



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:07 AM BST

PDB ID : 2H89  
Title : Avian Respiratory Complex II with Malonate Bound  
Authors : Huang, L.S.; Shen, J.T.; Wang, A.C.; Berry, E.A.  
Deposited on : 2006-06-06  
Resolution : 2.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

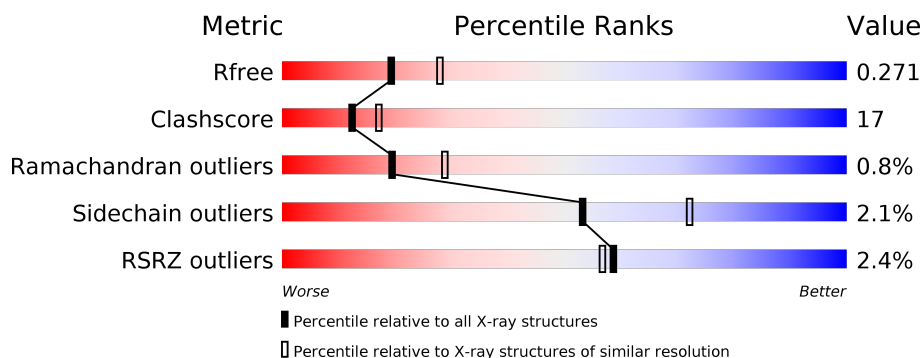
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div>..</div> </div> </div>
2	B	252	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>.</div> </div> </div>
3	C	140	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>38%</div> <div>..</div> </div> </div>
4	D	103	<div> <div></div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	BHG	C	141	X	-	-	-
7	MLI	A	1002	-	-	X	-
8	UNL	A	1008	-	-	-	X
8	UNL	A	1014	-	-	-	X
8	UNL	A	1015	-	-	-	X
8	UNL	B	1005	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 9302 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	613	Total	C	N	O	S	0	0	1
			4727	2957	843	898	29			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ARG	CYS	conflict	UNP Q9YHT1
A	556	LEU	PHE	conflict	UNP Q9YHT1
A	560	GLU	ASP	conflict	UNP Q9YHT1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	1
			1925	1218	326	359	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			

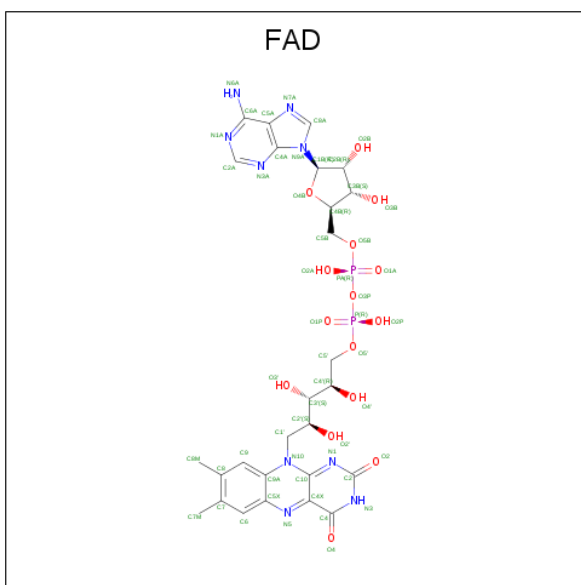
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			771	508	122	138	3			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



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

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula:  $\text{C}_3\text{H}_2\text{O}_4$ ).

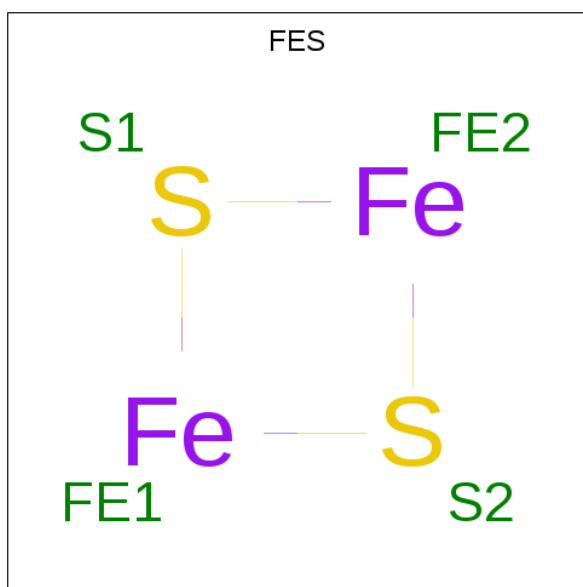


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 8 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

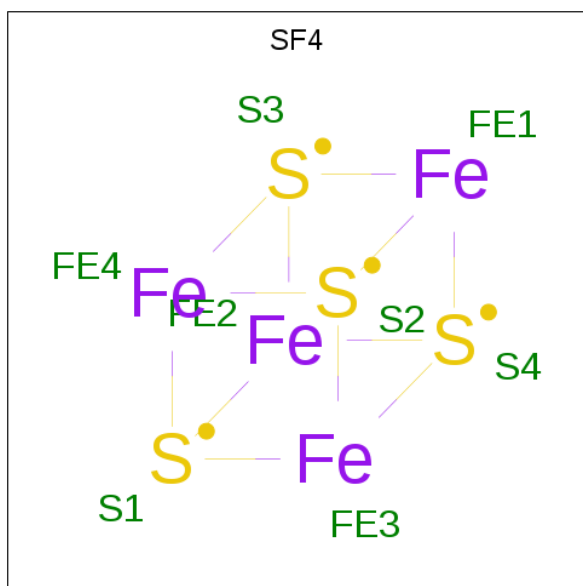
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	10	Total	C	O	0	0
			15	3	12		
8	A	15	Total	O		0	0
			15	15			
8	D	6	Total	O		0	0
			6	6			
8	C	9	Total	O		0	0
			11	11			

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



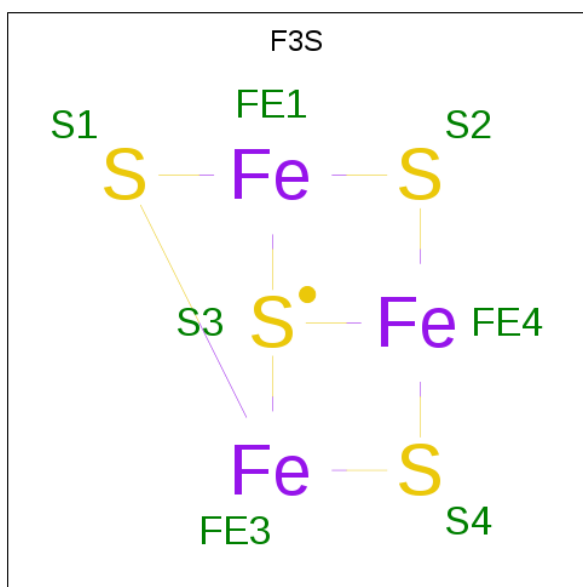
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



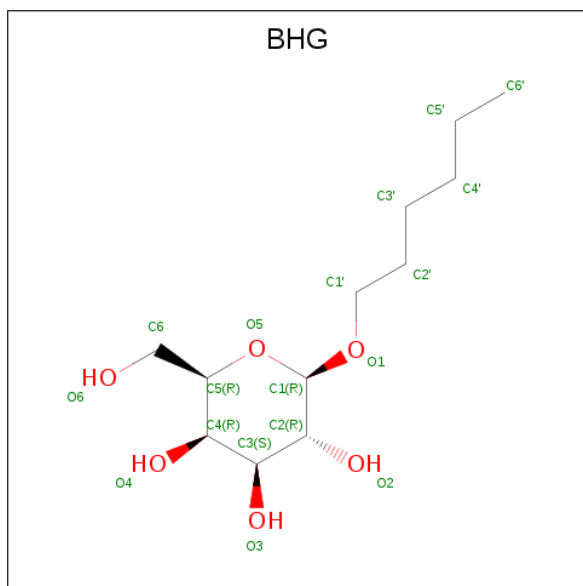
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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

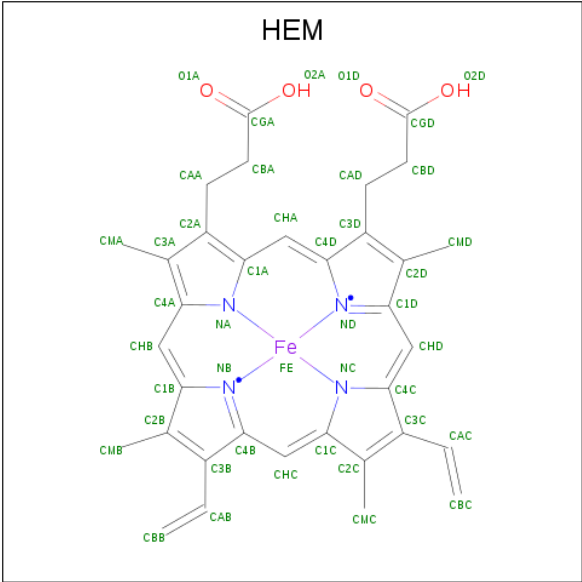
- Molecule 12 is hexyl beta-D-galactopyranoside (three-letter code: BHG) (formula:  $C_{12}H_{24}O_6$ ).



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

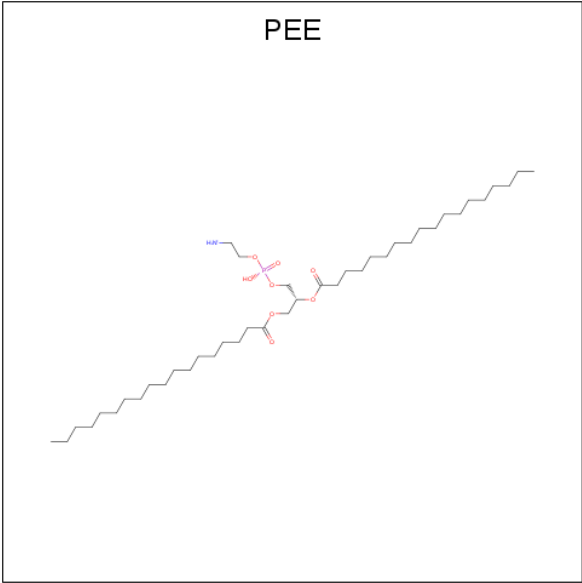
- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

- Molecule 14 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	1	Total	C	0	0
			11	11		
14	D	1	Total	C	0	0
			24	24		

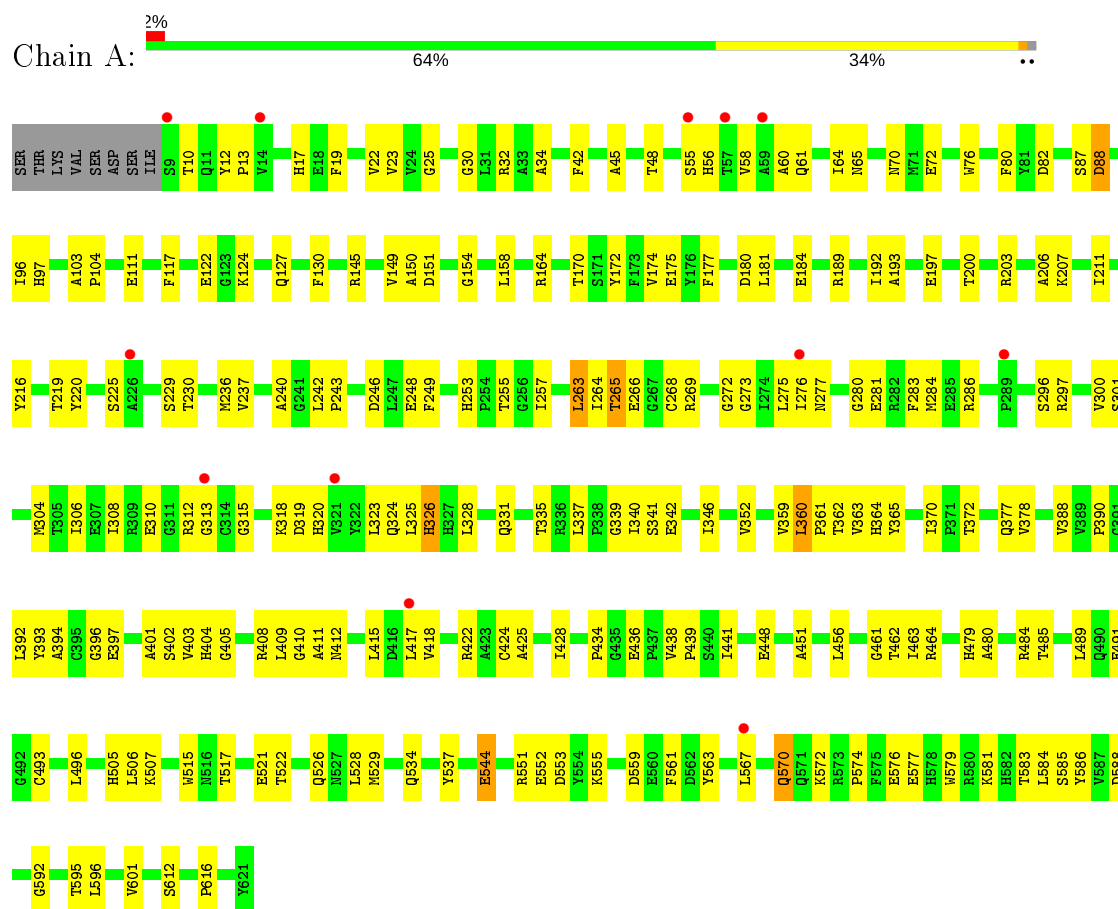
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	292	Total 292	O 292	0	0
15	B	166	Total 166	O 166	0	0
15	C	61	Total 61	O 61	0	0
15	D	61	Total 61	O 61	0	0

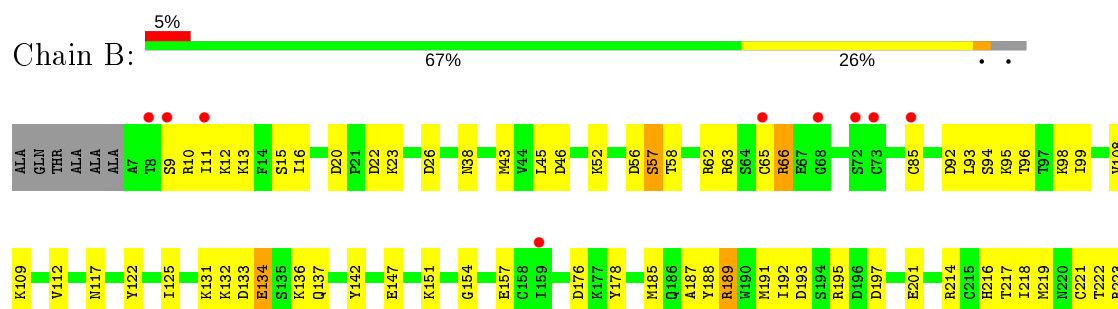
### 3 Residue-property plots [i](#)

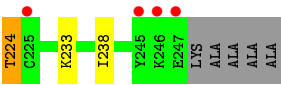
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT



#### • Molecule 2: Succinate dehydrogenase Ip subunit

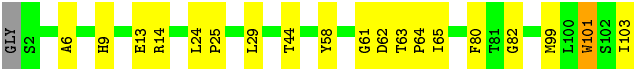
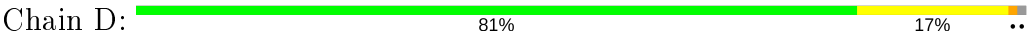




• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



• 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, $\alpha$ , $\beta$ , $\gamma$	70.52Å 84.12Å 292.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.74 – 2.40 50.74 – 2.29	Depositor EDS
% Data completeness (in resolution range)	86.3 (50.74-2.40) 79.7 (50.74-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.279 0.217 , 0.271	Depositor DCC
$R_{free}$ test set	3091 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SF4, MLI, BHG, F3S, FES, PEE, HEM, UNL, K, FAD

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	0.41	0/4827	0.66	0/6535
2	B	0.44	0/1966	0.68	0/2651
3	C	0.44	0/1106	0.61	0/1503
4	D	0.42	0/794	0.56	0/1089
All	All	0.42	0/8693	0.65	0/11778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4727	0	4609	181	0
2	B	1925	0	1918	58	0
3	C	1077	0	1112	45	0
4	D	771	0	763	18	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	53	0	29	2	0
7	A	7	0	2	4	0
8	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	15	0	0	1	0
8	C	11	0	0	0	0
8	D	6	0	0	0	0
9	B	4	0	0	0	0
10	B	8	0	0	0	0
11	B	7	0	0	0	0
12	C	18	0	24	1	0
13	C	41	0	24	0	0
14	C	11	0	18	0	0
14	D	24	0	40	1	0
15	A	292	0	0	22	0
15	B	166	0	0	4	0
15	C	61	0	0	3	0
15	D	61	0	0	2	0
All	All	9302	0	8539	291	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 17.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HH22	7:A:1002:MLI:C3	1.65	1.08
1:A:365:TYR:CE1	1:A:397:GLU:HG3	2.11	0.86
3:C:4:THR:OG1	3:C:7:GLU:HG3	1.77	0.85
1:A:401:ALA:N	1:A:402:SER:HA	1.98	0.77
3:C:115:LYS:HB3	3:C:118:GLN:OE1	1.86	0.76
2:B:187:ALA:O	2:B:191:MET:HG3	1.88	0.73
3:C:70:TYR:O	3:C:74:VAL:HG23	1.87	0.73
3:C:74:VAL:HA	3:C:77:LEU:HD12	1.70	0.73
1:A:297:ARG:HH22	7:A:1002:MLI:C1	2.03	0.71
1:A:297:ARG:NH2	7:A:1002:MLI:C3	2.49	0.71
1:A:464:ARG:HB3	1:A:507:LYS:HE3	1.73	0.71
1:A:277:ASN:HD21	1:A:281:GLU:HB3	1.55	0.70
1:A:177:PHE:O	1:A:193:ALA:HB1	1.90	0.70
4:D:24:LEU:N	4:D:25:PRO:HD2	2.07	0.70
1:A:281:GLU:HG2	1:A:283:PHE:N	2.07	0.70
2:B:65:CYS:O	2:B:66:ARG:HG3	1.93	0.69
2:B:15:SER:HB3	2:B:98:LYS:HG2	1.76	0.68
2:B:216:HIS:HB2	15:C:1145:HOH:O	1.92	0.68
1:A:424:CYS:O	1:A:428:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG21	1:A:370:ILE:HD13	1.77	0.67
2:B:23:LYS:HB3	2:B:26:ASP:HB2	1.75	0.67
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.75	0.67
1:A:207:LYS:NZ	1:A:436:GLU:HB3	2.10	0.66
3:C:8:GLU:HG2	3:C:11:ARG:NH2	2.10	0.66
3:C:5:ALA:O	3:C:9:MET:HG3	1.97	0.65
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.78	0.64
3:C:69:HIS:O	3:C:73:VAL:HG23	1.97	0.64
1:A:306:ILE:O	1:A:310:GLU:HB2	1.97	0.64
2:B:45:LEU:HD22	2:B:85:CYS:HB3	1.80	0.64
1:A:403:VAL:HG23	1:A:404:HIS:CE1	2.34	0.63
3:C:106:LEU:HD22	15:D:1267:HOH:O	1.97	0.63
2:B:134:GLU:CD	2:B:134:GLU:H	2.02	0.62
2:B:133:ASP:OD1	2:B:136:LYS:HE3	2.00	0.62
3:C:26:HIS:CD2	3:C:27:ILE:H	2.16	0.62
1:A:410:GLY:O	1:A:411:ALA:HB3	1.98	0.62
1:A:122:GLU:HG3	15:A:1062:HOH:O	1.98	0.62
2:B:10:ARG:HD3	2:B:38:ASN:HD21	1.66	0.61
1:A:103:ALA:HB3	1:A:104:PRO:HD3	1.81	0.61
1:A:237:VAL:HG12	1:A:242:LEU:HB2	1.84	0.60
1:A:61:GLN:HB3	1:A:151:ASP:O	2.01	0.60
1:A:127:GLN:NE2	1:A:145:ARG:HA	2.17	0.60
1:A:563:TYR:HE1	15:A:1258:HOH:O	1.85	0.59
1:A:324:GLN:HG3	1:A:326:HIS:CE1	2.37	0.59
1:A:197:GLU:HB2	15:A:1262:HOH:O	2.03	0.59
1:A:574:PRO:HD2	1:A:577:GLU:HB2	1.84	0.59
1:A:189:ARG:HH11	1:A:439:PRO:HB2	1.68	0.58
1:A:340:ILE:HD12	1:A:341:SER:N	2.18	0.58
1:A:32:ARG:HH22	1:A:422:ARG:NH1	2.02	0.58
1:A:296:SER:O	1:A:300:VAL:HG23	2.03	0.58
2:B:13:LYS:HB3	2:B:96:THR:HG23	1.86	0.58
1:A:230:THR:HG22	1:A:528:LEU:HD11	1.86	0.57
2:B:122:TYR:O	2:B:125:ILE:HG12	2.04	0.57
2:B:11:ILE:O	2:B:93:LEU:HD22	2.04	0.57
1:A:263:LEU:HG	1:A:264:ILE:N	2.19	0.57
1:A:64:ILE:HD11	1:A:415:LEU:HA	1.87	0.57
2:B:189:ARG:HD3	2:B:189:ARG:C	2.25	0.57
1:A:402:SER:HB2	15:A:1060:HOH:O	2.03	0.57
2:B:217:THR:HG22	2:B:217:THR:O	2.04	0.57
1:A:515:TRP:HD1	15:A:1271:HOH:O	1.88	0.56
3:C:65:GLU:HB2	3:C:70:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:GLY:O	4:D:65:ILE:HG13	2.04	0.56
1:A:25:GLY:HA2	6:A:1001:FAD:H1B	1.86	0.56
1:A:479:HIS:O	1:A:489:LEU:HD23	2.04	0.56
1:A:448:GLU:O	1:A:451:ALA:HB3	2.04	0.56
2:B:151:LYS:HB3	2:B:192:ILE:HD12	1.87	0.56
1:A:493:CYS:HB3	1:A:537:TYR:CZ	2.40	0.56
1:A:277:ASN:ND2	1:A:281:GLU:HB3	2.21	0.56
1:A:19:PHE:CD2	1:A:45:ALA:HB2	2.41	0.55
1:A:576:GLU:CD	1:A:576:GLU:H	2.10	0.55
1:A:563:TYR:CD1	1:A:616:PRO:HB2	2.41	0.55
1:A:10:THR:O	1:A:10:THR:HG23	2.07	0.55
1:A:377:GLN:HG2	1:A:393:TYR:CE1	2.41	0.55
1:A:207:LYS:HZ2	1:A:436:GLU:HB3	1.72	0.55
1:A:340:ILE:HD12	1:A:340:ILE:C	2.27	0.55
1:A:312:ARG:HG3	1:A:312:ARG:HH11	1.72	0.54
2:B:154:GLY:H	2:B:157:GLU:CD	2.10	0.54
2:B:10:ARG:HD3	2:B:38:ASN:ND2	2.22	0.54
1:A:174:VAL:HG12	1:A:175:GLU:HG3	1.89	0.54
2:B:147:GLU:CD	2:B:147:GLU:H	2.11	0.54
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.21	0.54
1:A:32:ARG:NH2	1:A:422:ARG:HD2	2.22	0.54
3:C:81:PRO:O	3:C:84:ILE:HB	2.07	0.54
1:A:22:VAL:HG23	1:A:206:ALA:CB	2.37	0.54
2:B:131:LYS:HE3	2:B:195:ARG:O	2.08	0.54
3:C:93:PHE:N	3:C:94:PRO:HD2	2.23	0.54
1:A:300:VAL:HG12	15:A:1279:HOH:O	2.07	0.54
2:B:20:ASP:HB3	2:B:23:LYS:HB2	1.90	0.54
1:A:184:GLU:HB3	1:A:189:ARG:HE	1.74	0.53
1:A:276:ILE:HA	1:A:281:GLU:O	2.09	0.53
1:A:372:THR:HG21	1:A:394:ALA:HB3	1.90	0.53
4:D:63:THR:HB	4:D:64:PRO:HD3	1.89	0.53
1:A:237:VAL:CG1	1:A:242:LEU:HB2	2.39	0.53
1:A:253:HIS:O	1:A:361:PRO:HA	2.07	0.53
1:A:266:GLU:HG3	1:A:269:ARG:CZ	2.38	0.53
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.91	0.53
1:A:70:ASN:ND2	1:A:124:LYS:HB3	2.24	0.53
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.44	0.53
4:D:9:HIS:O	4:D:13:GLU:HG3	2.08	0.53
2:B:136:LYS:HB2	15:B:1138:HOH:O	2.09	0.53
1:A:534:GLN:NE2	1:A:585:SER:OG	2.42	0.52
3:C:137:ILE:HA	3:C:140:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG23	1:A:206:ALA:HB2	1.92	0.52
2:B:52:LYS:HG2	2:B:57:SER:HA	1.90	0.52
3:C:77:LEU:O	3:C:78:SER:C	2.48	0.52
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.45	0.51
4:D:62:ASP:HA	15:D:1384:HOH:O	2.11	0.51
2:B:15:SER:O	2:B:98:LYS:HA	2.11	0.51
1:A:461:GLY:H	1:A:507:LYS:HB3	1.76	0.51
1:A:263:LEU:HD13	1:A:364:HIS:CE1	2.46	0.51
1:A:378:VAL:HG21	1:A:392:LEU:HG	1.93	0.51
4:D:61:GLY:O	4:D:64:PRO:HD2	2.11	0.51
1:A:559:ASP:HB3	15:A:1258:HOH:O	2.10	0.50
1:A:19:PHE:O	1:A:206:ALA:HA	2.11	0.50
1:A:496:LEU:HD22	1:A:529:MET:CE	2.41	0.50
3:C:45:THR:O	3:C:49:LEU:HG	2.11	0.50
1:A:237:VAL:O	1:A:240:ALA:HB3	2.12	0.50
1:A:489:LEU:HD12	1:A:551:ARG:NH1	2.26	0.50
1:A:342:GLU:OE2	1:A:346:ILE:HD11	2.12	0.50
1:A:372:THR:CG2	1:A:394:ALA:HB3	2.42	0.50
1:A:269:ARG:HA	1:A:273:GLY:O	2.12	0.50
1:A:438:VAL:HG23	1:A:439:PRO:HD2	1.94	0.49
1:A:441:ILE:HG13	1:A:441:ILE:O	2.11	0.49
1:A:418:VAL:HB	15:A:1042:HOH:O	2.12	0.49
2:B:62:ARG:NH1	2:B:112:VAL:HG13	2.27	0.49
1:A:170:THR:HB	1:A:172:TYR:HE1	1.76	0.49
2:B:20:ASP:OD1	2:B:22:ASP:N	2.45	0.49
1:A:189:ARG:HH11	1:A:439:PRO:CB	2.25	0.49
2:B:12:LYS:NZ	2:B:95:LYS:O	2.34	0.49
1:A:308:ILE:HD13	1:A:319:ASP:O	2.12	0.49
1:A:275:LEU:HD12	1:A:284:MET:HG3	1.94	0.49
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.94	0.49
2:B:189:ARG:NH1	2:B:193:ASP:OD2	2.38	0.49
4:D:24:LEU:N	4:D:25:PRO:CD	2.75	0.49
3:C:37:ALA:O	3:C:40:ILE:HG22	2.13	0.49
4:D:25:PRO:O	4:D:29:LEU:HG	2.12	0.49
4:D:63:THR:HG22	4:D:64:PRO:N	2.27	0.49
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.94	0.49
1:A:19:PHE:CE2	1:A:45:ALA:HB2	2.48	0.49
1:A:255:THR:HG22	1:A:359:VAL:HG21	1.94	0.48
1:A:401:ALA:N	1:A:402:SER:CA	2.71	0.48
3:C:8:GLU:HG2	3:C:11:ARG:HH21	1.78	0.48
1:A:87:SER:O	1:A:88:ASP:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:VAL:O	3:C:51:LEU:HG	2.13	0.48
2:B:176:ASP:HB3	3:C:13:TRP:CZ2	2.48	0.48
2:B:188:TYR:HD1	2:B:191:MET:CE	2.27	0.48
1:A:207:LYS:HZ3	1:A:436:GLU:HB3	1.77	0.48
1:A:82:ASP:HA	15:A:1125:HOH:O	2.12	0.48
1:A:266:GLU:HA	15:A:1092:HOH:O	2.13	0.48
1:A:55:SER:O	1:A:58:VAL:HG12	2.13	0.48
1:A:409:LEU:O	1:A:412:ASN:HB2	2.14	0.47
2:B:223:ARG:HG3	2:B:223:ARG:HH11	1.79	0.47
1:A:65:ASN:ND2	1:A:411:ALA:HB3	2.29	0.47
2:B:189:ARG:O	2:B:189:ARG:HD3	2.15	0.47
4:D:101:TRP:CD1	14:D:105:PEE:H28	2.49	0.47
8:B:1013:UNL:O1	4:D:6:ALA:HB2	2.14	0.47
1:A:584:LEU:O	1:A:596:LEU:HA	2.13	0.47
1:A:586:TYR:HB2	1:A:595:THR:HB	1.96	0.47
3:C:89:PHE:HE1	3:C:135:ALA:N	2.12	0.47
1:A:216:TYR:CD1	1:A:216:TYR:O	2.68	0.47
1:A:544:GLU:HG2	1:A:579:TRP:CG	2.49	0.47
2:B:56:ASP:C	2:B:58:THR:H	2.18	0.47
3:C:57:SER:HB2	4:D:82:GLY:HA3	1.96	0.47
1:A:266:GLU:HB2	7:A:1002:MLI:O6	2.15	0.47
1:A:13:PRO:HG2	1:A:200:THR:HG22	1.97	0.47
1:A:65:ASN:O	1:A:415:LEU:HD22	2.15	0.47
1:A:461:GLY:HA3	1:A:505:HIS:O	2.15	0.47
1:A:517:THR:O	1:A:521:GLU:HG3	2.15	0.47
1:A:242:LEU:HB3	15:A:1048:HOH:O	2.14	0.46
3:C:40:ILE:HG23	3:C:41:THR:N	2.30	0.46
3:C:41:THR:HG22	3:C:97:TYR:CE2	2.50	0.46
1:A:365:TYR:CE2	1:A:408:ARG:HD3	2.50	0.46
2:B:201:GLU:OE1	2:B:201:GLU:N	2.47	0.46
1:A:388:VAL:O	1:A:390:PRO:HD3	2.15	0.46
1:A:456:LEU:HD13	1:A:522:THR:HG22	1.98	0.46
1:A:561:PHE:CZ	1:A:572:LYS:HB2	2.51	0.46
1:A:61:GLN:HB2	1:A:265:THR:HB	1.98	0.46
2:B:108:VAL:HG23	2:B:112:VAL:O	2.15	0.46
3:C:13:TRP:O	3:C:17:THR:HG23	2.16	0.46
1:A:581:LYS:HA	1:A:601:VAL:HG23	1.96	0.46
2:B:185:MET:HB3	15:B:1027:HOH:O	2.14	0.46
3:C:67:PHE:N	3:C:68:PRO:CD	2.79	0.46
1:A:301:SER:HA	15:A:1279:HOH:O	2.15	0.46
2:B:43:MET:O	2:B:46:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HG22	1:A:340:ILE:HG21	1.98	0.45
1:A:312:ARG:HG3	1:A:312:ARG:NH1	2.31	0.45
1:A:422:ARG:O	1:A:425:ALA:HB3	2.16	0.45
2:B:223:ARG:HA	3:C:116:LEU:HD22	1.98	0.45
1:A:17:HIS:HB3	1:A:19:PHE:HE1	1.80	0.45
1:A:479:HIS:HE1	1:A:491:GLU:OE1	2.00	0.45
1:A:403:VAL:HG23	1:A:404:HIS:ND1	2.31	0.45
1:A:58:VAL:HB	1:A:158:LEU:HD23	1.99	0.45
1:A:56:HIS:CE1	1:A:225:SER:HA	2.52	0.45
1:A:561:PHE:N	15:A:1258:HOH:O	2.37	0.45
1:A:76:TRP:HH2	1:A:97:HIS:NE2	2.14	0.45
1:A:276:ILE:CG2	1:A:280:GLY:HA2	2.47	0.45
2:B:62:ARG:HD2	15:B:1067:HOH:O	2.16	0.44
3:C:107:VAL:HA	3:C:110:MET:CE	2.46	0.44
1:A:177:PHE:O	1:A:193:ALA:CB	2.63	0.44
2:B:221:CYS:O	2:B:224:THR:HG22	2.16	0.44
1:A:111:GLU:OE2	2:B:142:TYR:HB2	2.16	0.44
1:A:164:ARG:HH22	2:B:137:GLN:HE22	1.65	0.44
1:A:552:GLU:O	1:A:555:LYS:HE3	2.17	0.44
2:B:219:MET:HE3	2:B:222:THR:HB	1.99	0.44
1:A:42:PHE:CD1	1:A:434:PRO:HG3	2.53	0.44
1:A:192:ILE:HD12	1:A:203:ARG:HG2	1.99	0.44
1:A:276:ILE:HG23	1:A:280:GLY:HA2	1.98	0.44
1:A:339:GLY:HA3	15:A:1090:HOH:O	2.18	0.44
1:A:365:TYR:HE1	1:A:397:GLU:HG3	1.76	0.44
1:A:464:ARG:HB3	1:A:507:LYS:CE	2.46	0.44
3:C:65:GLU:O	3:C:70:TYR:HE1	2.00	0.44
1:A:315:GLY:HA3	1:A:320:HIS:CE1	2.53	0.43
2:B:191:MET:HB2	2:B:191:MET:HE3	1.83	0.43
3:C:107:VAL:HA	3:C:110:MET:HE3	1.99	0.43
1:A:283:PHE:O	1:A:286:ARG:HB3	2.18	0.43
1:A:313:GLY:O	1:A:318:LYS:HD2	2.18	0.43
1:A:396:GLY:HA2	1:A:417:LEU:CD2	2.48	0.43
1:A:567:LEU:O	1:A:570:GLN:HB2	2.17	0.43
2:B:188:TYR:HA	2:B:191:MET:HE2	2.00	0.43
1:A:87:SER:HB2	1:A:405:GLY:HA3	2.00	0.43
1:A:170:THR:O	3:C:2:ALA:HB2	2.18	0.43
3:C:63:LEU:HB3	3:C:70:TYR:OH	2.19	0.43
1:A:401:ALA:H	1:A:402:SER:HA	1.78	0.43
2:B:191:MET:CE	2:B:238:ILE:HG12	2.49	0.43
1:A:25:GLY:O	1:A:30:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:ARG:NH1	4:D:58:TYR:OH	2.48	0.43
3:C:68:PRO:HA	4:D:99:MET:HE1	2.01	0.43
1:A:246:ASP:HB3	1:A:249:PHE:HD1	1.84	0.43
1:A:275:LEU:HD12	1:A:284:MET:CG	2.49	0.43
1:A:463:ILE:O	1:A:506:LEU:HA	2.19	0.43
3:C:74:VAL:HG11	4:D:103:ILE:HD13	2.00	0.43
3:C:81:PRO:HA	3:C:84:ILE:HB	2.00	0.43
1:A:246:ASP:HB3	1:A:249:PHE:CD1	2.54	0.43
1:A:284:MET:HB2	15:A:1074:HOH:O	2.19	0.43
2:B:233:LYS:HB2	3:C:114:PHE:HB3	2.00	0.42
1:A:237:VAL:HG21	1:A:370:ILE:CD1	2.47	0.42
1:A:275:LEU:HB2	15:A:1074:HOH:O	2.18	0.42
1:A:403:VAL:CG2	1:A:404:HIS:CE1	3.02	0.42
2:B:117:ASN:HB2	3:C:12:PHE:CD2	2.55	0.42
2:B:178:TYR:CD1	2:B:214:ARG:HB2	2.55	0.42
2:B:20:ASP:HB2	15:B:1080:HOH:O	2.18	0.42
3:C:137:ILE:O	3:C:140:GLU:HG2	2.18	0.42
1:A:362:THR:O	1:A:363:VAL:C	2.56	0.42
2:B:108:VAL:O	2:B:109:LYS:HB2	2.19	0.42
1:A:313:GLY:O	1:A:318:LYS:CD	2.67	0.42
1:A:456:LEU:HD11	1:A:526:GLN:CD	2.40	0.42
1:A:180:ASP:HA	1:A:236:MET:HG2	2.00	0.42
2:B:16:ILE:HG12	2:B:99:ILE:HB	2.02	0.42
1:A:255:THR:HG21	1:A:323:LEU:HD22	2.01	0.42
1:A:331:GLN:NE2	1:A:335:THR:OG1	2.53	0.42
1:A:588:ASP:O	1:A:592:GLY:N	2.36	0.42
2:B:132:LYS:HE2	2:B:197:ASP:O	2.20	0.42
1:A:10:THR:OG1	1:A:12:TYR:O	2.38	0.42
1:A:216:TYR:O	1:A:216:TYR:HD1	2.03	0.42
1:A:310:GLU:OE1	1:A:312:ARG:NH2	2.42	0.42
12:C:141:BHG:H6'1	15:C:1339:HOH:O	2.20	0.42
1:A:229:SER:HA	15:A:1257:HOH:O	2.18	0.42
1:A:263:LEU:HD22	6:A:1001:FAD:H6	2.02	0.41
1:A:304:MET:HE1	1:A:360:LEU:HA	2.02	0.41
1:A:304:MET:CE	1:A:361:PRO:HD3	2.50	0.41
1:A:484:ARG:HA	15:A:1070:HOH:O	2.19	0.41
4:D:63:THR:CB	4:D:64:PRO:HD3	2.50	0.41
1:A:268:CYS:HA	1:A:337:LEU:HD11	2.02	0.41
15:A:1269:HOH:O	3:C:15:LYS:HD2	2.21	0.41
1:A:23:VAL:HG21	1:A:34:ALA:HA	2.02	0.41
15:A:1271:HOH:O	2:B:108:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:VAL:HG21	4:D:99:MET:CE	2.50	0.41
4:D:44:THR:HG21	4:D:80:PHE:HB2	2.03	0.41
1:A:378:VAL:HG11	1:A:392:LEU:HD23	2.02	0.41
1:A:485:THR:HG22	15:A:1274:HOH:O	2.19	0.41
3:C:115:LYS:HG3	15:C:1096:HOH:O	2.21	0.41
1:A:76:TRP:CH2	1:A:97:HIS:CD2	3.08	0.41
1:A:534:GLN:HG2	1:A:585:SER:HB2	2.02	0.41
1:A:284:MET:HE1	1:A:300:VAL:HA	2.03	0.41
1:A:438:VAL:CG2	1:A:439:PRO:HD2	2.50	0.41
3:C:27:ILE:HG23	3:C:28:SER:N	2.36	0.41
1:A:170:THR:HB	1:A:172:TYR:CE1	2.55	0.40
1:A:61:GLN:CD	1:A:263:LEU:HD23	2.41	0.40
1:A:272:GLY:HA3	1:A:328:LEU:HD21	2.03	0.40
2:B:191:MET:HE2	2:B:238:ILE:HG12	2.04	0.40
2:B:92:ASP:OD1	2:B:94:SER:OG	2.33	0.40
1:A:319:ASP:N	1:A:319:ASP:OD1	2.55	0.40
1:A:553:ASP:N	1:A:553:ASP:OD1	2.48	0.40
2:B:218:ILE:O	2:B:219:MET:HB2	2.20	0.40
3:C:65:GLU:HG3	3:C:69:HIS:CE1	2.56	0.40
15:A:1270:HOH:O	2:B:137:GLN:HG2	2.22	0.40
1:A:248:GLU:OE2	1:A:583:THR:OG1	2.30	0.40
1:A:410:GLY:O	1:A:411:ALA:CB	2.63	0.40
2:B:131:LYS:HD2	2:B:142:TYR:CE2	2.57	0.40
1:A:149:VAL:O	1:A:150:ALA:C	2.60	0.40
1:A:80:PHE:CD1	1:A:96:ILE:HG22	2.57	0.40
3:C:106:LEU:HA	3:C:106:LEU:HD23	1.89	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	610/621 (98%)	551 (90%)	53 (9%)	6 (1%)	15	23
2	B	238/252 (94%)	216 (91%)	20 (8%)	2 (1%)	19	29
3	C	137/140 (98%)	130 (95%)	6 (4%)	1 (1%)	22	32
4	D	100/103 (97%)	94 (94%)	6 (6%)	0	100	100
All	All	1085/1116 (97%)	991 (91%)	85 (8%)	9 (1%)	19	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	SER
1	A	326	HIS
2	B	9	SER
1	A	480	ALA
3	C	78	SER
1	A	88	ASP
1	A	265	THR
1	A	257	ILE
1	A	352	VAL

### 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	497/506 (98%)	487 (98%)	10 (2%)	55	74
2	B	215/219 (98%)	210 (98%)	5 (2%)	50	70
3	C	118/119 (99%)	116 (98%)	2 (2%)	60	78
4	D	78/79 (99%)	76 (97%)	2 (3%)	46	66
All	All	908/923 (98%)	889 (98%)	19 (2%)	53	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	72	GLU

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Mol	Chain	Res	Type
1	A	130	PHE
1	A	219	THR
1	A	263	LEU
1	A	360	LEU
1	A	462	THR
1	A	544	GLU
1	A	570	GLN
1	A	612	SER
2	B	63	ARG
2	B	66	ARG
2	B	134	GLU
2	B	189	ARG
2	B	224	THR
3	C	50	SER
3	C	91	LEU
4	D	14	ARG
4	D	101	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	155	HIS
1	A	159	HIS
1	A	251	GLN
1	A	326	HIS
1	A	331	GLN
1	A	479	HIS
1	A	534	GLN
2	B	38	ASN
2	B	121	GLN
2	B	137	GLN
3	C	26	HIS
4	D	9	HIS
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 40 are unknown and 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	PEE	C	143	-	10,10,50	1.19	1 (10%)	9,9,55	1.41	2 (22%)
10	SF4	B	1003	2	0,12,12	0.00	-	-		
12	BHG	C	141	-	18,18,18	1.91	6 (33%)	23,23,23	0.86	0
14	PEE	D	105	-	22,22,50	0.92	1 (4%)	20,20,55	1.00	2 (10%)
7	MLI	A	1002	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	A	1001	1	51,58,58	2.71	21 (41%)	60,89,89	2.05	13 (21%)
11	F3S	B	1004	2	0,9,9	0.00	-	-		
13	HEM	C	142	3,4	26,48,50	1.92	4 (15%)	21,80,82	1.07	1 (4%)
9	FES	B	1002	2	0,4,4	0.00	-	-		

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
14	PEE	C	143	-	-	5/8/8/54	-
11	F3S	B	1004	2	-	-	0/3/3/3
10	SF4	B	1003	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BHG	C	141	-	1/1/5/5	4/9/29/29	0/1/1/1
14	PEE	D	105	-	-	13/18/18/54	-
7	MLI	A	1002	-	-	0/0/4/4	-
6	FAD	A	1001	1	-	9/30/50/50	0/6/6/6
9	FES	B	1002	2	-	-	0/1/1/1
13	HEM	C	142	3,4	-	0/6/50/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	FAD	C4-N3	6.12	1.43	1.33
13	C	142	HEM	CAB-C3B	-5.55	1.40	1.51
6	A	1001	FAD	C10-N1	5.52	1.40	1.33
6	A	1001	FAD	C4X-N5	5.29	1.40	1.33
13	C	142	HEM	CAC-C3C	-5.21	1.39	1.51
6	A	1001	FAD	PA-O2A	-5.16	1.31	1.55
6	A	1001	FAD	C4X-C10	5.04	1.43	1.38
6	A	1001	FAD	C9A-N10	4.85	1.45	1.38
12	C	141	BHG	O1-C1	4.85	1.48	1.40
6	A	1001	FAD	C1'-N10	4.73	1.53	1.48
6	A	1001	FAD	PA-O1A	-4.26	1.35	1.50
6	A	1001	FAD	C2A-N3A	3.97	1.38	1.32
6	A	1001	FAD	C2-N3	3.96	1.46	1.38
6	A	1001	FAD	C4-C4X	3.89	1.48	1.41
6	A	1001	FAD	C6-C7	3.58	1.46	1.37
6	A	1001	FAD	C4A-N3A	3.31	1.40	1.35
6	A	1001	FAD	C6-C5X	3.25	1.46	1.41
6	A	1001	FAD	C9-C8	2.96	1.45	1.37
12	C	141	BHG	O5-C1	2.92	1.49	1.41
14	C	143	PEE	C19-C18	-2.89	1.35	1.51
14	D	105	PEE	C19-C18	-2.73	1.36	1.51
6	A	1001	FAD	O4B-C1B	2.62	1.44	1.41
12	C	141	BHG	C3-C2	2.55	1.58	1.52
6	A	1001	FAD	C2A-N1A	2.54	1.38	1.33
6	A	1001	FAD	C5X-N5	2.43	1.39	1.35
6	A	1001	FAD	C8-C7	2.33	1.46	1.40
13	C	142	HEM	C1C-C2C	2.30	1.47	1.42
6	A	1001	FAD	C2B-C1B	-2.25	1.50	1.53
12	C	141	BHG	C4-C5	2.17	1.57	1.53
13	C	142	HEM	C4D-C3D	2.14	1.47	1.42
6	A	1001	FAD	C9-C9A	2.10	1.44	1.40
12	C	141	BHG	C4-C3	2.05	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	141	BHG	O1-C1'	2.01	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	FAD	C4X-N5-C5X	7.79	124.55	116.77
6	A	1001	FAD	N3A-C2A-N1A	-5.59	119.94	128.68
6	A	1001	FAD	C4-N3-C2	5.29	119.61	115.14
6	A	1001	FAD	C4-C4X-N5	4.43	123.66	118.60
6	A	1001	FAD	C4-C4X-C10	-4.26	117.13	119.95
13	C	142	HEM	C1B-C2B-C3B	-3.72	104.29	106.85
6	A	1001	FAD	C4X-C10-N10	-3.02	117.19	120.30
6	A	1001	FAD	P-O3P-PA	2.97	143.02	132.83
6	A	1001	FAD	C10-C4X-N5	-2.97	119.21	121.26
14	D	105	PEE	C20-C19-C18	2.89	129.09	114.42
6	A	1001	FAD	C4'-C3'-C2'	-2.86	107.40	113.36
14	C	143	PEE	C20-C19-C18	2.77	128.50	114.42
14	D	105	PEE	C19-C18-C17	2.72	128.24	114.42
6	A	1001	FAD	C4X-C4-N3	-2.71	119.73	123.43
14	C	143	PEE	C19-C18-C17	2.62	127.70	114.42
6	A	1001	FAD	C5'-C4'-C3'	2.34	116.72	112.20
6	A	1001	FAD	C1'-C2'-C3'	2.28	116.15	109.79
6	A	1001	FAD	C5X-C9A-N10	-2.07	116.22	117.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	141	BHG	C4

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	FAD	N10-C1'-C2'-O2'
6	A	1001	FAD	N10-C1'-C2'-C3'
6	A	1001	FAD	O4'-C4'-C5'-O5'
6	A	1001	FAD	C5'-O5'-P-O1P
6	A	1001	FAD	C5'-O5'-P-O2P
6	A	1001	FAD	PA-O3P-P-O5'
12	C	141	BHG	O1-C1'-C2'-C3'
14	D	105	PEE	C31-C32-C33-C34
14	C	143	PEE	C13-C14-C15-C16
14	C	143	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
14	D	105	PEE	C16-C17-C18-C19
14	D	105	PEE	C18-C19-C20-C21
12	C	141	BHG	C2'-C3'-C4'-C5'
14	D	105	PEE	C32-C33-C34-C35
6	A	1001	FAD	C3'-C4'-C5'-O5'
14	C	143	PEE	C15-C16-C17-C18
14	D	105	PEE	C13-C14-C15-C16
12	C	141	BHG	C3'-C4'-C5'-C6'
12	C	141	BHG	C1'-C2'-C3'-C4'
14	D	105	PEE	C34-C35-C36-C37
14	D	105	PEE	C11-C12-C13-C14
14	D	105	PEE	C12-C13-C14-C15
14	D	105	PEE	C38-C39-C40-C41
14	C	143	PEE	C12-C13-C14-C15
14	D	105	PEE	C17-C18-C19-C20
14	D	105	PEE	C35-C36-C37-C38
14	D	105	PEE	C33-C34-C35-C36
14	C	143	PEE	C14-C15-C16-C17
6	A	1001	FAD	O4B-C4B-C5B-O5B
14	D	105	PEE	C37-C38-C39-C40
6	A	1001	FAD	C5'-O5'-P-O3P

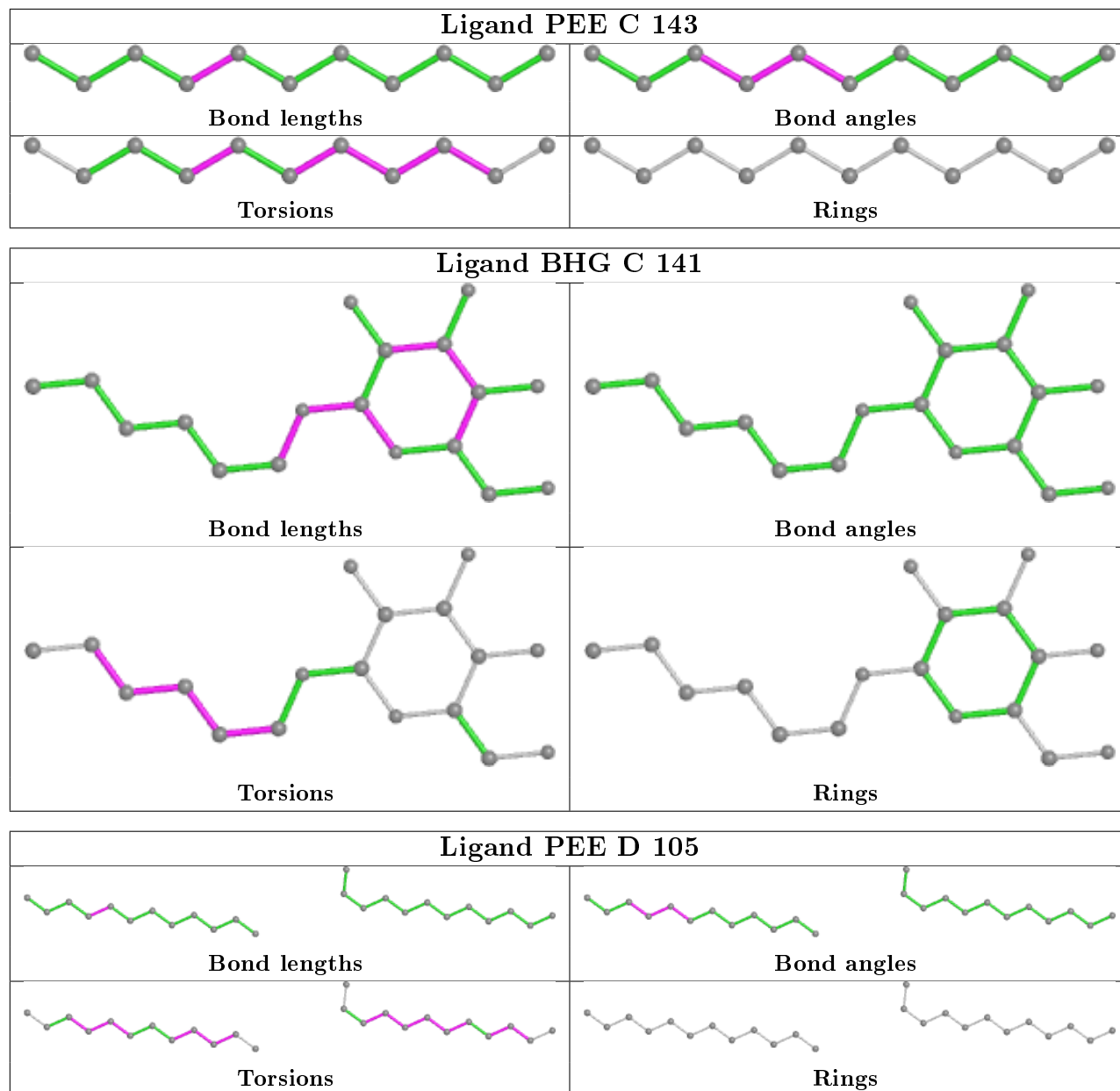
There are no ring outliers.

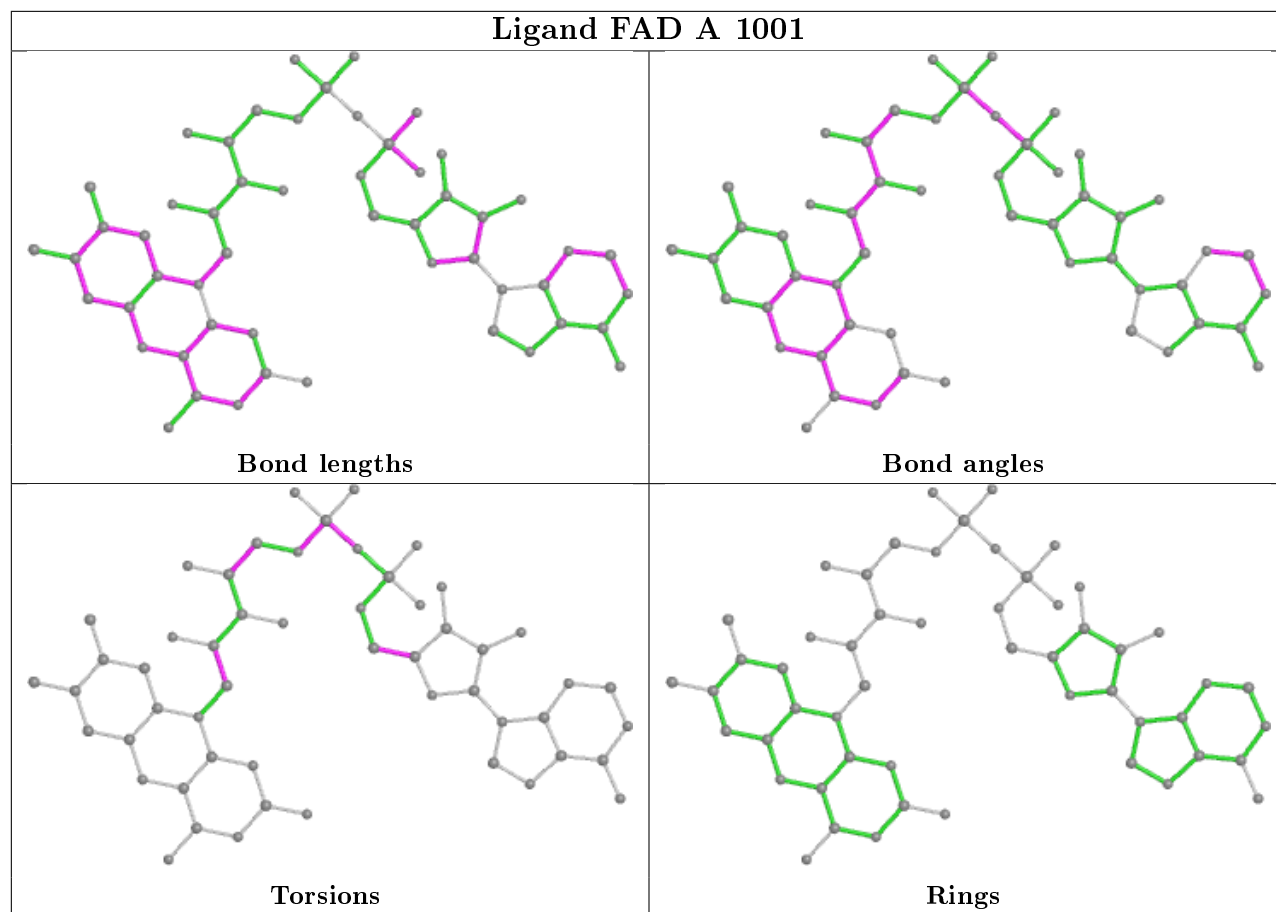
4 monomers are involved in 8 short contacts:

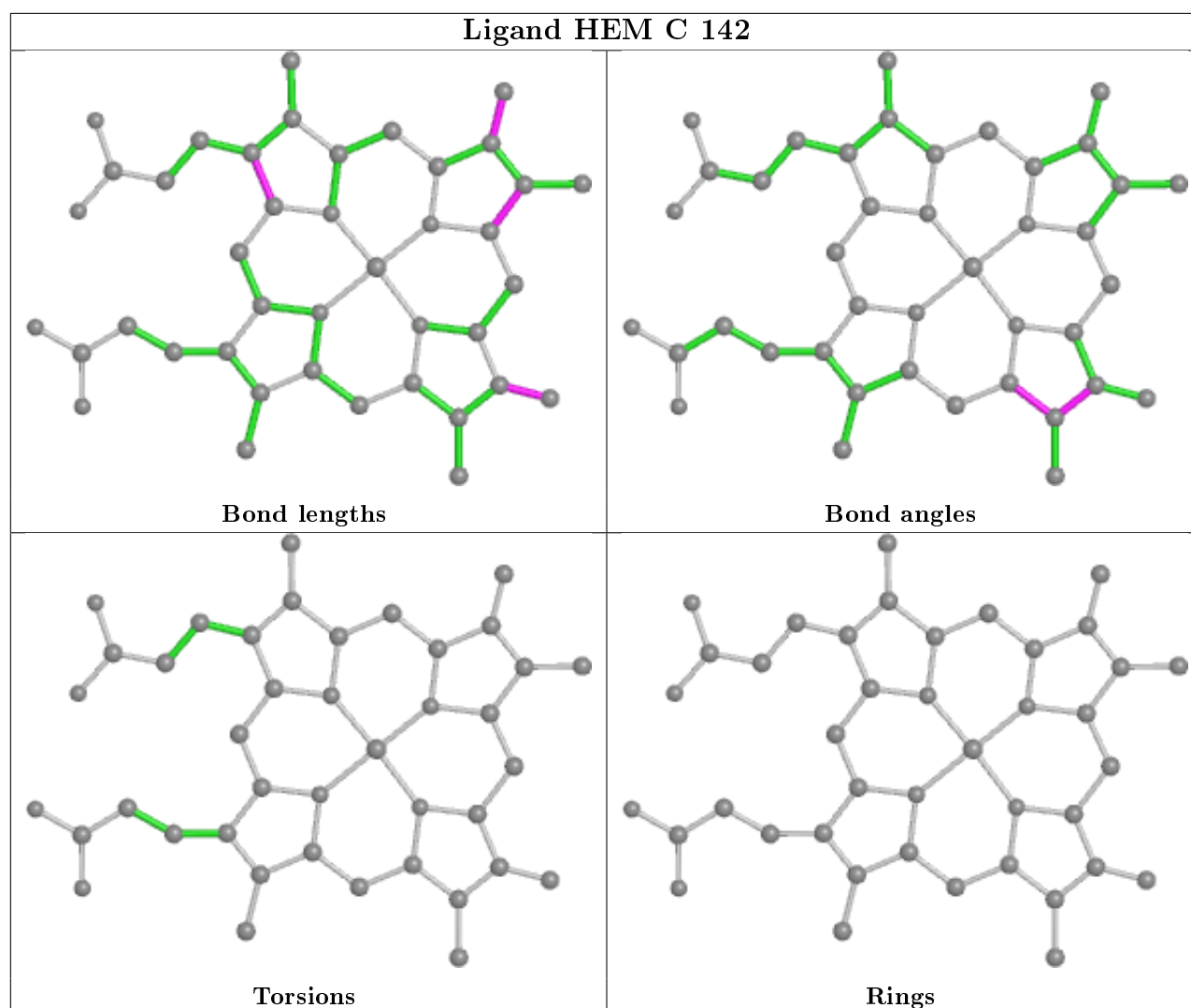
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	141	BHG	1	0
14	D	105	PEE	1	0
7	A	1002	MLI	4	0
6	A	1001	FAD	2	0

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	613/621 (98%)	-0.27	12 (1%) 65 63	34, 58, 92, 123	0
2	B	241/252 (95%)	-0.20	13 (5%) 25 24	34, 50, 86, 115	0
3	C	139/140 (99%)	-0.52	1 (0%) 87 86	35, 55, 82, 93	0
4	D	102/103 (99%)	-0.69	0 100 100	39, 53, 78, 96	0
All	All	1095/1116 (98%)	-0.33	26 (2%) 59 57	34, 56, 89, 123	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	8	THR	4.2
1	A	289	PRO	3.7
2	B	9	SER	3.7
2	B	247	GLU	3.6
2	B	11	ILE	3.0
1	A	9	SER	3.0
2	B	245	TYR	2.9
2	B	65	CYS	2.8
2	B	246	LYS	2.7
1	A	59	ALA	2.6
2	B	68	GLY	2.6
1	A	417	LEU	2.5
2	B	225	CYS	2.5
1	A	567	LEU	2.4
3	C	79	LEU	2.4
1	A	276	ILE	2.4
1	A	57	THR	2.4
1	A	14	VAL	2.3
2	B	85	CYS	2.3
2	B	159	ILE	2.3
1	A	226	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	VAL	2.1
1	A	55	SER	2.1
1	A	313	GLY	2.1
2	B	73	CYS	2.1
2	B	72	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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
8	UNL	A	1014	1/-	0.31	0.55	91,91,91,91	0
8	UNL	B	1005	6/-	0.37	0.87	154,157,158,158	0
8	UNL	A	1009	1/-	0.53	0.20	70,70,70,70	0
8	UNL	B	1008	1/-	0.59	0.25	74,74,74,74	0
8	UNL	A	1015	1/-	0.62	0.56	84,84,84,84	0
8	UNL	A	1005	1/-	0.67	0.13	73,73,73,73	0
8	UNL	B	1011	1/-	0.68	0.23	71,71,71,71	0
8	UNL	C	151	1/-	0.68	0.24	77,77,77,77	0
8	UNL	A	1010	1/-	0.70	0.33	63,63,63,63	0
8	UNL	A	1004	1/-	0.73	0.09	56,56,56,56	0
8	UNL	C	146	1/-	0.73	0.38	147,147,147,147	0
14	PEE	D	105	24/51	0.74	0.29	59,70,82,83	0
14	PEE	C	143	11/51	0.74	0.34	57,60,65,66	0
8	UNL	C	148	2/-	0.76	0.18	68,68,68,71	0
8	UNL	C	150	1/-	0.77	0.26	48,48,48,48	0
8	UNL	A	1008	1/-	0.78	0.65	63,63,63,63	0
8	UNL	B	1009	1/-	0.79	0.28	70,70,70,70	0
8	UNL	C	144	2/-	0.80	0.25	74,74,74,75	0

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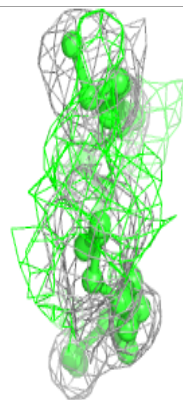
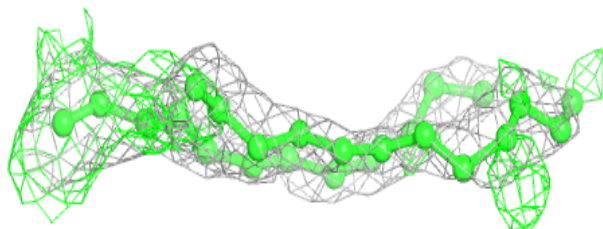
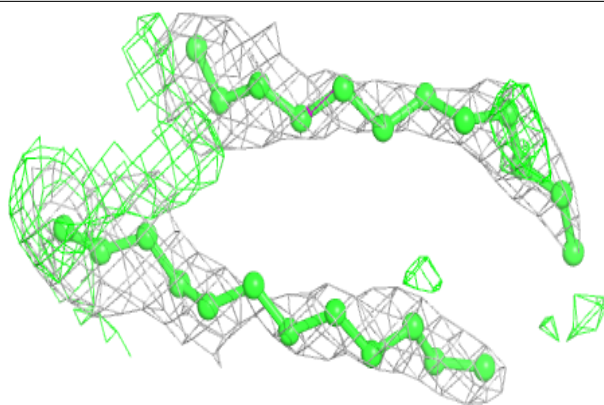
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	UNL	A	1012	1/-	0.81	0.20	49,49,49,49	0
8	UNL	B	1012	1/-	0.81	0.12	57,57,57,57	0
8	UNL	D	132	1/-	0.86	0.30	47,47,47,47	0
8	UNL	B	1007	1/-	0.87	0.22	58,58,58,58	0
8	UNL	D	110	1/-	0.87	0.23	79,79,79,79	0
8	UNL	B	1010	1/-	0.88	0.18	55,55,55,55	0
12	BHG	C	141	18/18	0.88	0.17	49,52,59,60	0
8	UNL	B	1013	1/-	0.89	0.20	63,63,63,63	0
8	UNL	A	1006	1/-	0.90	0.18	69,69,69,69	0
8	UNL	A	1017	1/-	0.92	0.30	56,56,56,56	0
8	UNL	C	152	1/-	0.92	0.28	53,53,53,53	0
8	UNL	A	1003	1/-	0.92	0.32	58,58,58,58	0
8	UNL	B	1014	1/-	0.92	0.39	65,65,65,65	0
8	UNL	D	125	1/-	0.93	0.14	50,50,50,50	0
8	UNL	A	1013	1/-	0.93	0.04	61,61,61,61	0
5	K	B	253	1/1	0.94	0.06	91,91,91,91	0
8	UNL	A	1007	1/-	0.94	0.12	60,60,60,60	0
8	UNL	A	1011	1/-	0.95	0.10	68,68,68,68	0
8	UNL	D	122	1/-	0.95	0.14	54,54,54,54	0
7	MLI	A	1002	7/7	0.96	0.21	59,60,62,62	0
8	UNL	D	142	1/-	0.96	0.11	54,54,54,54	0
8	UNL	C	145	1/-	0.97	0.24	43,43,43,43	0
8	UNL	B	1006	1/-	0.97	0.07	41,41,41,41	0
13	HEM	C	142	41/43	0.97	0.12	41,52,59,60	0
8	UNL	A	1016	1/-	0.97	0.09	43,43,43,43	0
8	UNL	C	149	1/-	0.97	0.22	54,54,54,54	0
6	FAD	A	1001	53/53	0.98	0.24	35,46,54,58	0
8	UNL	D	109	1/-	0.98	0.19	53,53,53,53	0
10	SF4	B	1003	8/8	0.99	0.17	39,46,50,51	0
8	UNL	C	147	1/-	0.99	0.21	49,49,49,49	0
9	FES	B	1002	4/4	0.99	0.18	38,44,48,52	0
11	F3S	B	1004	7/7	0.99	0.14	31,36,37,43	0
5	K	A	622	1/1	0.99	0.14	50,50,50,50	0

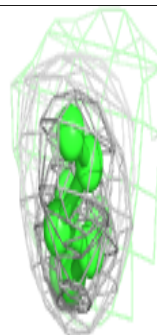
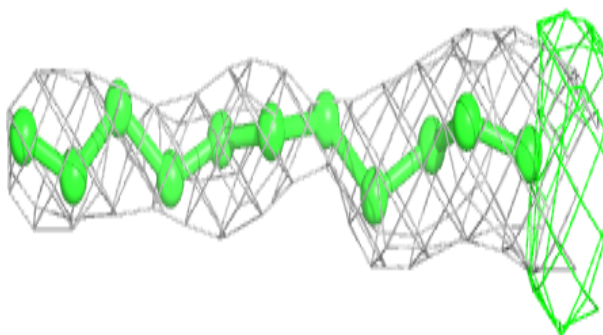
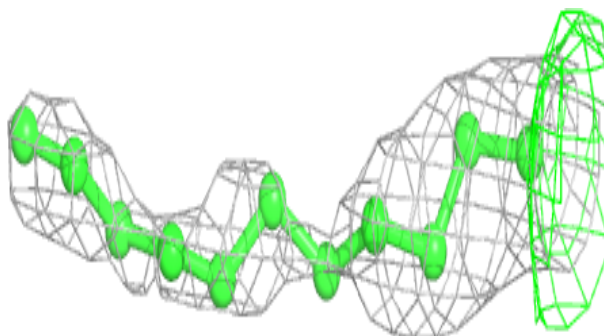
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PEE D 105:**

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

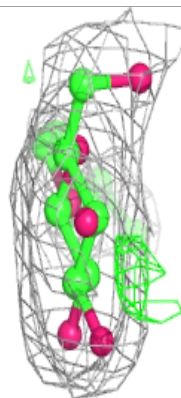
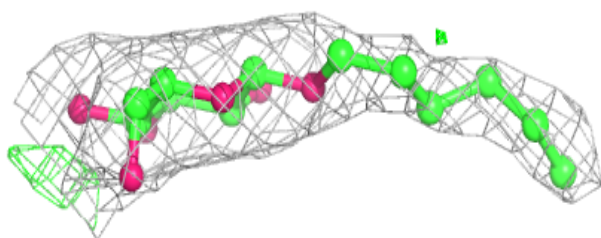
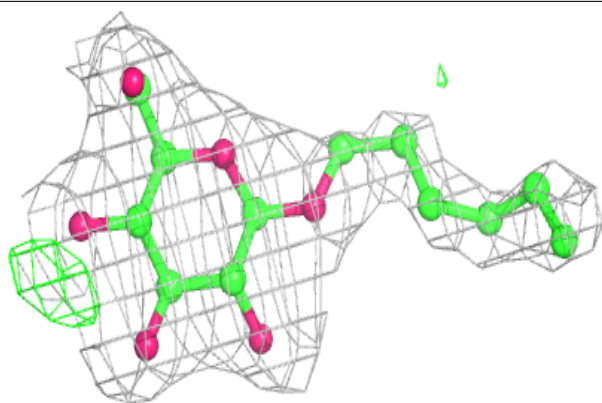
**Electron density around PEE C 143:**

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

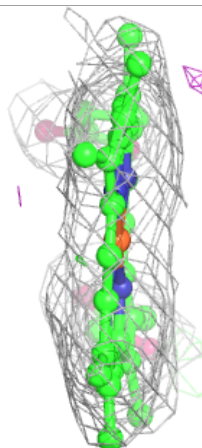
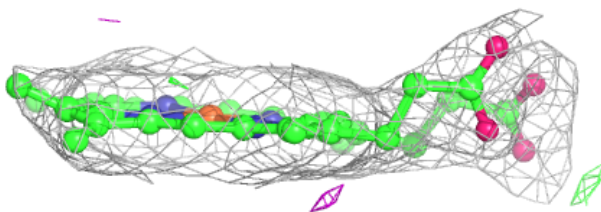
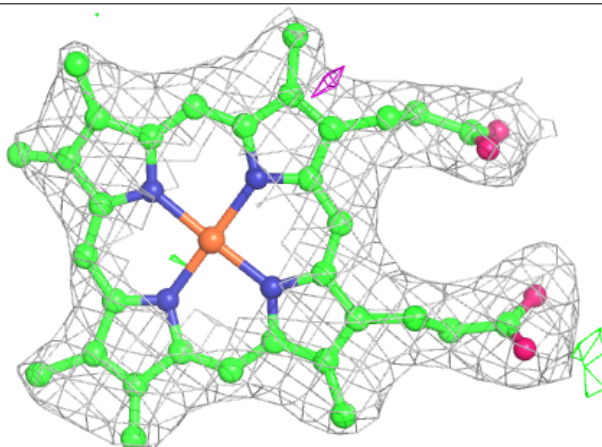


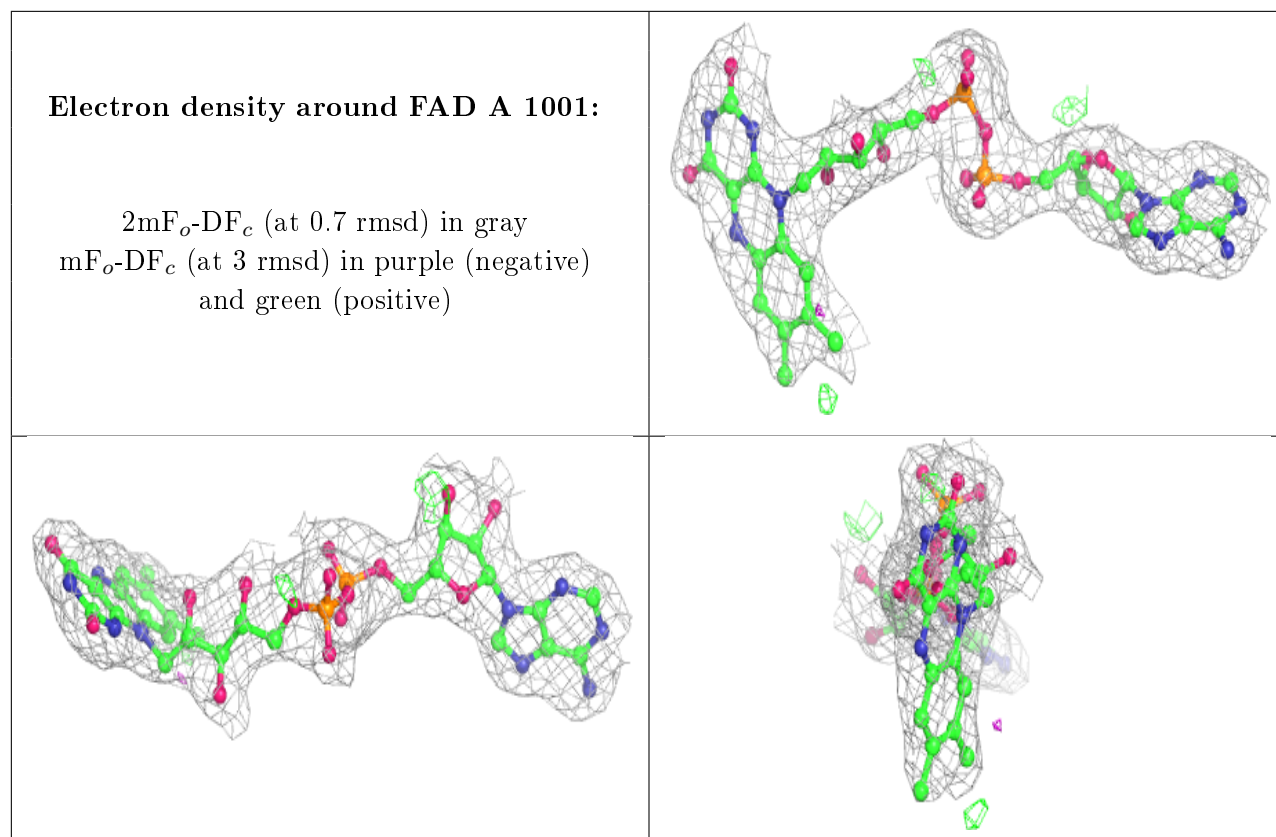
**Electron density around BHG C 141:**

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

**Electron density around HEM 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.