



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:57 am GMT

PDB ID : 4NBG  
Title : Oxygenase with Gln282 replaced by Tyr and ferredoxin complex of carbazole  
1,9a-dioxygenase  
Authors : Ashikawa, Y.; Usami, Y.; Inoue, K.; Nojiri, H.  
Deposited on : 2013-10-23  
Resolution : 1.85 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

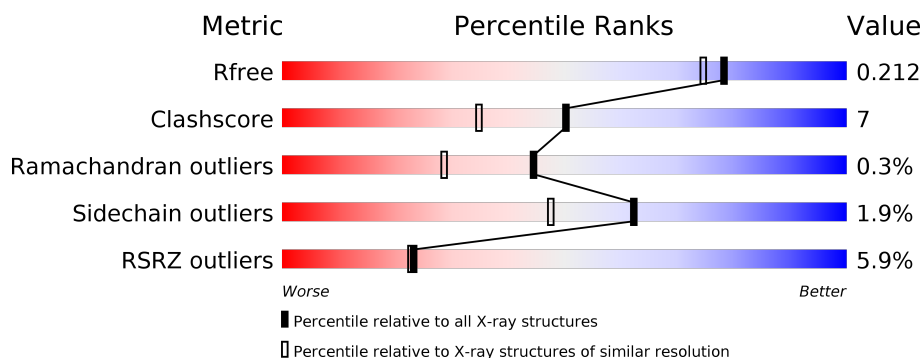
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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. 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	392	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	392	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	C	392	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
2	D	115	<div> <div>28%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>.</div> <div>10%</div> </div> </div>
2	E	115	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
2	F	115	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12957 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3131	2003	533	582	13			
1	B	388	Total	C	N	O	S	0	0	0
			3131	2003	533	582	13			
1	C	388	Total	C	N	O	S	0	0	0
			3131	2003	533	582	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	TYR	GLN	ENGINEERED MUTATION	UNP Q84II6
A	385	LEU	-	EXPRESSION TAG	UNP Q84II6
A	386	GLU	-	EXPRESSION TAG	UNP Q84II6
A	387	HIS	-	EXPRESSION TAG	UNP Q84II6
A	388	HIS	-	EXPRESSION TAG	UNP Q84II6
A	389	HIS	-	EXPRESSION TAG	UNP Q84II6
A	390	HIS	-	EXPRESSION TAG	UNP Q84II6
A	391	HIS	-	EXPRESSION TAG	UNP Q84II6
A	392	HIS	-	EXPRESSION TAG	UNP Q84II6
B	282	TYR	GLN	ENGINEERED MUTATION	UNP Q84II6
B	385	LEU	-	EXPRESSION TAG	UNP Q84II6
B	386	GLU	-	EXPRESSION TAG	UNP Q84II6
B	387	HIS	-	EXPRESSION TAG	UNP Q84II6
B	388	HIS	-	EXPRESSION TAG	UNP Q84II6
B	389	HIS	-	EXPRESSION TAG	UNP Q84II6
B	390	HIS	-	EXPRESSION TAG	UNP Q84II6
B	391	HIS	-	EXPRESSION TAG	UNP Q84II6
B	392	HIS	-	EXPRESSION TAG	UNP Q84II6
C	282	TYR	GLN	ENGINEERED MUTATION	UNP Q84II6
C	385	LEU	-	EXPRESSION TAG	UNP Q84II6
C	386	GLU	-	EXPRESSION TAG	UNP Q84II6
C	387	HIS	-	EXPRESSION TAG	UNP Q84II6
C	388	HIS	-	EXPRESSION TAG	UNP Q84II6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	389	HIS	-	EXPRESSION TAG	UNP Q84II6
C	390	HIS	-	EXPRESSION TAG	UNP Q84II6
C	391	HIS	-	EXPRESSION TAG	UNP Q84II6
C	392	HIS	-	EXPRESSION TAG	UNP Q84II6

- Molecule 2 is a protein called Ferredoxin CarAc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			
2	E	112	Total	C	N	O	S	0	0	0
			844	529	148	160	7			
2	F	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			

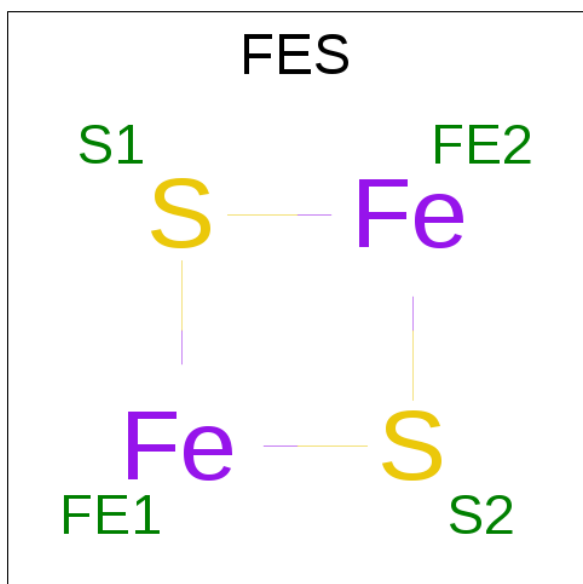
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	EXPRESSION TAG	UNP Q8GI16
D	109	GLU	-	EXPRESSION TAG	UNP Q8GI16
D	110	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	111	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	112	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	113	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	114	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	115	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	108	LEU	-	EXPRESSION TAG	UNP Q8GI16
E	109	GLU	-	EXPRESSION TAG	UNP Q8GI16
E	110	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	111	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	112	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	113	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	114	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	115	HIS	-	EXPRESSION TAG	UNP Q8GI16
F	108	LEU	-	EXPRESSION TAG	UNP Q8GI16
F	109	GLU	-	EXPRESSION TAG	UNP Q8GI16
F	110	HIS	-	EXPRESSION TAG	UNP Q8GI16
F	111	HIS	-	EXPRESSION TAG	UNP Q8GI16
F	112	HIS	-	EXPRESSION TAG	UNP Q8GI16
F	113	HIS	-	EXPRESSION TAG	UNP Q8GI16
F	114	HIS	-	EXPRESSION TAG	UNP Q8GI16
F	115	HIS	-	EXPRESSION TAG	UNP Q8GI16

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

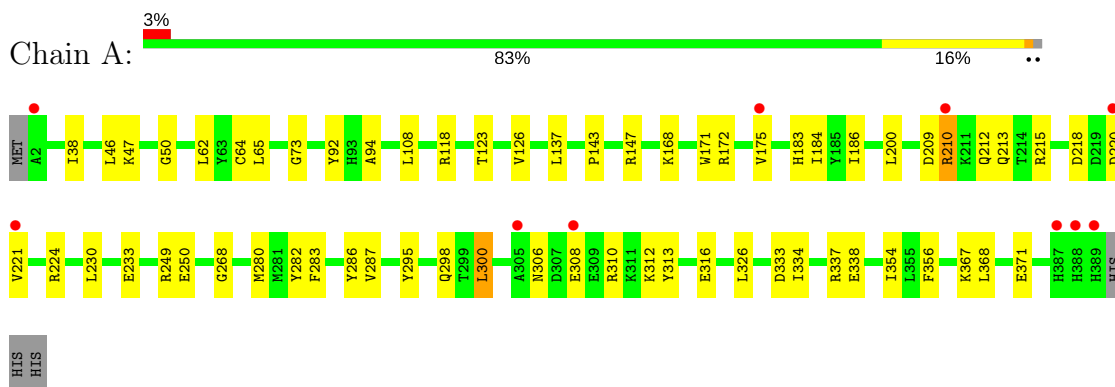
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	338	Total 338	O 338	0	0
5	B	308	Total 308	O 308	0	0
5	C	347	Total 347	O 347	0	0
5	D	35	Total 35	O 35	0	0
5	E	61	Total 61	O 61	0	0
5	F	68	Total 68	O 68	0	0

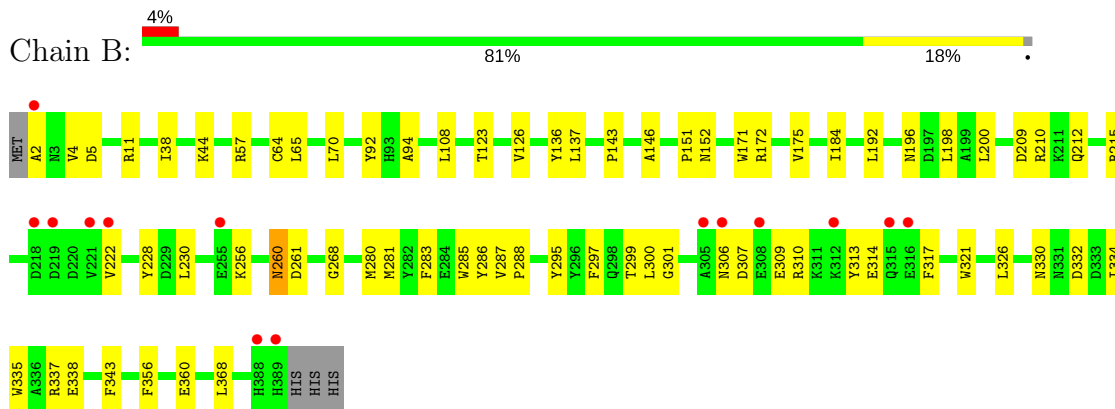
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

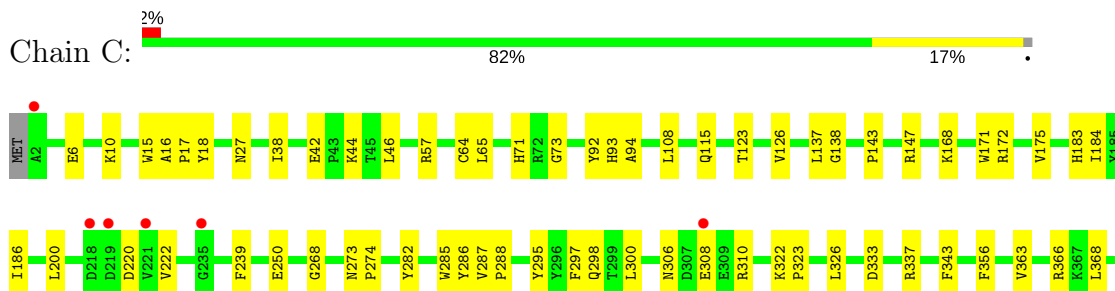
- Molecule 1: Terminal oxygenase component of carbazole

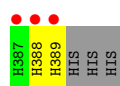


- Molecule 1: Terminal oxygenase component of carbazole



- Molecule 1: Terminal oxygenase component of carbazole

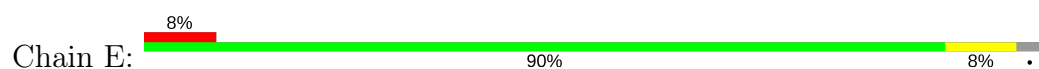




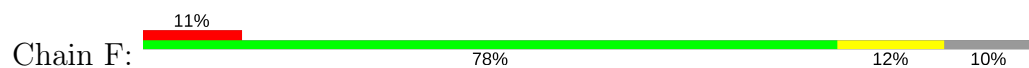
• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.35Å 89.94Å 105.26Å 90.00° 104.23° 90.00°	Depositor
Resolution (Å)	39.22 – 1.85 39.22 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.22-1.85) 99.9 (39.22-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 1.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.213 0.188 , 0.212	Depositor DCC
$R_{free}$ test set	7485 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/3217	0.61	0/4368
1	B	0.29	0/3217	0.58	0/4368
1	C	0.29	0/3217	0.59	0/4368
2	D	0.28	0/784	0.58	0/1066
2	E	0.27	0/865	0.57	0/1176
2	F	0.30	0/784	0.59	0/1066
All	All	0.29	0/12084	0.59	0/16412

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

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	3131	0	3031	40	0
1	B	3131	0	3031	51	0
1	C	3131	0	3031	38	0
2	D	768	0	745	13	0
2	E	844	0	805	5	0
2	F	768	0	745	11	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	A	338	0	0	3	0
5	B	308	0	0	2	1
5	C	347	0	0	1	1
5	D	35	0	0	1	0
5	E	61	0	0	0	0
5	F	68	0	0	2	0
All	All	12957	0	11388	154	1

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 7.

All (154) 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:280:MET:HE1	1:A:300:LEU:HD13	1.57	0.86
1:C:6:GLU:O	1:C:10:LYS:HG2	1.79	0.83
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.65	0.79
1:B:281:MET:HE3	1:B:283:PHE:HZ	1.50	0.76
2:D:7:LYS:HG2	2:D:101:TYR:CE1	2.24	0.73
1:A:118:ARG:HD2	5:A:760:HOH:O	1.88	0.72
2:D:7:LYS:HG2	2:D:101:TYR:HE1	1.57	0.69
1:C:220:ASP:OD1	1:C:222:VAL:HG22	1.93	0.68
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.74	0.68
2:F:4:ILE:HG23	2:F:5:TRP:H	1.60	0.67
1:A:280:MET:HE1	1:A:300:LEU:CD1	2.27	0.65
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.79	0.64
1:B:38:ILE:HG23	1:B:57:ARG:HH21	1.63	0.64
1:A:210:ARG:HA	1:A:213:GLN:HG2	1.79	0.64
1:B:11:ARG:HH21	1:C:388:HIS:CD2	2.16	0.63
1:C:333:ASP:O	1:C:337:ARG:HG3	2.00	0.61
1:A:280:MET:HE3	1:A:313:TYR:HE1	1.65	0.61
1:B:360:GLU:HG3	5:B:685:HOH:O	1.99	0.61
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.83	0.60
1:B:300:LEU:HD23	1:B:301:GLY:N	2.17	0.60
2:F:4:ILE:HG12	2:F:5:TRP:N	2.15	0.60
2:E:90:VAL:HG23	2:E:107:LYS:HB3	1.83	0.60
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.84	0.60
2:D:92:GLU:OE2	2:D:107:LYS:HD3	2.01	0.59
1:B:260:ASN:ND2	1:B:260:ASN:H	2.01	0.58
1:B:260:ASN:H	1:B:260:ASN:HD22	1.52	0.58
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.86	0.57
1:B:310:ARG:O	1:B:314:GLU:HG3	2.04	0.57
2:E:10:ALA:HB3	2:E:13:ASP:OD2	2.05	0.57
2:F:4:ILE:HG23	2:F:5:TRP:N	2.20	0.57
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.35	0.56
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.88	0.55
1:A:280:MET:CE	1:A:313:TYR:HE1	2.20	0.55
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.89	0.55
1:B:281:MET:HE3	1:B:283:PHE:CZ	2.38	0.54
1:C:306:ASN:O	1:C:310:ARG:HG3	2.07	0.54
1:A:220:ASP:OD1	1:A:221:VAL:N	2.40	0.54
1:A:312:LYS:O	1:A:316:GLU:HG3	2.07	0.54
1:A:38:ILE:HD13	1:A:62:LEU:HD22	1.90	0.53
2:D:4:ILE:HG22	2:D:5:TRP:N	2.22	0.53
2:D:19:ILE:HG21	2:D:54:SER:HA	1.91	0.53
1:C:168:LYS:HE2	5:C:810:HOH:O	2.09	0.53
1:B:260:ASN:N	1:B:260:ASN:HD22	2.05	0.53
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.44	0.53
1:C:184:ILE:HD11	1:C:200:LEU:CD1	2.38	0.52
2:E:47:THR:HG23	2:E:88:LEU:HD23	1.91	0.52
1:C:42:GLU:HG2	1:C:44:LYS:HE3	1.90	0.52
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.40	0.52
1:C:282:TYR:HE1	1:C:326:LEU:HD21	1.75	0.52
1:C:38:ILE:HG23	1:C:57:ARG:HH21	1.75	0.52
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.40	0.51
1:B:283:PHE:HB2	1:B:299:THR:OG1	2.11	0.51
2:F:4:ILE:HG12	2:F:5:TRP:H	1.76	0.51
1:A:220:ASP:HB2	1:A:224:ARG:HB2	1.93	0.50
1:B:317:PHE:HA	1:B:321:TRP:HB2	1.93	0.50
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.94	0.50
2:D:61:ASP:O	2:D:74:VAL:HG22	2.12	0.50
1:B:334:ILE:O	1:B:338:GLU:HG3	2.12	0.49
1:B:215:ARG:HB3	1:B:228:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:HG12	1:B:222:VAL:O	2.14	0.48
2:F:90:VAL:HG13	5:F:364:HOH:O	2.14	0.48
1:B:280:MET:HB3	1:B:300:LEU:HD21	1.95	0.48
1:B:334:ILE:O	1:B:337:ARG:HG2	2.14	0.48
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.49	0.47
1:B:215:ARG:HB2	1:B:230:LEU:HD11	1.96	0.47
2:F:19:ILE:HG21	2:F:54:SER:HA	1.97	0.47
1:B:196:ASN:O	1:B:256:LYS:HD2	2.15	0.47
2:F:96:LYS:HG3	5:F:331:HOH:O	2.15	0.47
1:A:47:LYS:HE2	5:A:818:HOH:O	2.14	0.47
1:A:334:ILE:O	1:A:338:GLU:HG3	2.14	0.47
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.30	0.47
1:A:298:GLN:HB3	1:A:326:LEU:HD22	1.96	0.47
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.50	0.47
1:B:64:CYS:HB2	1:B:126:VAL:HG21	1.97	0.46
1:B:260:ASN:HD22	1:B:261:ASP:N	2.13	0.46
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.51	0.46
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.50	0.46
1:A:282:TYR:HE1	1:A:326:LEU:HD21	1.80	0.46
2:F:106:LYS:O	2:F:107:LYS:HB2	2.16	0.46
1:C:282:TYR:CE1	1:C:326:LEU:HD21	2.50	0.46
1:A:47:LYS:HE3	1:A:50:GLY:HA2	1.98	0.46
1:B:64:CYS:HB2	1:B:126:VAL:CG2	2.45	0.45
1:B:171:TRP:CG	1:B:288:PRO:HG3	2.51	0.45
1:A:218:ASP:OD1	1:A:218:ASP:O	2.34	0.45
1:B:192:LEU:HG	1:B:198:LEU:HD11	1.98	0.45
1:B:209:ASP:OD1	1:B:212:GLN:HG3	2.15	0.45
1:C:285:TRP:HB2	1:C:297:PHE:HB3	1.98	0.45
2:D:15:GLN:HG2	5:D:332:HOH:O	2.16	0.45
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.50	0.45
1:B:326:LEU:O	1:B:330:ASN:HB2	2.16	0.45
1:C:306:ASN:OD1	1:C:308:GLU:HB2	2.16	0.45
1:A:280:MET:HE1	1:A:300:LEU:HD22	1.99	0.45
2:F:96:LYS:HE2	2:F:101:TYR:CZ	2.52	0.45
1:A:184:ILE:HD11	1:A:200:LEU:CD1	2.46	0.44
2:D:95:VAL:HA	2:D:99:GLU:O	2.17	0.44
1:B:280:MET:CE	1:B:313:TYR:HE1	2.30	0.44
1:B:2:ALA:HB2	5:B:797:HOH:O	2.17	0.44
1:A:333:ASP:O	1:A:337:ARG:HG3	2.18	0.44
1:B:38:ILE:HG23	1:B:57:ARG:NH2	2.31	0.44
1:C:239:PHE:O	1:C:250:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASP:OD1	1:A:212:GLN:HG3	2.18	0.44
1:A:280:MET:CE	1:A:300:LEU:HD13	2.37	0.44
1:B:306:ASN:OD1	1:B:309:GLU:HG3	2.18	0.44
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.83	0.43
1:A:64:CYS:HB2	1:A:126:VAL:HG21	2.00	0.43
1:B:287:VAL:HA	1:B:288:PRO:HD3	1.91	0.43
1:A:168:LYS:HE2	5:A:872:HOH:O	2.18	0.43
1:C:184:ILE:HD11	1:C:200:LEU:HD11	1.99	0.43
2:F:51:ALA:HB2	2:F:67:PHE:CG	2.53	0.43
1:A:354:ILE:HD12	1:B:70:LEU:HB3	2.00	0.43
1:C:183:HIS:O	1:C:186:ILE:HG12	2.19	0.43
1:C:108:LEU:HD12	1:C:108:LEU:N	2.33	0.43
1:C:93:HIS:HB2	4:C:502:FES:S1	2.58	0.43
1:B:175:VAL:HG22	1:B:286:TYR:CD2	2.53	0.43
1:A:367:LYS:O	1:A:371:GLU:HG3	2.19	0.42
2:D:10:ALA:HB3	2:D:13:ASP:OD2	2.18	0.42
1:B:343:PHE:CG	1:C:73:GLY:HA3	2.55	0.42
1:A:73:GLY:HA3	1:C:343:PHE:CG	2.55	0.42
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.49	0.42
2:E:90:VAL:CG2	2:E:107:LYS:HB3	2.48	0.42
1:B:300:LEU:HD22	1:B:313:TYR:OH	2.20	0.42
1:A:64:CYS:HB2	1:A:126:VAL:CG2	2.49	0.42
2:D:92:GLU:HB2	2:D:103:ALA:HB2	2.01	0.42
2:D:4:ILE:CG2	2:D:5:TRP:N	2.83	0.42
1:B:146:ALA:HB1	1:B:222:VAL:HG11	2.02	0.42
1:C:273:ASN:ND2	1:C:274:PRO:HA	2.35	0.42
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.50	0.42
1:C:16:ALA:HB3	1:C:17:PRO:HD3	2.02	0.42
1:C:322:LYS:HB3	1:C:323:PRO:CD	2.49	0.42
1:C:15:TRP:CZ3	1:C:363:VAL:HG13	2.55	0.42
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.85	0.42
1:B:321:TRP:HA	1:B:321:TRP:CE3	2.55	0.42
1:C:175:VAL:HG22	1:C:286:TYR:CD2	2.54	0.42
2:F:53:LEU:CD1	2:F:88:LEU:HD11	2.50	0.42
1:A:306:ASN:O	1:A:310:ARG:HG3	2.20	0.41
1:B:196:ASN:HD22	1:B:198:LEU:HD21	1.86	0.41
1:C:298:GLN:NE2	1:C:326:LEU:HD22	2.36	0.41
1:C:64:CYS:HB2	1:C:126:VAL:CG2	2.51	0.41
2:D:11:ALA:O	2:D:34:ARG:NH1	2.54	0.41
1:C:115:GLN:HA	1:C:115:GLN:OE1	2.21	0.41
1:B:285:TRP:HB2	1:B:297:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HA	1:B:44:LYS:HZ2	1.86	0.41
1:C:27:ASN:HA	1:C:138:GLY:HA3	2.02	0.41
1:B:184:ILE:HD11	1:B:200:LEU:CD1	2.50	0.41
1:C:273:ASN:HA	1:C:274:PRO:HA	1.91	0.41
1:A:249:ARG:HG3	1:A:250:GLU:N	2.36	0.41
1:A:175:VAL:HG22	1:A:286:TYR:CD2	2.56	0.41
1:C:171:TRP:CG	1:C:288:PRO:HG3	2.55	0.41
1:B:151:PRO:O	1:B:152:ASN:HB2	2.21	0.40
1:A:308:GLU:H	1:A:308:GLU:CD	2.24	0.40
1:B:136:TYR:CE1	1:B:143:PRO:HD2	2.56	0.40
1:A:183:HIS:O	1:A:186:ILE:HG12	2.21	0.40
1:B:4:VAL:HG12	1:B:5:ASP:N	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:858:HOH:O	5:C:945:HOH:O[2_545]	2.19	0.01

## 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	386/392 (98%)	367 (95%)	18 (5%)	1 (0%)	44	29
1	B	386/392 (98%)	369 (96%)	16 (4%)	1 (0%)	44	29
1	C	386/392 (98%)	367 (95%)	17 (4%)	2 (0%)	32	16
2	D	102/115 (89%)	96 (94%)	5 (5%)	1 (1%)	18	5
2	E	110/115 (96%)	107 (97%)	3 (3%)	0	100	100
2	F	102/115 (89%)	99 (97%)	3 (3%)	0	100	100
All	All	1472/1521 (97%)	1405 (95%)	62 (4%)	5 (0%)	44	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLY
1	B	268	GLY
1	C	268	GLY
1	C	71	HIS
2	D	5	TRP

### 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	335/339 (99%)	326 (97%)	9 (3%)	50	33
1	B	335/339 (99%)	329 (98%)	6 (2%)	64	50
1	C	335/339 (99%)	328 (98%)	7 (2%)	59	43
2	D	82/93 (88%)	82 (100%)	0	100	100
2	E	90/93 (97%)	89 (99%)	1 (1%)	78	70
2	F	82/93 (88%)	81 (99%)	1 (1%)	75	67
All	All	1259/1296 (97%)	1235 (98%)	24 (2%)	62	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	92	TYR
1	A	137	LEU
1	A	210	ARG
1	A	233	GLU
1	A	283	PHE
1	A	300	LEU
1	A	356	PHE
1	A	368	LEU
1	B	92	TYR
1	B	137	LEU
1	B	260	ASN

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Mol	Chain	Res	Type
1	B	307	ASP
1	B	356	PHE
1	B	368	LEU
1	C	46	LEU
1	C	92	TYR
1	C	137	LEU
1	C	300	LEU
1	C	356	PHE
1	C	368	LEU
1	C	389	HIS
2	E	6	LEU
2	F	37	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	B	165	GLN
1	B	260	ASN
1	C	165	GLN
1	C	273	ASN
2	E	112	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z  > 2$
4	FES	A	502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	B	502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	C	502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	D	201	2	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	E	201	2	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	F	201	2	0,4,4	0.00	-	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
4	FES	A	502	1	-	0/0/4/4	0/1/1/1
4	FES	B	502	1	-	0/0/4/4	0/1/1/1
4	FES	C	502	1	-	0/0/4/4	0/1/1/1
4	FES	D	201	2	-	0/0/4/4	0/1/1/1
4	FES	E	201	2	-	0/0/4/4	0/1/1/1
4	FES	F	201	2	-	0/0/4/4	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
4	C	502	FES	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	388/392 (98%)	-0.02	10 (2%) 56 55	11, 19, 32, 36	0
1	B	388/392 (98%)	0.10	14 (3%) 43 41	11, 23, 34, 39	0
1	C	388/392 (98%)	-0.01	9 (2%) 61 59	13, 22, 31, 37	0
2	D	104/115 (90%)	1.21	32 (30%) 0 0	16, 30, 37, 39	0
2	E	112/115 (97%)	0.38	9 (8%) 13 13	19, 27, 33, 37	0
2	F	104/115 (90%)	0.45	13 (12%) 4 4	17, 27, 34, 38	0
All	All	1484/1521 (97%)	0.16	87 (5%) 23 23	11, 22, 34, 39	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	VAL	7.2
1	C	389	HIS	5.8
1	C	388	HIS	5.7
2	D	4	ILE	5.5
1	B	305	ALA	5.4
1	A	221	VAL	5.2
2	F	25	VAL	5.1
2	D	6	LEU	5.0
1	A	389	HIS	5.0
1	B	389	HIS	4.9
2	D	5	TRP	4.9
2	D	95	VAL	4.8
2	D	104	GLY	4.8
2	F	4	ILE	4.7
2	D	25	VAL	4.6
1	A	2	ALA	4.6
2	D	99	GLU	4.5
1	C	221	VAL	4.5
2	D	101	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
2	E	37	ASP	4.3
2	F	107	LYS	4.2
2	D	105	GLU	4.1
2	D	93	VAL	4.1
2	D	97	GLU	4.1
1	A	388	HIS	4.1
2	D	92	GLU	4.0
2	D	98	GLY	4.0
2	D	37	ASP	4.0
2	D	38	GLN	4.0
2	D	7	LYS	3.9
2	F	95	VAL	3.7
1	B	308	GLU	3.6
2	D	12	SER	3.6
2	F	105	GLU	3.6
1	C	387	HIS	3.6
1	B	222	VAL	3.6
1	A	387	HIS	3.5
2	E	97	GLU	3.5
2	F	26	GLY	3.5
1	B	2	ALA	3.3
1	B	388	HIS	3.3
2	F	106	LYS	3.2
2	D	96	LYS	3.2
2	F	96	LYS	3.1
1	B	255	GLU	3.1
2	D	39	PHE	3.0
2	D	9	CYS	3.0
2	E	25	VAL	3.0
1	B	219	ASP	2.9
1	B	312	LYS	2.9
2	E	96	LYS	2.9
2	D	107	LYS	2.9
2	D	100	VAL	2.8
2	F	92	GLU	2.8
2	F	104	GLY	2.8
1	C	219	ASP	2.8
2	D	106	LYS	2.7
2	E	3	GLN	2.7
2	F	101	TYR	2.7
1	A	308	GLU	2.7
1	B	218	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	218	ASP	2.6
1	B	306	ASN	2.5
2	F	6	LEU	2.5
2	D	16	PRO	2.5
1	C	235	GLY	2.5
1	A	220	ASP	2.5
2	D	11	ALA	2.5
2	E	114	HIS	2.5
1	C	2	ALA	2.4
2	D	26	GLY	2.4
1	B	315	GLN	2.4
1	A	210	ARG	2.3
1	A	175	VAL	2.3
2	D	94	GLU	2.3
2	E	98	GLY	2.2
1	C	308	GLU	2.2
2	E	99	GLU	2.2
1	A	305	ALA	2.2
2	D	15	GLN	2.2
2	E	7	LYS	2.2
2	D	13	ASP	2.1
2	F	100	VAL	2.1
2	D	40	TYR	2.1
1	B	316	GLU	2.0
2	D	10	ALA	2.0
2	D	36	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FE2	B	501	1/1	0.99	0.11	0.55	31,31,31,31	0
4	FES	A	502	4/4	0.99	0.13	0.54	14,15,15,19	0
4	FES	D	201	4/4	1.00	0.08	-0.26	16,17,18,18	0
4	FES	E	201	4/4	0.99	0.09	-0.43	18,19,19,20	0
4	FES	F	201	4/4	1.00	0.08	-0.56	16,16,17,18	0
3	FE2	A	501	1/1	1.00	0.11	-0.61	18,18,18,18	0
4	FES	C	502	4/4	0.99	0.09	-0.74	16,19,19,19	0
4	FES	B	502	4/4	1.00	0.13	-0.98	13,14,15,16	0
3	FE2	C	501	1/1	1.00	0.04	-3.75	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.