



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2021 – 05:34 PM JST

PDB ID : 7C3B  
Title : Ferredoxin reductase in carbazole 1,9a-dioxygenase (FAD apo form)  
Authors : Ashikawa, Y.; Fujimoto, Z.; Nojiri, H.  
Deposited on : 2020-05-11  
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 : 2.18  
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) : 2.18

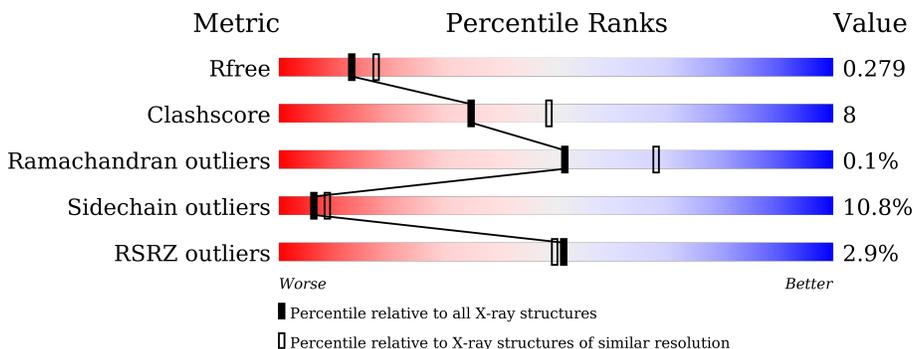
# 1 Overall quality at a glance

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 of 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	335	
1	B	335	
1	C	335	

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
4	CL	B	405	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7657 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.

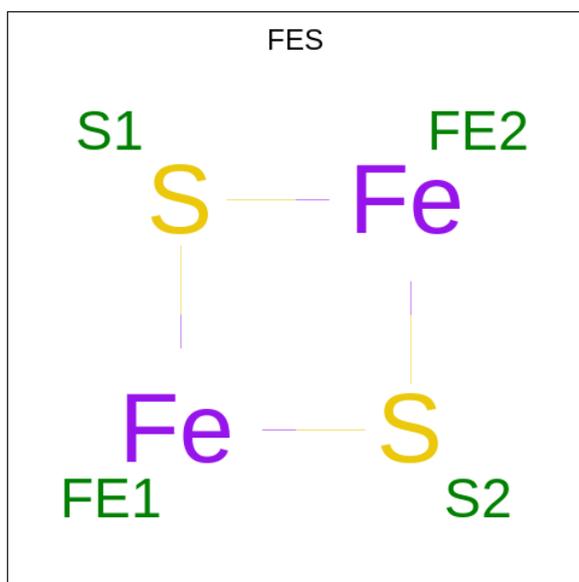
- Molecule 1 is a protein called Ferredoxin reductase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2504	1599	439	451	15	0	0	0
1	B	306	2361	1512	408	426	15	0	0	0
1	C	334	2584	1648	451	470	15	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q84II0
A	-4	HIS	-	expression tag	UNP Q84II0
A	-3	HIS	-	expression tag	UNP Q84II0
A	-2	HIS	-	expression tag	UNP Q84II0
A	-1	HIS	-	expression tag	UNP Q84II0
A	0	HIS	-	expression tag	UNP Q84II0
A	1	HIS	-	expression tag	UNP Q84II0
B	-5	MET	-	expression tag	UNP Q84II0
B	-4	HIS	-	expression tag	UNP Q84II0
B	-3	HIS	-	expression tag	UNP Q84II0
B	-2	HIS	-	expression tag	UNP Q84II0
B	-1	HIS	-	expression tag	UNP Q84II0
B	0	HIS	-	expression tag	UNP Q84II0
B	1	HIS	-	expression tag	UNP Q84II0
C	-5	MET	-	expression tag	UNP Q84II0
C	-4	HIS	-	expression tag	UNP Q84II0
C	-3	HIS	-	expression tag	UNP Q84II0
C	-2	HIS	-	expression tag	UNP Q84II0
C	-1	HIS	-	expression tag	UNP Q84II0
C	0	HIS	-	expression tag	UNP Q84II0
C	1	HIS	-	expression tag	UNP Q84II0

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



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

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		
3	B	1	Total	I	0	0
			1	1		
3	C	1	Total	I	0	0
			1	1		

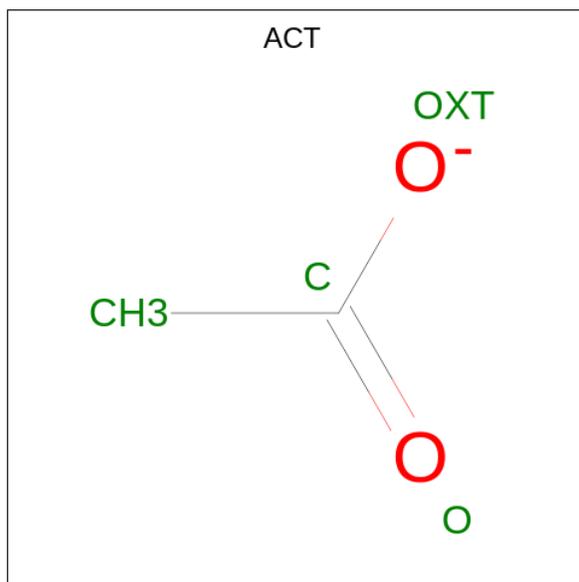
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Cl	0	0
			7	7		
4	B	6	Total	Cl	0	0
			6	6		
4	C	5	Total	Cl	0	0
			5	5		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ni 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0

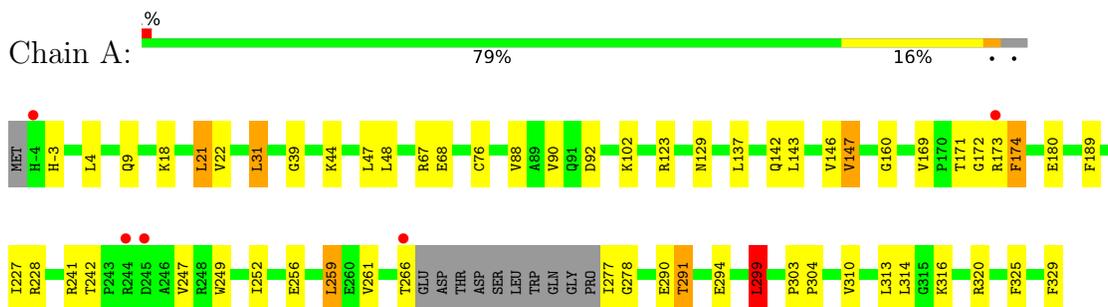
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	77	Total O 77 77	0	0
7	B	36	Total O 36 36	0	0
7	C	57	Total O 57 57	0	0

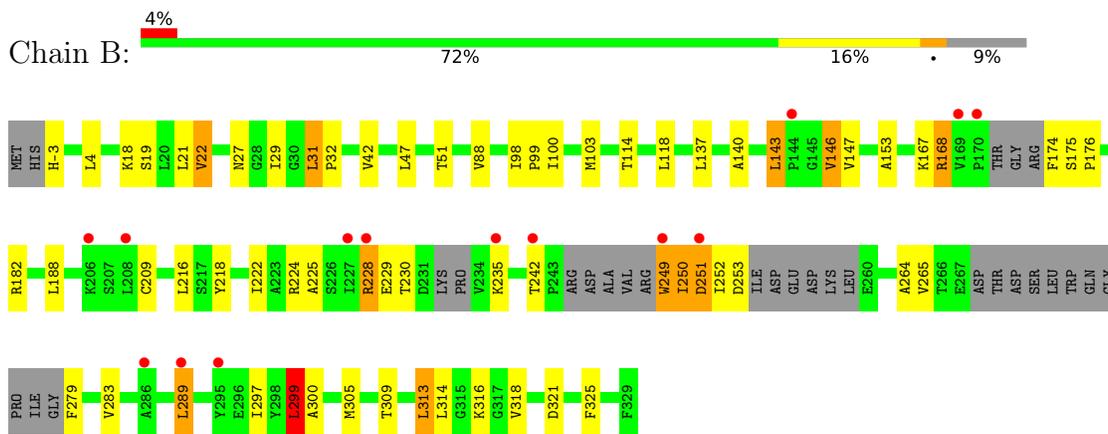
### 3 Residue-property plots [i](#)

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.

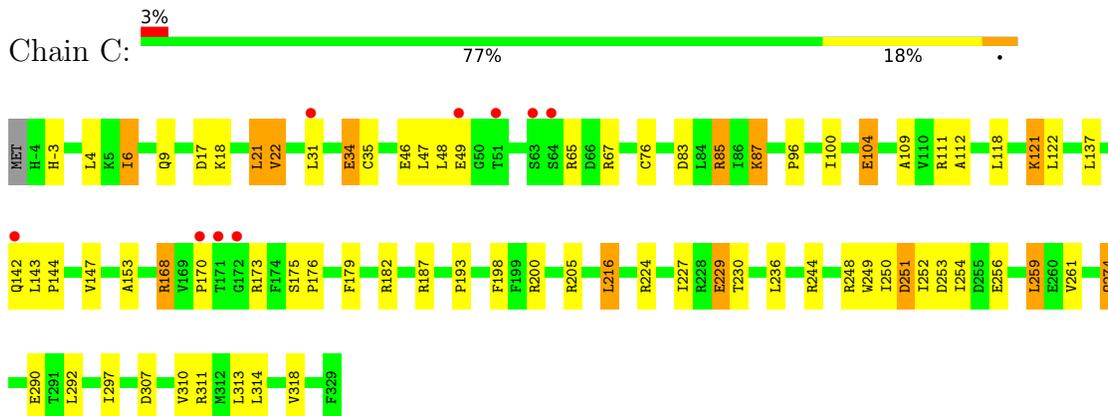
- Molecule 1: Ferredoxin reductase component of carbazole



- Molecule 1: Ferredoxin reductase component of carbazole



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.92Å 161.92Å 79.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.07 – 2.40 43.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.07-2.40) 99.7 (43.07-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.227 , 0.281 0.228 , 0.279	Depositor DCC
$R_{free}$ test set	2106 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.0	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: ACT, NI, CL, FES, IOD

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	0.42	0/2565	0.64	3/3476 (0.1%)
1	B	0.39	0/2416	0.61	1/3270 (0.0%)
1	C	0.40	0/2649	0.63	1/3594 (0.0%)
All	All	0.40	0/7630	0.63	5/10340 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	299	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	299	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	228	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	31	LEU	CA-CB-CG	5.02	126.84	115.30

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	2504	0	2502	36	0
1	B	2361	0	2347	40	0
1	C	2584	0	2568	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	A	7	0	0	1	0
4	B	6	0	0	3	0
4	C	5	0	0	0	0
5	A	1	0	0	0	0
6	C	4	0	3	1	0
7	A	77	0	0	3	0
7	B	36	0	0	1	0
7	C	57	0	0	0	0
All	All	7657	0	7420	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:O	1:B:224:ARG:NH2	2.14	0.81
1:A:171:THR:HG23	1:A:172:GLY:H	1.47	0.80
1:C:6:ILE:HG12	1:C:9:GLN:HB2	1.66	0.78
1:C:259:LEU:HD13	1:C:261:VAL:HG23	1.67	0.77
1:B:224:ARG:HH12	1:B:252:ILE:HG22	1.52	0.73
1:A:146:VAL:O	1:A:146:VAL:HG13	1.88	0.72
1:C:104:GLU:H	1:C:104:GLU:CD	1.94	0.71
1:C:227:ILE:HD11	1:C:259:LEU:HG	1.75	0.68
1:B:249:TRP:HB3	1:B:250:ILE:HD12	1.77	0.67
1:B:140:ALA:HA	1:B:188:LEU:HD23	1.77	0.66
1:B:114:THR:O	1:B:168:ARG:NH1	2.28	0.65
1:A:172:GLY:O	1:A:173:ARG:HG2	1.97	0.65
1:A:171:THR:HG23	1:A:172:GLY:N	2.12	0.64
1:B:167:LYS:O	1:B:182:ARG:NH2	2.31	0.63
1:B:31:LEU:HD22	1:B:88:VAL:HG11	1.79	0.62
1:C:216:LEU:HD11	1:C:252:ILE:HD11	1.82	0.60
1:C:249:TRP:NE1	1:C:261:VAL:HG11	2.16	0.60
1:A:277:ILE:HG22	1:A:278:GLY:H	1.67	0.60
1:C:229:GLU:HG3	1:C:230:THR:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:HD12	1:C:76:CYS:HB3	1.84	0.59
1:A:241:ARG:HA	1:A:266:THR:HB	1.84	0.59
1:A:310:VAL:HG21	7:A:565:HOH:O	2.02	0.59
1:A:291:THR:O	1:A:294:GLU:HG2	2.03	0.57
1:B:209:CYS:SG	1:B:222:ILE:HG22	2.44	0.57
1:B:143:LEU:HD22	1:B:174:PHE:HE1	1.70	0.56
1:C:274:GLN:H	1:C:274:GLN:CD	2.08	0.56
1:B:249:TRP:HA	1:B:249:TRP:CE3	2.41	0.56
1:C:6:ILE:CG1	1:C:9:GLN:HB2	2.34	0.55
1:C:307:ASP:HB3	1:C:311:ARG:NH2	2.21	0.55
1:B:299:LEU:HD13	1:B:325:PHE:HB3	1.87	0.55
1:A:18:LYS:HB2	1:A:22:VAL:CG2	2.37	0.55
1:B:225:ALA:HA	1:B:228:ARG:HD2	1.89	0.55
1:C:34:GLU:CG	1:C:35:CYS:N	2.70	0.54
1:C:18:LYS:HB2	1:C:22:VAL:HG22	1.89	0.54
1:A:249:TRP:CZ2	1:A:261:VAL:HG21	2.44	0.53
1:A:143:LEU:HB2	1:A:146:VAL:HG11	1.91	0.53
1:C:118:LEU:HD13	1:C:168:ARG:HD3	1.90	0.53
1:C:250:ILE:HD12	1:C:250:ILE:H	1.74	0.53
1:B:250:ILE:HD12	1:B:250:ILE:N	2.24	0.53
1:B:264:ALA:CB	1:B:283:VAL:HG21	2.39	0.53
1:B:249:TRP:HA	1:B:249:TRP:HE3	1.74	0.52
1:A:249:TRP:HA	1:A:252:ILE:HG12	1.94	0.50
1:C:49:GLU:HB3	1:C:85:ARG:HB3	1.93	0.50
1:C:297:ILE:HD12	1:C:318:VAL:HG11	1.94	0.50
1:A:172:GLY:C	1:A:173:ARG:CG	2.80	0.50
1:C:111:ARG:NH2	1:C:251:ASP:O	2.34	0.50
1:B:218:TYR:CD2	1:B:300:ALA:HB2	2.47	0.49
1:C:249:TRP:CE2	1:C:261:VAL:CG1	2.95	0.49
1:C:153:ALA:O	1:C:224:ARG:NH2	2.45	0.49
1:B:289:LEU:O	1:B:316:LYS:HD2	2.13	0.49
1:B:18:LYS:HE2	4:B:405:CL:CL	2.50	0.49
1:B:137:LEU:HB3	1:B:147:VAL:CG1	2.44	0.48
1:A:142:GLN:HG2	1:A:180:GLU:OE2	2.14	0.48
1:B:297:ILE:HD12	1:B:318:VAL:HG11	1.96	0.48
1:C:143:LEU:HA	1:C:144:PRO:HD2	1.75	0.48
1:A:171:THR:O	1:A:172:GLY:C	2.50	0.48
1:A:143:LEU:HB2	1:A:146:VAL:CG1	2.44	0.47
1:B:250:ILE:O	1:B:251:ASP:CG	2.52	0.47
1:C:229:GLU:CG	1:C:230:THR:N	2.76	0.47
1:B:140:ALA:HB3	1:B:143:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:HG22	1:B:251:ASP:N	2.30	0.47
1:B:143:LEU:HB2	1:B:146:VAL:CG1	2.45	0.46
1:A:299:LEU:HD13	1:A:325:PHE:HB3	1.96	0.46
1:A:123:ARG:NH2	7:A:504:HOH:O	2.48	0.46
1:A:227:ILE:HD11	1:A:259:LEU:HD23	1.97	0.46
1:A:303:PRO:HB2	1:A:304:PRO:HD3	1.98	0.46
1:C:112:ALA:HA	1:C:118:LEU:HD12	1.98	0.46
1:C:249:TRP:NE1	1:C:261:VAL:CG1	2.78	0.45
1:C:96:PRO:HB3	1:C:100:ILE:HD13	1.98	0.45
1:C:249:TRP:CZ2	1:C:261:VAL:HG13	2.51	0.45
1:C:170:PRO:HD3	1:C:179:PHE:HZ	1.81	0.45
1:C:168:ARG:O	1:C:182:ARG:NH2	2.34	0.45
1:A:21:LEU:HD12	1:A:76:CYS:HB3	1.99	0.45
1:B:224:ARG:HH11	1:B:253:ASP:HB2	1.80	0.45
1:C:249:TRP:CE2	1:C:261:VAL:HG13	2.51	0.45
1:C:104:GLU:CD	1:C:104:GLU:N	2.65	0.45
1:A:249:TRP:CD1	1:A:252:ILE:HD11	2.52	0.44
1:C:198:PHE:O	1:C:200:ARG:NH1	2.50	0.44
1:A:249:TRP:HD1	1:A:252:ILE:HD11	1.82	0.44
1:B:29:ILE:HD12	7:B:514:HOH:O	2.16	0.44
1:B:265:VAL:HG13	1:B:279:PHE:HB2	2.00	0.44
1:B:250:ILE:O	1:B:251:ASP:CB	2.66	0.44
1:C:224:ARG:NH1	1:C:253:ASP:HB3	2.33	0.44
1:B:175:SER:HB2	1:B:176:PRO:HD2	2.00	0.44
1:C:254:ILE:HA	3:C:402:IOD:I	2.87	0.44
1:A:39:GLY:HA3	1:A:329:PHE:CD1	2.53	0.43
1:B:250:ILE:O	1:B:251:ASP:OD1	2.36	0.43
1:B:250:ILE:N	1:B:250:ILE:CD1	2.82	0.43
1:A:249:TRP:HB2	1:A:256:GLU:HG3	1.99	0.43
1:B:18:LYS:HE3	1:B:22:VAL:HG22	2.00	0.43
1:C:143:LEU:HA	1:C:143:LEU:HD23	1.92	0.43
1:B:167:LYS:HE3	4:B:408:CL:CL	2.56	0.43
1:B:250:ILE:CD1	1:B:250:ILE:H	2.30	0.43
1:B:309:THR:O	1:B:313:LEU:HD22	2.19	0.43
1:C:216:LEU:CD1	1:C:252:ILE:HD11	2.47	0.43
1:A:172:GLY:O	1:A:173:ARG:CG	2.63	0.43
1:C:249:TRP:CD1	1:C:261:VAL:HG11	2.54	0.43
1:C:175:SER:HB2	1:C:176:PRO:HD2	2.01	0.42
1:B:264:ALA:HB1	1:B:283:VAL:HG21	2.00	0.42
1:B:98:ILE:HA	1:B:99:PRO:HD2	1.93	0.42
1:C:111:ARG:HH21	1:C:251:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CD1	1:A:174:PHE:N	2.88	0.42
1:A:9:GLN:OE1	1:A:90:VAL:HG11	2.20	0.42
1:A:102:LYS:HE2	1:A:189:PHE:HB3	2.01	0.42
1:C:6:ILE:H	1:C:6:ILE:HD13	1.85	0.42
1:C:307:ASP:HA	1:C:310:VAL:HG22	2.02	0.42
1:C:249:TRP:CE2	1:C:261:VAL:HG11	2.55	0.41
1:A:259:LEU:HD12	1:A:261:VAL:CG2	2.50	0.41
1:B:31:LEU:HD13	1:B:32:PRO:HD2	2.02	0.41
1:C:100:ILE:HD11	1:C:193:PRO:O	2.20	0.41
1:A:169:VAL:HG22	7:A:552:HOH:O	2.19	0.41
1:A:171:THR:CG2	1:A:172:GLY:H	2.18	0.41
1:B:18:LYS:CE	4:B:405:CL:CL	3.05	0.41
1:C:17:ASP:OD1	1:C:17:ASP:N	2.47	0.41
1:C:46:GLU:HB3	1:C:87:LYS:HG2	2.01	0.41
1:A:18:LYS:NZ	4:A:405:CL:CL	2.91	0.41
1:C:-3:HIS:HB3	6:C:408:ACT:H1	2.02	0.41
1:A:171:THR:CG2	1:A:172:GLY:N	2.79	0.41
1:C:109:ALA:HB3	1:C:121:LYS:HB3	2.03	0.41
1:C:137:LEU:HB3	1:C:147:VAL:CG1	2.51	0.40
1:A:137:LEU:HB3	1:A:147:VAL:HG23	2.03	0.40
1:B:19:SER:OG	1:B:22:VAL:HG12	2.21	0.40
1:A:123:ARG:HA	1:A:160:GLY:O	2.21	0.40
1:C:248:ARG:O	1:C:251:ASP:OD1	2.40	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	320/335 (96%)	301 (94%)	19 (6%)	0	100 100
1	B	294/335 (88%)	281 (96%)	12 (4%)	1 (0%)	41 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	332/335 (99%)	316 (95%)	16 (5%)	0	100	100
All	All	946/1005 (94%)	898 (95%)	47 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/275 (96%)	241 (91%)	24 (9%)	9	14
1	B	250/275 (91%)	221 (88%)	29 (12%)	5	7
1	C	274/275 (100%)	242 (88%)	32 (12%)	5	7
All	All	789/825 (96%)	704 (89%)	85 (11%)	6	9

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	A	4	LEU
1	A	21	LEU
1	A	31	LEU
1	A	44	LYS
1	A	47	LEU
1	A	48	LEU
1	A	67	ARG
1	A	68	GLU
1	A	88	VAL
1	A	92	ASP
1	A	129	ASN
1	A	147	VAL
1	A	174	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	242	THR
1	A	247	VAL
1	A	259	LEU
1	A	290	GLU
1	A	291	THR
1	A	299	LEU
1	A	313	LEU
1	A	314	LEU
1	A	316	LYS
1	A	320	ARG
1	B	-3	HIS
1	B	4	LEU
1	B	21	LEU
1	B	22	VAL
1	B	27	ASN
1	B	31	LEU
1	B	42	VAL
1	B	47	LEU
1	B	51	THR
1	B	100	ILE
1	B	103	MET
1	B	118	LEU
1	B	143	LEU
1	B	146	VAL
1	B	168	ARG
1	B	216	LEU
1	B	228	ARG
1	B	229	GLU
1	B	230	THR
1	B	235	LYS
1	B	242	THR
1	B	249	TRP
1	B	250	ILE
1	B	251	ASP
1	B	299	LEU
1	B	305	MET
1	B	313	LEU
1	B	314	LEU
1	B	321	ASP
1	C	4	LEU
1	C	6	ILE
1	C	21	LEU

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Mol	Chain	Res	Type
1	C	22	VAL
1	C	31	LEU
1	C	34	GLU
1	C	47	LEU
1	C	48	LEU
1	C	65	ARG
1	C	67	ARG
1	C	83	ASP
1	C	85	ARG
1	C	87	LYS
1	C	104	GLU
1	C	121	LYS
1	C	122	LEU
1	C	142	GLN
1	C	168	ARG
1	C	173	ARG
1	C	187	ARG
1	C	216	LEU
1	C	229	GLU
1	C	236	LEU
1	C	244	ARG
1	C	251	ASP
1	C	256	GLU
1	C	259	LEU
1	C	274	GLN
1	C	290	GLU
1	C	292	LEU
1	C	313	LEU
1	C	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	C	27	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 22 are monoatomic - leaving 4 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
2	FES	A	401	1	0,4,4	0.00	-	-		
2	FES	C	401	1	0,4,4	0.00	-	-		
2	FES	B	401	1	0,4,4	0.00	-	-		
6	ACT	C	408	-	1,3,3	2.31	1 (100%)	0,3,3	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
2	FES	A	401	1	-	-	0/1/1/1
2	FES	C	401	1	-	-	0/1/1/1
2	FES	B	401	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	408	ACT	CH3-C	2.31	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	408	ACT	1	0

## 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	324/335 (96%)	0.07	5 (1%) 73 72	42, 61, 97, 119	0
1	B	306/335 (91%)	0.22	14 (4%) 32 31	52, 70, 101, 117	0
1	C	334/335 (99%)	0.19	9 (2%) 54 52	48, 69, 105, 131	0
All	All	964/1005 (95%)	0.16	28 (2%) 51 50	42, 68, 102, 131	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	SER	6.2
1	C	49	GLU	5.1
1	B	169	VAL	4.8
1	B	144	PRO	4.5
1	A	244	ARG	4.3
1	B	208	LEU	4.2
1	B	251	ASP	3.9
1	B	227	ILE	3.4
1	C	171	THR	3.4
1	B	242	THR	3.2
1	C	172	GLY	3.1
1	B	249	TRP	2.8
1	A	266	THR	2.6
1	B	170	PRO	2.6
1	A	173	ARG	2.5
1	C	51	THR	2.5
1	C	170	PRO	2.4
1	C	31	LEU	2.4
1	B	286	ALA	2.4
1	B	235	LYS	2.3
1	B	228	ARG	2.3
1	A	245	ASP	2.3
1	B	289	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	206	LYS	2.1
1	C	142	GLN	2.1
1	C	63	SER	2.1
1	A	-4	HIS	2.0
1	B	295	TYR	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(Å <sup>2</sup> )	Q<0.9
4	CL	A	406	1/1	0.90	0.22	44,44,44,44	0
4	CL	A	408	1/1	0.90	0.25	46,46,46,46	0
4	CL	C	405	1/1	0.90	0.19	48,48,48,48	0
4	CL	C	407	1/1	0.90	0.18	46,46,46,46	0
4	CL	C	404	1/1	0.94	0.07	47,47,47,47	0
4	CL	B	404	1/1	0.94	0.12	47,47,47,47	0
4	CL	B	407	1/1	0.94	0.10	48,48,48,48	0
4	CL	A	404	1/1	0.95	0.13	48,48,48,48	0
4	CL	B	406	1/1	0.95	0.16	48,48,48,48	0
4	CL	C	406	1/1	0.96	0.17	47,47,47,47	0
4	CL	A	407	1/1	0.96	0.09	44,44,44,44	0
4	CL	A	405	1/1	0.97	0.23	44,44,44,44	0
4	CL	C	403	1/1	0.97	0.27	44,44,44,44	0
4	CL	A	409	1/1	0.97	0.29	45,45,45,45	0
6	ACT	C	408	4/4	0.97	0.07	47,47,49,50	0
4	CL	B	405	1/1	0.98	0.14	45,45,45,45	0
4	CL	B	408	1/1	0.99	0.24	41,41,41,41	0
2	FES	A	401	4/4	0.99	0.16	41,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	403	1/1	0.99	0.38	32,32,32,32	0
2	FES	B	401	4/4	0.99	0.15	40,43,43,45	0
2	FES	C	401	4/4	0.99	0.10	44,44,46,47	0
3	IOD	B	402	1/1	0.99	0.14	51,51,51,51	0
3	IOD	C	402	1/1	0.99	0.10	52,52,52,52	0
3	IOD	A	402	1/1	1.00	0.02	49,49,49,49	0
5	NI	A	410	1/1	1.00	0.13	46,46,46,46	0
4	CL	A	403	1/1	1.00	0.33	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.