



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:01 PM UTC

PDB ID : 7C3B / pdb_00007c3b
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

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
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

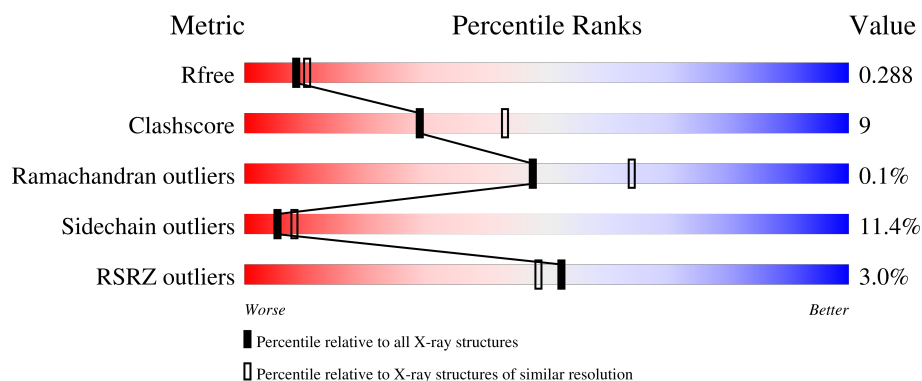
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 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	3% 78% 17% • •
1	B	335	4% 71% 17% • 9%
1	C	335	% 76% 19% 5%

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
1	A	324	Total	C	N	O	S	0	0	0
			2504	1599	439	451	15			
1	B	306	Total	C	N	O	S	0	0	0
			2361	1512	408	426	15			
1	C	334	Total	C	N	O	S	0	0	0
			2584	1648	451	470	15			

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 (CCD ID: FES) (formula: Fe₂S₂).



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 (CCD ID: 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		

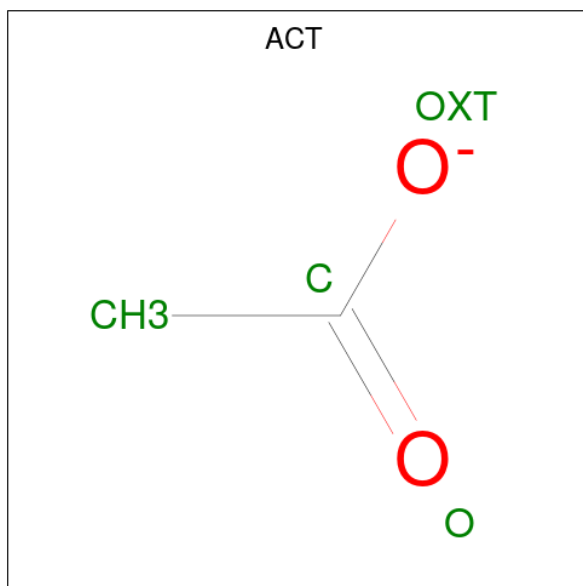
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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 (CCD ID: NI) (formula: Ni).

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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

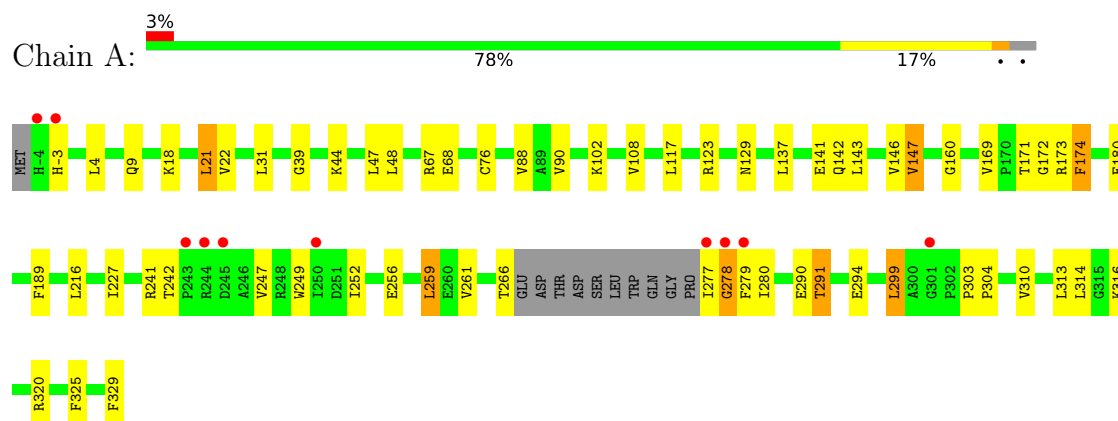
- Molecule 7 is water.

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

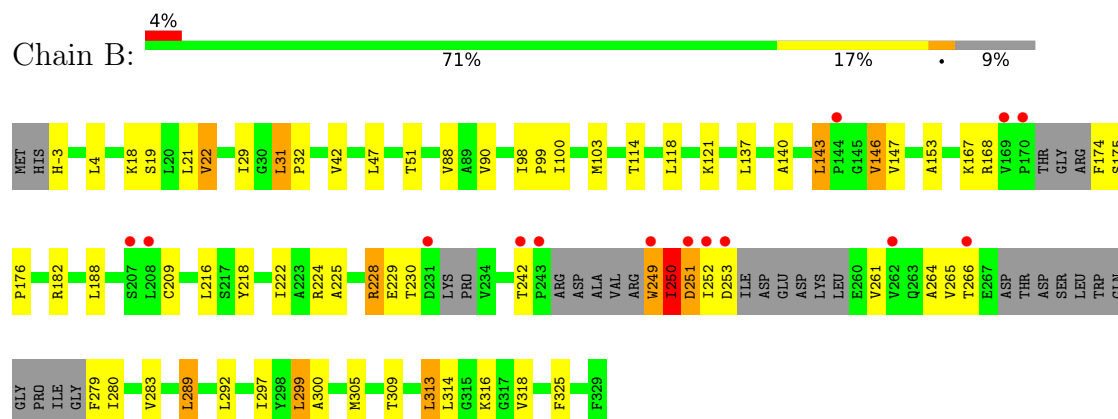
3 Residue-property plots [i](#)

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.

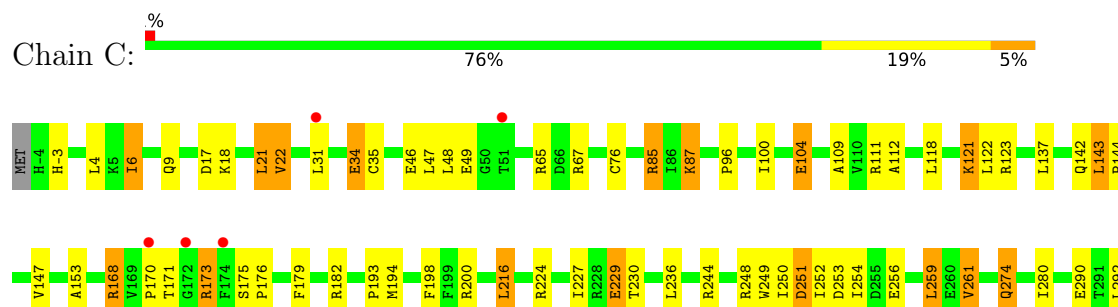
- Molecule 1: Ferredoxin reductase component of carbazole



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L297	M305	V306	D307	V310	R311	M312	L313	L314	G315	K316	G317	V318	F329
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4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	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) 99.6 (43.07-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.227 , 0.281 (Not available) , 0.288	Depositor DCC
R_{free} test set	2106 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7657	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, NI, ACT, CL, 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	0.55	0/2565	0.78	3/3476 (0.1%)
1	B	0.52	0/2416	0.76	1/3270 (0.0%)
1	C	0.54	0/2649	0.81	4/3594 (0.1%)
All	All	0.54	0/7630	0.78	8/10340 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	PHE	N-CA-C	8.03	119.15	108.07
1	C	143	LEU	CA-C-N	6.97	128.56	119.84
1	C	143	LEU	C-N-CA	6.97	128.56	119.84
1	B	250	ILE	N-CA-C	-6.70	102.64	110.21
1	C	173	ARG	N-CA-C	-6.50	100.26	108.45
1	C	171	THR	N-CA-C	5.91	118.39	110.35
1	A	280	ILE	N-CA-C	5.87	121.54	109.34
1	A	278	GLY	N-CA-C	-5.25	104.82	112.17

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	2504	0	2502	37	0
1	B	2361	0	2347	40	0
1	C	2584	0	2568	52	0
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	129	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 9.

All (129) 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:C:104:GLU:H	1:C:104:GLU:CD	1.94	0.76
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: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:274:GLN:H	1:C:274:GLN:CD	2.08	0.61
1:C:216:LEU:HD11	1:C:252:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:172:GLY:C	1:A:173:ARG:CG	2.80	0.54
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:A:171:THR:O	1:A:172:GLY:C	2.50	0.52
1:B:249:TRP:HA	1:B:249:TRP:HE3	1.74	0.52
1:B:250:ILE:O	1:B:251:ASP:CG	2.52	0.52
1:C:312:MET:HE2	1:C:316:LYS:HG3	1.93	0.50
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:280:ILE:HG21	1:C:305:MET:HE2	1.93	0.50
1:C:297:ILE:HD12	1:C:318:VAL:HG11	1.94	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:C:104:GLU:CD	1:C:104:GLU:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:LEU:HB2	1:A:146:VAL:CG1	2.44	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
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:A:172:GLY:C	1:A:173:ARG:HG3	2.42	0.44
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: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:B:250:ILE:O	1:B:251:ASP:CB	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:312:MET:HE2	1:C:316:LYS:CG	2.51	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:C:194:MET:HE3	1:C:194:MET:HB3	1.98	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/335 (96%)	301 (94%)	19 (6%)	0	100	100
1	B	294/335 (88%)	281 (96%)	12 (4%)	1 (0%)	36	50
1	C	332/335 (99%)	316 (95%)	16 (5%)	0	100	100
All	All	946/1005 (94%)	898 (95%)	47 (5%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	LEU

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	265/275 (96%)	238 (90%)	27 (10%)	7	11
1	B	250/275 (91%)	219 (88%)	31 (12%)	4	6
1	C	274/275 (100%)	242 (88%)	32 (12%)	5	7
All	All	789/825 (96%)	699 (89%)	90 (11%)	5	8

All (90) 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

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Mol	Chain	Res	Type
1	A	88	VAL
1	A	108	VAL
1	A	117	LEU
1	A	129	ASN
1	A	141	GLU
1	A	147	VAL
1	A	174	PHE
1	A	216	LEU
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	31	LEU
1	B	42	VAL
1	B	47	LEU
1	B	51	THR
1	B	90	VAL
1	B	100	ILE
1	B	103	MET
1	B	118	LEU
1	B	121	LYS
1	B	143	LEU
1	B	146	VAL
1	B	216	LEU
1	B	228	ARG
1	B	229	GLU
1	B	230	THR
1	B	242	THR
1	B	249	TRP
1	B	250	ILE
1	B	251	ASP
1	B	261	VAL

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Mol	Chain	Res	Type
1	B	266	THR
1	B	280	ILE
1	B	292	LEU
1	B	299	LEU
1	B	305	MET
1	B	313	LEU
1	B	314	LEU
1	C	4	LEU
1	C	6	ILE
1	C	21	LEU
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	85	ARG
1	C	87	LYS
1	C	104	GLU
1	C	121	LYS
1	C	122	LEU
1	C	123	ARG
1	C	142	GLN
1	C	168	ARG
1	C	173	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	261	VAL
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	9	GLN
1	A	27	ASN
1	A	73	HIS
1	B	73	HIS
1	B	281	HIS
1	C	1	HIS
1	C	9	GLN
1	C	27	ASN
1	C	281	HIS
1	C	282	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	401	1	0,4,4	-	-	-		
2	FES	C	401	1	0,4,4	-	-	-		
2	FES	A	401	1	0,4,4	-	-	-		
6	ACT	C	408	-	3,3,3	0.92	0	3,3,3	1.18	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
2	FES	B	401	1	-	-	0/1/1/1
2	FES	C	401	1	-	-	0/1/1/1
2	FES	A	401	1	-	-	0/1/1/1

There are no bond length outliers.

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, 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	324/335 (96%)	0.25	10 (3%)	51	47	42, 61, 97, 119	0
1	B	306/335 (91%)	0.46	14 (4%)	37	33	52, 70, 101, 117	0
1	C	334/335 (99%)	0.33	5 (1%)	72	68	48, 69, 105, 131	0
All	All	964/1005 (95%)	0.34	29 (3%)	52	48	42, 68, 102, 131	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	ILE	3.5
1	A	244	ARG	2.9
1	A	277	ILE	2.9
1	A	-4	HIS	2.8
1	A	250	ILE	2.7
1	B	169	VAL	2.7
1	B	243	PRO	2.7
1	C	170	PRO	2.7
1	B	249	TRP	2.5
1	B	251	ASP	2.5
1	C	31	LEU	2.5
1	B	208	LEU	2.5
1	B	253	ASP	2.5
1	A	279	PHE	2.4
1	C	174	PHE	2.3
1	B	170	PRO	2.3
1	C	172	GLY	2.3
1	B	231	ASP	2.3
1	A	278	GLY	2.3
1	B	262	VAL	2.2
1	B	242	THR	2.2
1	A	245	ASP	2.2
1	B	266	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	207	SER	2.1
1	B	144	PRO	2.1
1	A	243	PRO	2.1
1	A	301	GLY	2.1
1	C	51	THR	2.1
1	A	-3	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	C	407	1/1	0.90	0.07	46,46,46,46	0
6	ACT	C	408	4/4	0.90	0.09	47,47,49,50	0
4	CL	A	406	1/1	0.93	0.10	44,44,44,44	0
4	CL	A	408	1/1	0.93	0.08	46,46,46,46	0
4	CL	C	406	1/1	0.94	0.07	47,47,47,47	0
4	CL	B	407	1/1	0.94	0.07	48,48,48,48	0
4	CL	C	404	1/1	0.94	0.08	47,47,47,47	0
4	CL	C	405	1/1	0.95	0.06	48,48,48,48	0
4	CL	B	404	1/1	0.96	0.06	47,47,47,47	0
4	CL	A	407	1/1	0.97	0.05	44,44,44,44	0
4	CL	B	408	1/1	0.97	0.13	41,41,41,41	0
4	CL	A	404	1/1	0.97	0.05	48,48,48,48	0
4	CL	A	409	1/1	0.97	0.12	45,45,45,45	0
3	IOD	C	402	1/1	0.97	0.21	52,52,52,52	0
4	CL	B	405	1/1	0.97	0.06	45,45,45,45	0
4	CL	B	406	1/1	0.97	0.07	48,48,48,48	0
4	CL	C	403	1/1	0.98	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	405	1/1	0.98	0.11	44,44,44,44	0
3	IOD	B	402	1/1	0.98	0.26	51,51,51,51	0
4	CL	B	403	1/1	0.99	0.20	32,32,32,32	0
3	IOD	A	402	1/1	0.99	0.13	49,49,49,49	0
2	FES	A	401	4/4	0.99	0.04	41,42,42,42	0
2	FES	B	401	4/4	0.99	0.03	40,43,43,45	0
4	CL	A	403	1/1	0.99	0.18	32,32,32,32	0
2	FES	C	401	4/4	0.99	0.04	44,44,46,47	0
5	NI	A	410	1/1	1.00	0.02	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.