/1117 (98%)	1020 (94%)	62 (6%)	8 (1%)	18	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	THR
2	B	8	THR
3	C	78	SER
1	A	568	GLN
2	B	57	SER
2	B	64	SER
1	A	9	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	443	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	498/506 (98%)	479 (96%)	19 (4%)	29	38
2	B	215/219 (98%)	209 (97%)	6 (3%)	38	50
3	C	117/119 (98%)	114 (97%)	3 (3%)	40	53
4	D	78/79 (99%)	74 (95%)	4 (5%)	21	26
All	All	908/923 (98%)	876 (96%)	32 (4%)	32	41

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	THR
1	A	72	GLU
1	A	128	ARG
1	A	130	PHE
1	A	136	GLN
1	A	243	PRO
1	A	360	LEU
1	A	388	VAL
1	A	402	SER
1	A	462	THR
1	A	478	SER
1	A	496	LEU
1	A	498	GLN
1	A	536	ILE
1	A	562	ASP
1	A	570	GLN
1	A	589	VAL
1	A	590	LYS
2	B	66	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	116	SER
2	B	141	GLN
2	B	170	SER
2	B	224	THR
2	B	229	LEU
3	C	35	PRO
3	C	40	ILE
3	C	91	LEU
4	D	14	ARG
4	D	19	LEU
4	D	64	PRO
4	D	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	43	ASN
1	A	112	ASN
1	A	144	HIS
1	A	155	HIS
1	A	185	ASN
1	A	326	HIS
1	A	331	GLN
1	A	366	ASN
1	A	381	HIS
1	A	383	ASN
1	A	452	ASN
1	A	526	GLN
1	A	534	GLN
1	A	607	ASN
2	B	104	HIS
2	B	121	GLN
2	B	137	GLN
2	B	144	GLN
2	B	220	ASN
3	C	26	HIS
3	C	42	HIS
3	C	66	GLN
3	C	69	HIS
3	C	101	ASN
4	D	9	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	53	GLN
4	D	69	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 ⓘ

11 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
8	SF4	B	1003	2	0,12,12	-	-	-		
6	3NP	A	1002	1	5,5,7	3.73	3 (60%)	5,5,8	4.21	2 (40%)
9	F3S	B	1004	2	0,9,9	-	-	-		
14	PEE	C	145	-	19,19,50	1.39	3 (15%)	19,19,55	0.85	2 (10%)
7	FES	B	1002	2	0,4,4	-	-	-		
10	GOL	B	1005	-	5,5,5	1.36	0	5,5,5	0.61	0
5	FAD	A	1001	1	58,58,58	2.74	26 (44%)	85,89,89	1.76	21 (24%)
14	PEE	D	104	-	22,22,50	1.55	4 (18%)	20,20,55	1.17	2 (10%)
12	HEM	C	143	3,4	48,48,50	1.68	8 (16%)	66,80,82	1.88	17 (25%)
11	JZR	C	142	-	18,18,18	2.03	3 (16%)	23,23,23	1.01	2 (8%)
13	UQ	C	144	-	14,14,63	2.00	8 (57%)	20,20,79	0.45	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
6	3NP	A	1002	1	-	3/3/3/5	-
8	SF4	B	1003	2	-	-	0/6/5/5
9	F3S	B	1004	2	-	-	0/3/3/3
14	PEE	C	145	-	-	11/17/17/54	-
10	GOL	B	1005	-	-	3/4/4/4	-
7	FES	B	1002	2	-	-	0/1/1/1
5	FAD	A	1001	1	-	11/34/50/50	0/6/6/6
14	PEE	D	104	-	-	11/18/18/54	-
12	HEM	C	143	3,4	-	4/10/50/54	-
11	JZR	C	142	-	-	3/9/29/29	0/1/1/1
13	UQ	C	144	-	-	2/4/28/87	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	FAD	PA-O3P	-11.25	1.47	1.59
5	A	1001	FAD	P-O3P	6.63	1.66	1.59
11	C	142	JZR	O1-C1	6.09	1.50	1.40
6	A	1002	3NP	C2-C1	-5.82	1.37	1.50
5	A	1001	FAD	PA-O2A	-5.12	1.31	1.55
12	C	143	HEM	CAB-C3B	-5.01	1.40	1.50
6	A	1002	3NP	C3-C2	-4.92	1.31	1.51
5	A	1001	FAD	PA-O1A	-4.86	1.34	1.50
14	D	104	PEE	C39-C38	4.10	1.55	1.31
12	C	143	HEM	CAC-C3C	-4.02	1.42	1.50
5	A	1001	FAD	C10-N10	3.97	1.45	1.37
14	D	104	PEE	C18-C19	3.95	1.54	1.31
12	C	143	HEM	FE-NC	3.86	2.07	1.95
5	A	1001	FAD	C9-C8	3.83	1.44	1.39
5	A	1001	FAD	C5'-C4'	-3.78	1.46	1.51
5	A	1001	FAD	C9A-C5X	3.66	1.47	1.41
5	A	1001	FAD	C6-C7	3.66	1.44	1.39
5	A	1001	FAD	C4A-N3A	3.51	1.41	1.34
12	C	143	HEM	CMC-C2C	3.41	1.57	1.50
14	C	145	PEE	C21-C22	-3.40	1.34	1.51
14	C	145	PEE	O2-C10	3.39	1.42	1.30
12	C	143	HEM	C1C-NC	-3.09	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	FAD	C2'-C3'	-3.08	1.48	1.53
13	C	144	UQ	C7-C6	3.01	1.56	1.50
6	A	1002	3NP	O2-C1	2.96	1.31	1.22
12	C	143	HEM	CAD-C3D	2.94	1.58	1.51
5	A	1001	FAD	C5A-N7A	-2.92	1.33	1.39
11	C	142	JZR	O5-C1	2.91	1.49	1.41
13	C	144	UQ	C6-C1	2.81	1.56	1.47
5	A	1001	FAD	C4X-N5	2.74	1.36	1.30
5	A	1001	FAD	C10-N1	2.72	1.38	1.33
5	A	1001	FAD	O5'-C5'	-2.68	1.34	1.44
5	A	1001	FAD	C8-C7	2.68	1.47	1.40
13	C	144	UQ	O3-C3	2.65	1.43	1.36
12	C	143	HEM	C4B-C3B	2.59	1.49	1.44
14	C	145	PEE	C11-C10	2.54	1.56	1.50
5	A	1001	FAD	C9-C9A	2.49	1.43	1.39
5	A	1001	FAD	C8A-N9A	-2.49	1.33	1.37
13	C	144	UQ	C3-C4	2.46	1.55	1.48
14	D	104	PEE	C17-C18	-2.45	1.36	1.50
5	A	1001	FAD	C2A-N3A	2.36	1.38	1.33
5	A	1001	FAD	C2A-N1A	2.32	1.38	1.33
5	A	1001	FAD	PA-O5B	-2.30	1.50	1.59
5	A	1001	FAD	C4'-C3'	2.30	1.57	1.53
5	A	1001	FAD	C1'-N10	2.29	1.53	1.47
13	C	144	UQ	CM5-C5	2.29	1.55	1.50
11	C	142	JZR	O1-C1'	2.27	1.49	1.43
13	C	144	UQ	C2-C1	2.25	1.55	1.48
14	D	104	PEE	C21-C20	-2.25	1.34	1.49
12	C	143	HEM	C1A-C2A	-2.24	1.40	1.44
5	A	1001	FAD	C4A-N9A	-2.24	1.33	1.37
5	A	1001	FAD	C6-C5X	2.23	1.43	1.40
13	C	144	UQ	C5-C4	2.15	1.54	1.47
5	A	1001	FAD	C1'-C2'	2.14	1.55	1.52
13	C	144	UQ	O2-C2	2.03	1.41	1.36

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	3NP	C3-C2-C1	8.65	131.71	112.98
5	A	1001	FAD	N3A-C2A-N1A	-6.02	119.46	128.58
12	C	143	HEM	CMC-C2C-C1C	4.65	132.91	124.73
12	C	143	HEM	C3D-C4D-ND	4.54	115.15	110.17
12	C	143	HEM	CHC-C1C-NC	-4.31	119.76	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	FAD	N3A-C4A-N9A	3.95	133.89	127.17
12	C	143	HEM	CAB-C3B-C4B	3.74	130.88	125.03
5	A	1001	FAD	C2A-N3A-C4A	3.54	120.47	111.83
5	A	1001	FAD	O2P-P-O3P	3.52	116.80	107.27
12	C	143	HEM	CMA-C3A-C4A	3.49	130.74	125.42
5	A	1001	FAD	C5A-C4A-N3A	-3.49	121.92	126.72
5	A	1001	FAD	C4A-N9A-C8A	3.48	109.39	105.74
5	A	1001	FAD	C4-C4X-N5	3.33	122.81	118.21
12	C	143	HEM	C1B-NB-C4B	-3.26	101.34	105.21
12	C	143	HEM	C4D-C3D-C2D	-3.24	102.18	106.89
12	C	143	HEM	CMB-C2B-C1B	3.23	130.08	125.03
12	C	143	HEM	CAD-C3D-C4D	3.16	130.21	124.70
12	C	143	HEM	CHA-C4D-ND	-3.12	120.51	124.37
5	A	1001	FAD	C5X-N5-C4X	3.04	123.00	118.09
14	D	104	PEE	C21-C20-C19	3.00	127.21	112.96
5	A	1001	FAD	C5X-C9A-N10	-2.94	115.31	117.97
6	A	1002	3NP	C2-C3-N1	2.84	135.24	114.54
12	C	143	HEM	C2B-C1B-NB	2.84	113.11	109.84
5	A	1001	FAD	C1'-C2'-C3'	2.76	117.13	109.66
14	C	145	PEE	C22-C21-C20	2.74	127.04	113.86
14	D	104	PEE	C16-C17-C18	2.71	127.80	112.60
5	A	1001	FAD	C4-N3-C2	-2.64	120.96	125.64
5	A	1001	FAD	C4'-C3'-C2'	-2.62	109.21	113.57
5	A	1001	FAD	C4X-C4-N3	2.60	119.88	113.25
5	A	1001	FAD	C10-N1-C2	2.58	122.43	116.85
12	C	143	HEM	C4D-ND-C1D	-2.52	102.22	105.21
5	A	1001	FAD	O3'-C3'-C2'	-2.45	103.37	108.93
12	C	143	HEM	C1C-CHC-C4B	2.42	131.17	126.02
5	A	1001	FAD	C9-C9A-N10	2.35	125.01	121.85
5	A	1001	FAD	C10-C4X-N5	-2.34	120.02	124.81
14	C	145	PEE	C21-C22-C23	2.30	125.99	114.37
5	A	1001	FAD	O4B-C1B-N9A	2.29	112.50	108.09
5	A	1001	FAD	C7M-C7-C6	-2.29	115.53	119.57
12	C	143	HEM	CMD-C2D-C1D	2.21	128.49	125.03
11	C	142	JZR	O1-C1'-C2'	2.21	116.87	109.37
5	A	1001	FAD	O2'-C2'-C3'	-2.20	104.09	109.25
12	C	143	HEM	C1C-C2C-C3C	-2.15	104.74	107.22
12	C	143	HEM	CMC-C2C-C3C	-2.13	122.33	126.75
12	C	143	HEM	C1B-C2B-C3B	-2.10	105.13	107.09
11	C	142	JZR	C1'-O1-C1	2.04	117.16	113.68
5	A	1001	FAD	O4'-C4'-C5'	-2.04	105.50	109.99

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	O4'-C4'-C5'-O5'
5	A	1001	FAD	C5'-O5'-P-O1P
5	A	1001	FAD	C5'-O5'-P-O2P
5	A	1001	FAD	C5'-O5'-P-O3P
5	A	1001	FAD	PA-O3P-P-O5'
6	A	1002	3NP	C1-C2-C3-N1
14	D	104	PEE	C17-C18-C19-C20
14	D	104	PEE	C37-C38-C39-C40
10	B	1005	GOL	C1-C2-C3-O3
14	C	145	PEE	C11-C12-C13-C14
10	B	1005	GOL	O2-C2-C3-O3
14	C	145	PEE	C12-C13-C14-C15
11	C	142	JZR	O1-C1'-C2'-C3'
14	D	104	PEE	C33-C34-C35-C36
14	C	145	PEE	C23-C24-C25-C26
14	C	145	PEE	C22-C23-C24-C25
5	A	1001	FAD	C3'-C4'-C5'-O5'
14	C	145	PEE	C17-C18-C19-C20
14	C	145	PEE	C19-C20-C21-C22
14	D	104	PEE	C32-C33-C34-C35
14	D	104	PEE	C10-C11-C12-C13
14	D	104	PEE	C15-C16-C17-C18
14	D	104	PEE	C38-C39-C40-C41
14	D	104	PEE	C31-C32-C33-C34
14	D	104	PEE	C35-C36-C37-C38
5	A	1001	FAD	N10-C1'-C2'-C3'
13	C	144	UQ	C4-C3-O3-CM3
11	C	142	JZR	C2'-C3'-C4'-C5'
14	D	104	PEE	C34-C35-C36-C37
11	C	142	JZR	C3'-C4'-C5'-C6'
14	C	145	PEE	O2-C10-C11-C12
14	C	145	PEE	C24-C25-C26-C27
13	C	144	UQ	C2-C3-O3-CM3
14	C	145	PEE	O4-C10-C11-C12
12	C	143	HEM	C2A-CAA-CBA-CGA
12	C	143	HEM	CAD-CBD-CGD-O2D
14	C	145	PEE	C14-C15-C16-C17
14	C	145	PEE	C16-C17-C18-C19
10	B	1005	GOL	O1-C1-C2-O2
12	C	143	HEM	CAD-CBD-CGD-O1D
14	D	104	PEE	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

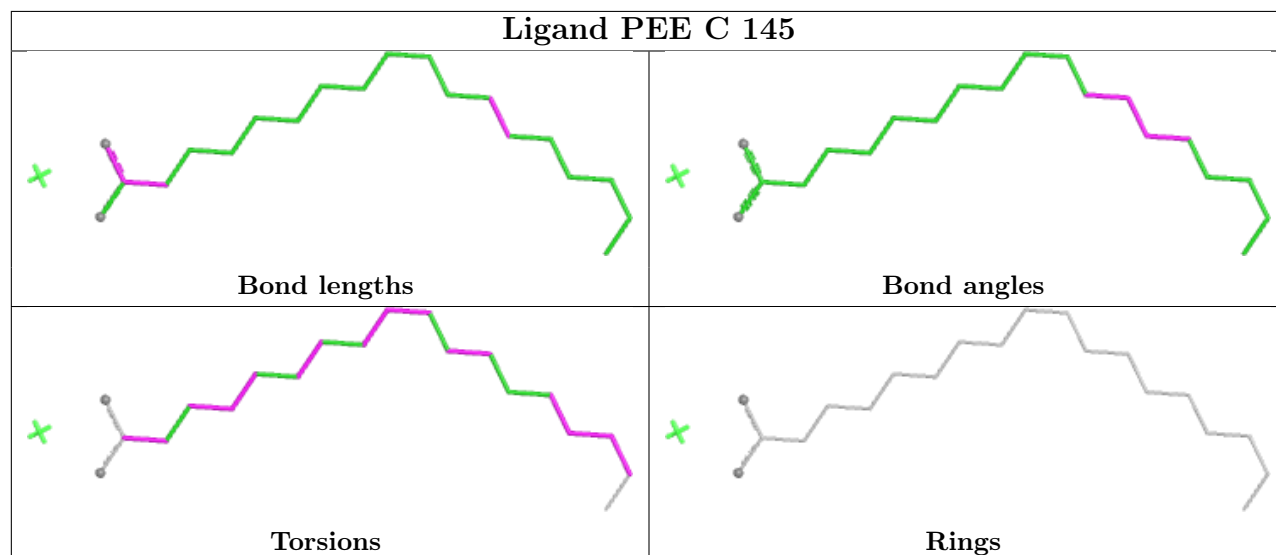
Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	PA-O3P-P-O1P
5	A	1001	FAD	O4B-C4B-C5B-O5B
6	A	1002	3NP	O1-C1-C2-C3
12	C	143	HEM	CAA-CBA-CGA-O2A
5	A	1001	FAD	PA-O3P-P-O2P
6	A	1002	3NP	O2-C1-C2-C3

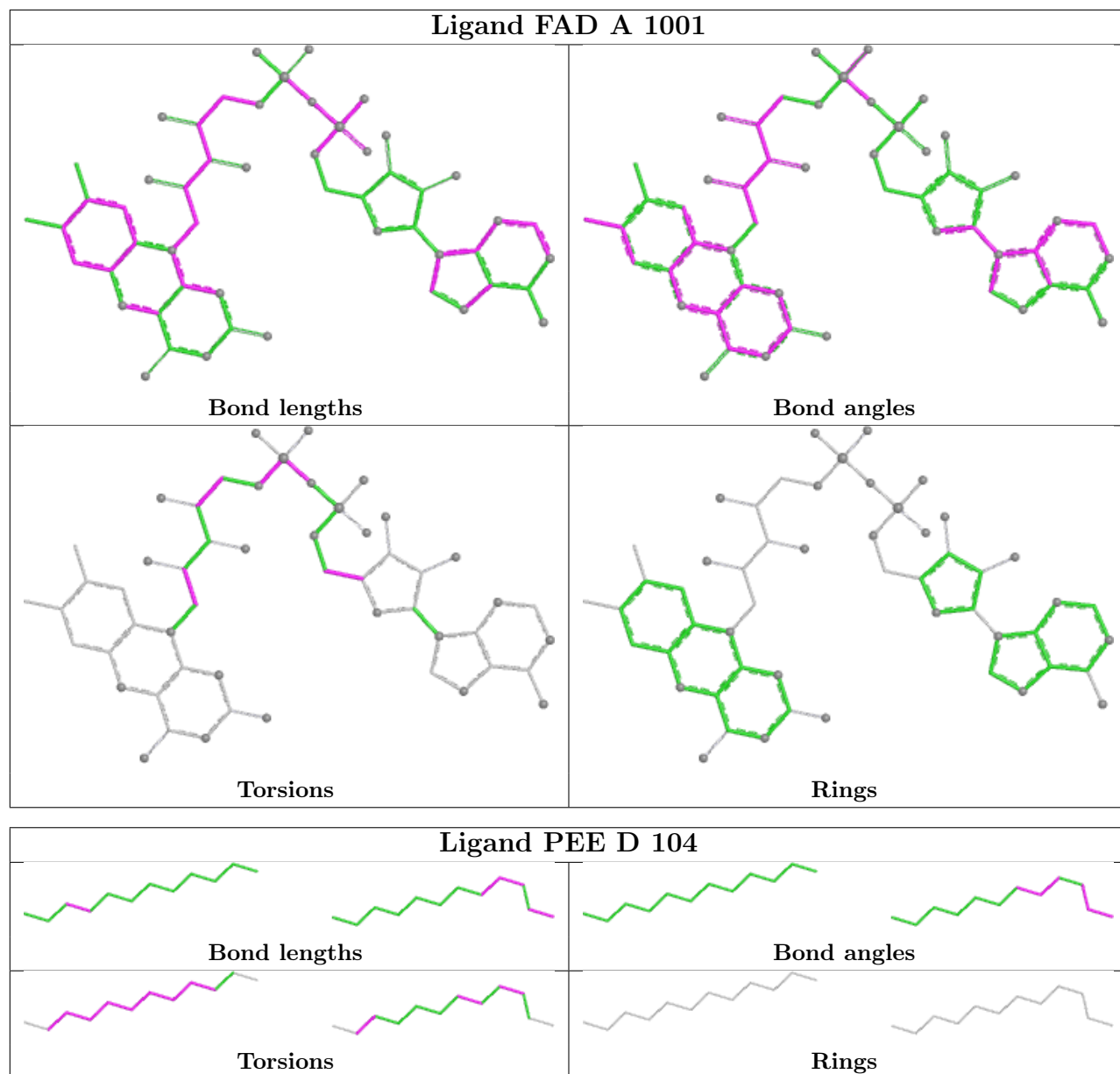
There are no ring outliers.

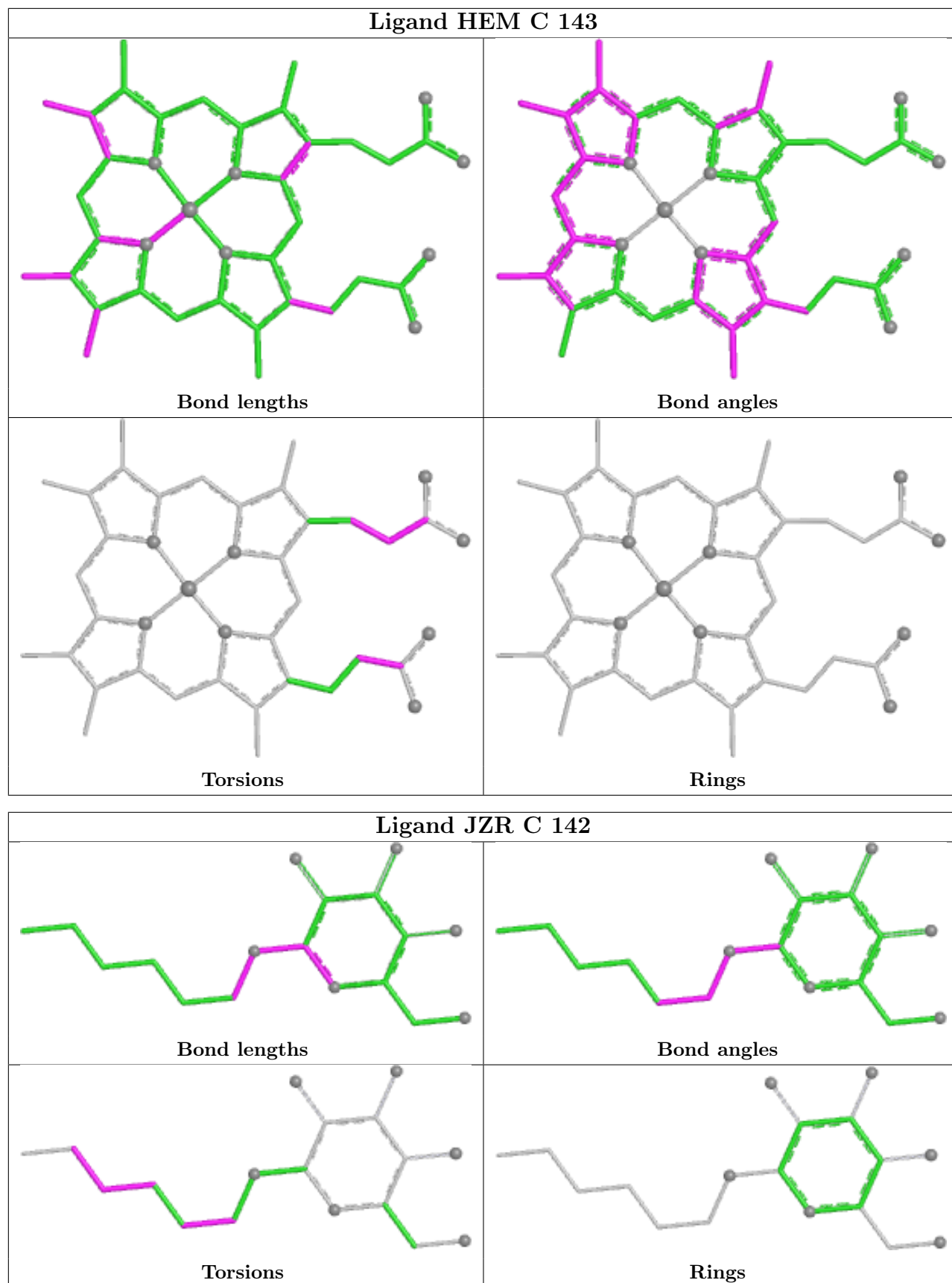
3 monomers are involved in 17 short contacts:

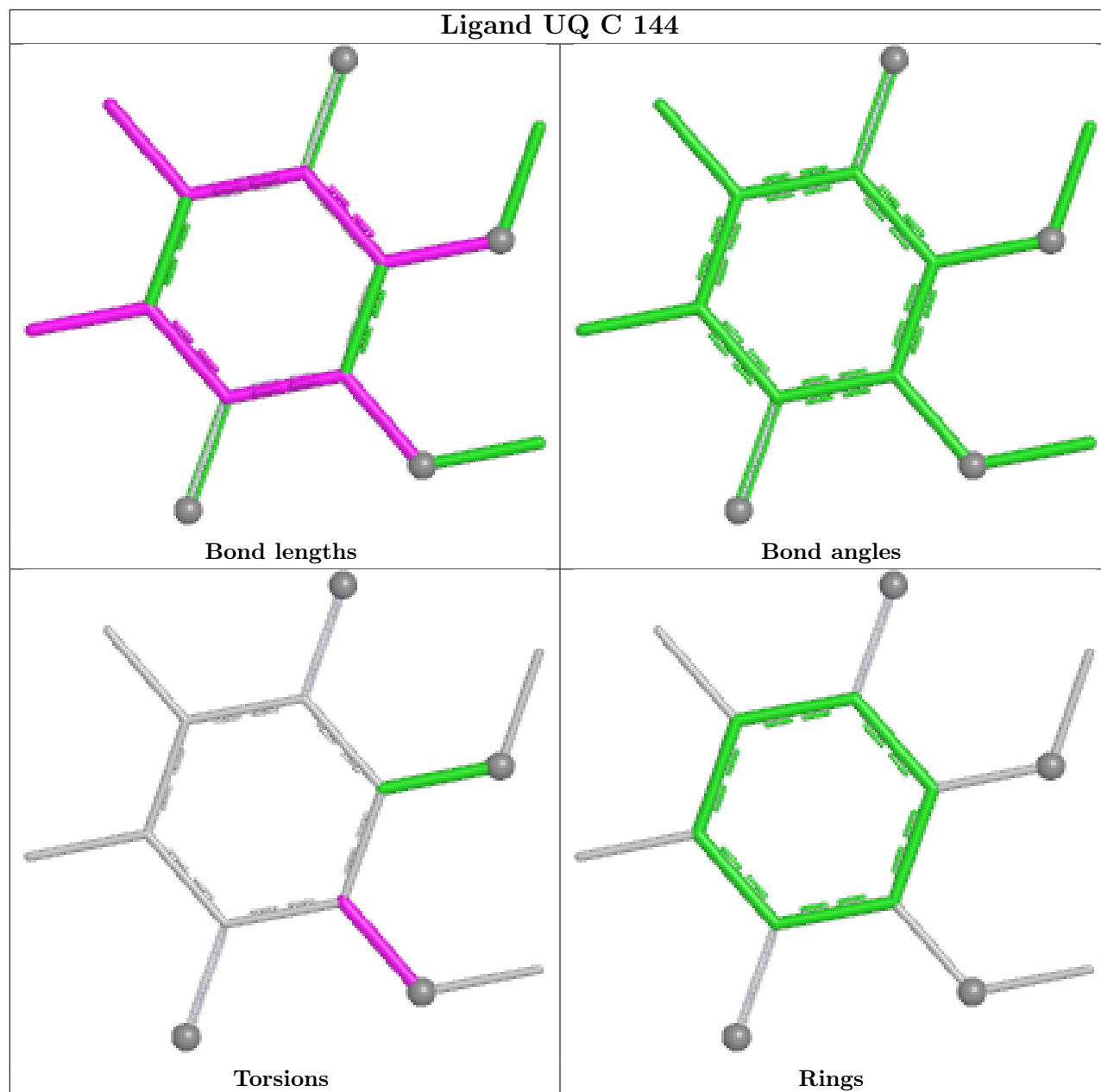
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	145	PEE	1	0
5	A	1001	FAD	6	0
13	C	144	UQ	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	614/621 (98%)	-0.02	5 (0%) 82 85	26, 47, 74, 152	0
2	B	242/252 (96%)	-0.16	7 (2%) 53 60	24, 40, 84, 124	0
3	C	140/141 (99%)	-0.03	2 (1%) 73 77	25, 45, 76, 91	0
4	D	102/103 (99%)	-0.03	1 (0%) 79 82	29, 42, 68, 84	0
All	All	1098/1117 (98%)	-0.05	15 (1%) 73 77	24, 45, 75, 152	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ILE	5.3
2	B	6	ALA	4.4
2	B	7	ALA	3.1
2	B	136	LYS	2.5
2	B	134	GLU	2.5
2	B	169	PRO	2.4
1	A	9	SER	2.4
4	D	73	TYR	2.3
1	A	10	THR	2.2
2	B	8	THR	2.2
3	C	140	ILE	2.2
1	A	441	ILE	2.1
2	B	246	LYS	2.1
1	A	494	GLU	2.1
3	C	141	SER	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

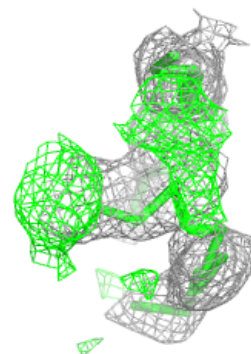
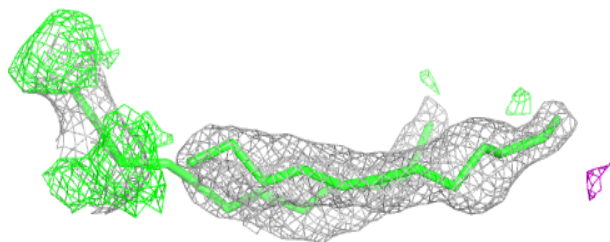
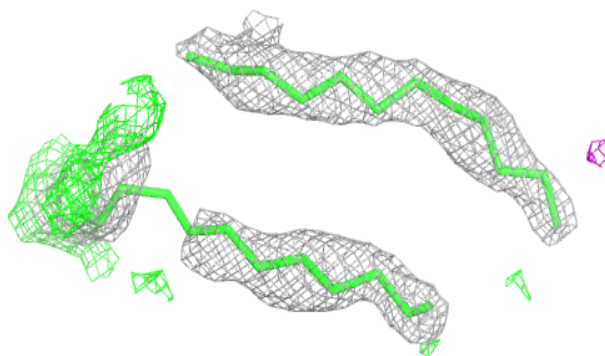
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	GOL	B	1005	6/6	0.77	0.24	156,160,161,162	0
14	PEE	D	104	24/51	0.82	0.24	53,72,98,99	0
13	UQ	C	144	14/63	0.85	0.28	90,99,109,113	0
14	PEE	C	145	21/51	0.87	0.18	45,74,88,92	0
11	JZR	C	142	18/18	0.93	0.11	38,48,61,63	0
6	3NP	A	1002	6/8	0.97	0.07	38,39,44,47	0
5	FAD	A	1001	53/53	0.97	0.06	18,32,43,52	0
12	HEM	C	143	41/43	0.98	0.08	29,41,65,67	0
8	SF4	B	1003	8/8	0.99	0.03	32,34,38,38	0
9	F3S	B	1004	7/7	0.99	0.03	26,27,28,30	0
7	FES	B	1002	4/4	1.00	0.02	30,32,34,37	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.

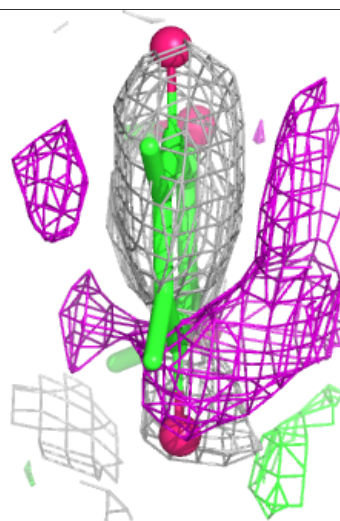
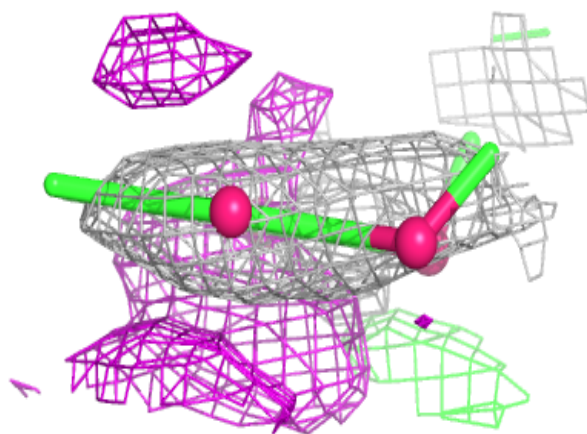
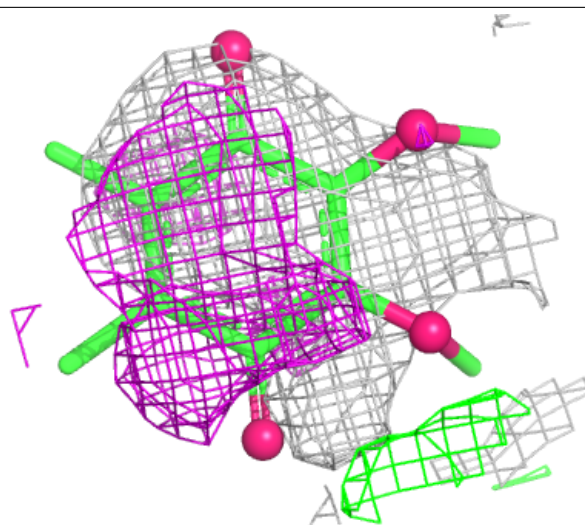
Electron density around PEE D 104:

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



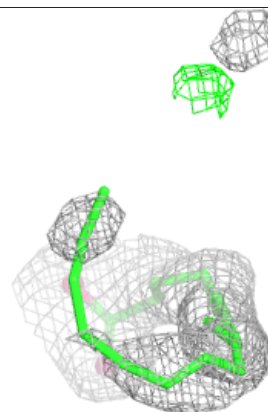
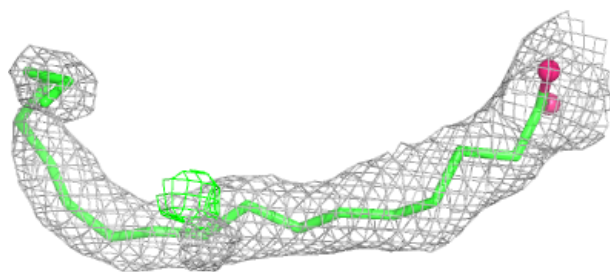
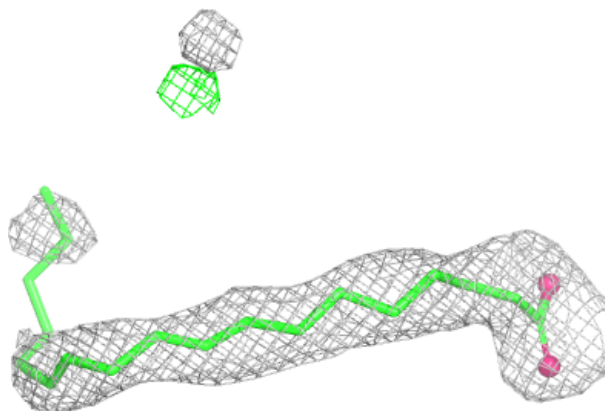
Electron density around UQ C 144:

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

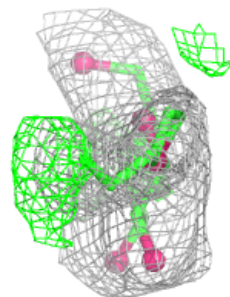
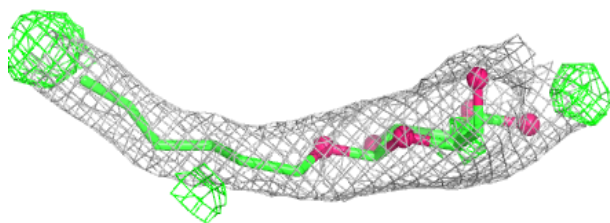
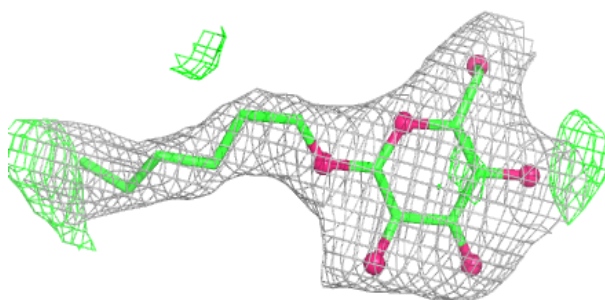


Electron density around PEE C 145:

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

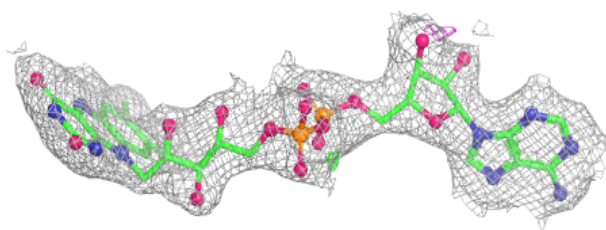
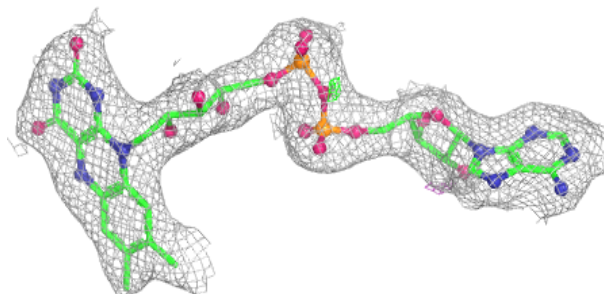
**Electron density around JZR C 142:**

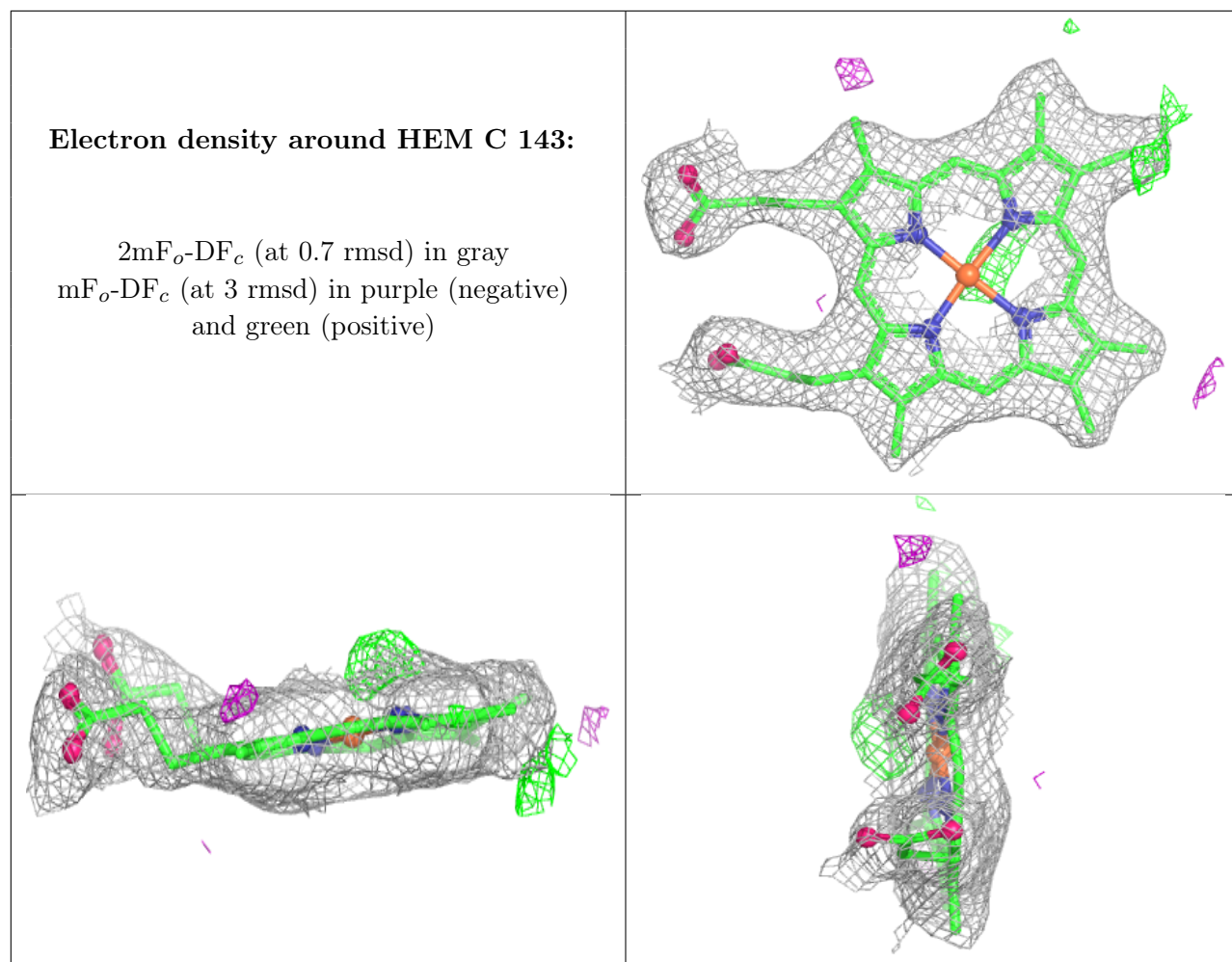
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD A 1001:

$2mF_o-DF_c$ (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.