



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:58 PM GMT

PDB ID : 4NBB  
Title : Carbazole- and oxygen-bound oxygenase with Ile262 replaced by Val and ferredoxin complex of carbazole 1,9a-dioxygenase  
Authors : Ashikawa, Y.; Usami, Y.; Inoue, K.; Nojiri, H.  
Deposited on : 2013-10-23  
Resolution : 2.05 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

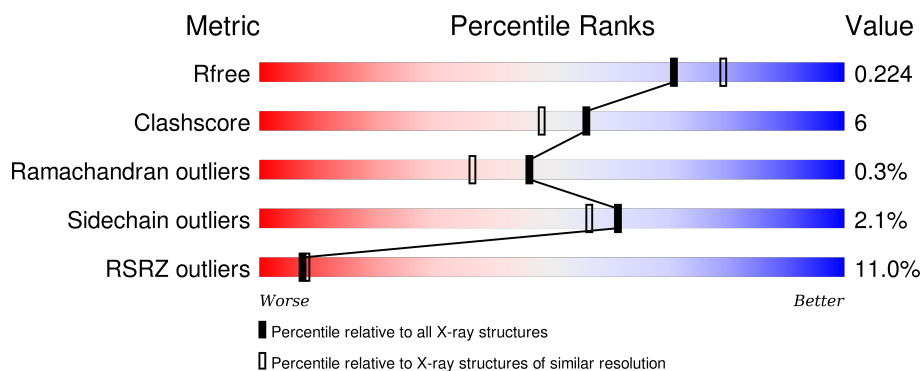
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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>8%</div> <div>83% 16%</div> </div>
1	B	392	<div> <div>6%</div> <div>83% 15%</div> </div>
1	C	392	<div> <div>7%</div> <div>82% 17%</div> </div>
2	D	115	<div> <div>32%</div> <div>73% 17% 10%</div> </div>
2	E	115	<div> <div>12%</div> <div>83% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	115	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	9CA	B	504	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12605 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	387	Total	C	N	O	S	0	0	0
			3117	1992	531	581	13			
1	B	387	Total	C	N	O	S	0	0	0
			3117	1992	531	581	13			
1	C	388	Total	C	N	O	S	0	0	0
			3127	1998	534	582	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	VAL	ILE	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	262	VAL	ILE	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	262	VAL	ILE	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	114	Total	C	N	O	S	0	0	0
			863	539	153	164	7			
2	F	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			

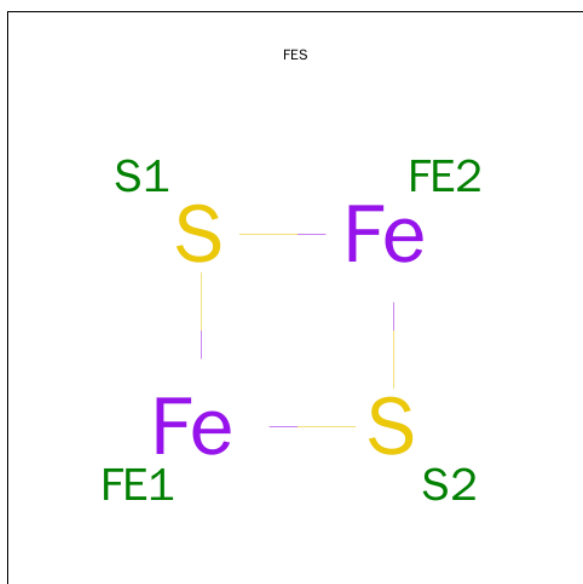
There are 24 discrepancies between the modelled and reference sequences:

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).

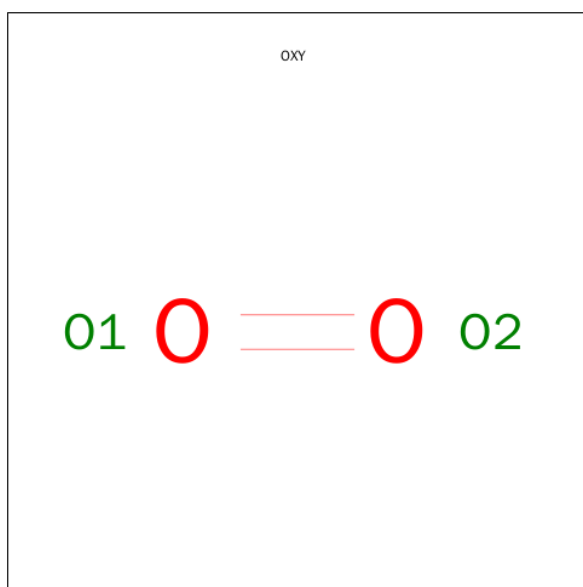
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

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



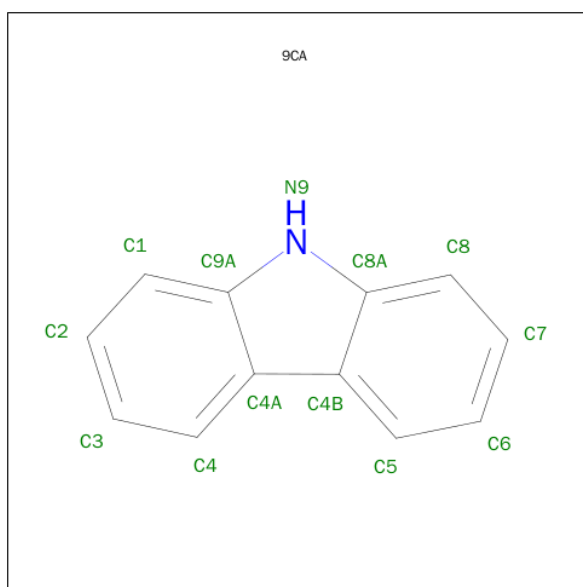
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	E	1	Total	Fe	S	0	0
			4	2	2		
4	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		
5	C	1	Total	O	0	0
			2	2		

- Molecule 6 is 9H-CARBAZOLE (three-letter code: 9CA) (formula: C<sub>12</sub>H<sub>9</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			13	12	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			13	12	1		

- Molecule 7 is water.

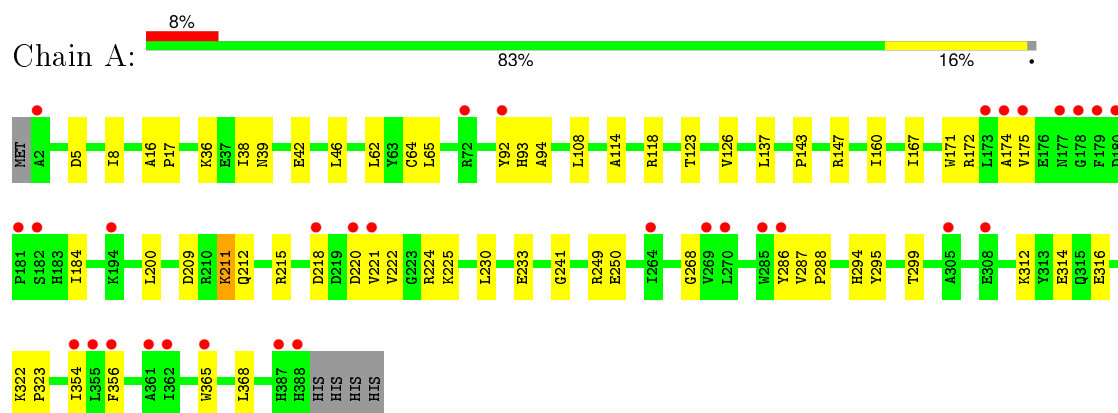
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	258	Total	O	0	0
			258	258		
7	B	225	Total	O	0	0
			225	225		
7	C	215	Total	O	0	0
			215	215		
7	D	21	Total	O	0	0
			21	21		
7	E	46	Total	O	0	0
			46	46		
7	F	21	Total	O	0	0
			21	21		



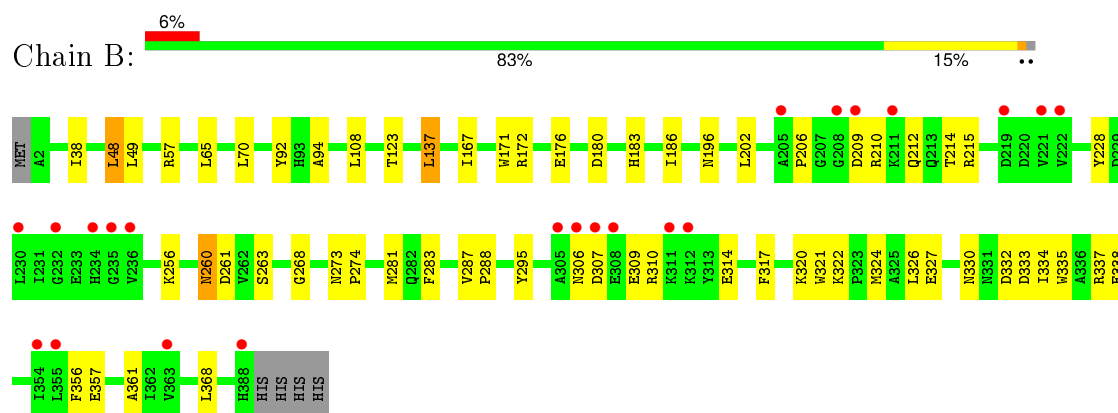
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

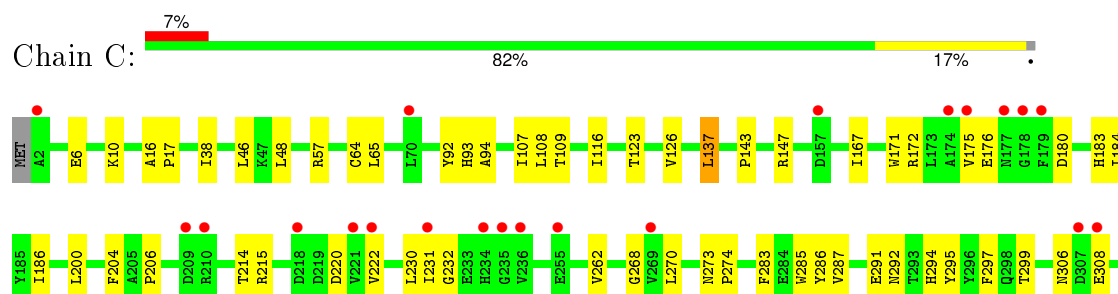
- Molecule 1: Terminal oxygenase component of carbazole

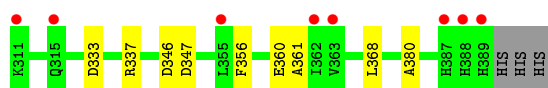


- Molecule 1: Terminal oxygenase component of carbazole

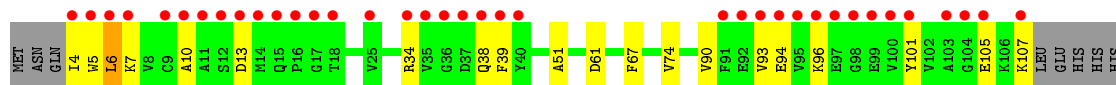


- Molecule 1: Terminal oxygenase component of carbazole

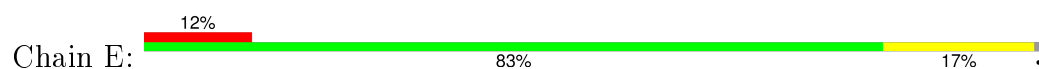




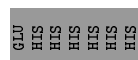
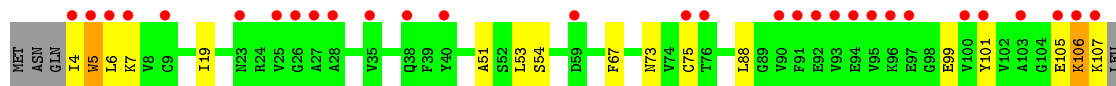
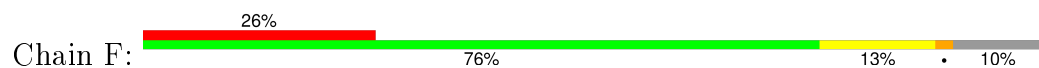
• Molecule 2: Ferredoxin CarAc



• 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, $\alpha$ , $\beta$ , $\gamma$	98.42Å 90.08Å 105.32Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	33.61 – 2.05 33.61 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.61-2.05) 99.3 (33.61-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.195 , 0.226 0.194 , 0.224	Depositor DCC
$R_{free}$ test set	5566 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 110832 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 9CA, FE2, OXY, 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	0.34	0/3201	0.61	0/4346
1	B	0.32	0/3201	0.60	0/4346
1	C	0.33	0/3212	0.59	0/4361
2	D	0.31	0/784	0.57	0/1066
2	E	0.31	0/885	0.57	0/1202
2	F	0.33	0/784	0.58	0/1066
All	All	0.33	0/12067	0.60	0/16387

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	3117	0	3021	40	0
1	B	3117	0	3021	37	0
1	C	3127	0	3028	36	0
2	D	768	0	745	12	0
2	E	863	0	818	11	0
2	F	768	0	745	10	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	1	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	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	B	13	0	9	0	0
6	C	13	0	9	0	0
7	A	258	0	0	2	0
7	B	225	0	0	1	0
7	C	215	0	0	3	0
7	D	21	0	0	0	0
7	E	46	0	0	1	0
7	F	21	0	0	0	0
All	All	12605	0	11396	144	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 6.

All (144) 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:211:LYS:H	1:A:211:LYS:HD3	1.44	0.82
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.65	0.78
1:C:6:GLU:O	1:C:10:LYS:HG2	1.86	0.75
1:B:281:MET:HE3	1:B:283:PHE:HZ	1.53	0.74
1:A:209:ASP:HB2	1:A:211:LYS:HE2	1.69	0.74
1:A:211:LYS:N	1:A:211:LYS:HD3	2.03	0.72
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.72	0.71
1:A:211:LYS:H	1:A:211:LYS:CD	2.03	0.70
2:D:7:LYS:HG2	2:D:101:TYR:CE1	2.30	0.67
1:B:281:MET:HE3	1:B:283:PHE:CZ	2.30	0.67
1:B:48:LEU:HD22	1:B:49:LEU:HD13	1.79	0.63
1:A:209:ASP:OD1	1:A:212:GLN:HG3	1.99	0.63
2:E:96:LYS:NZ	2:E:96:LYS:HB3	2.13	0.62
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.84	0.59
1:B:310:ARG:O	1:B:314:GLU:HG3	2.02	0.59
2:F:53:LEU:CD1	2:F:88:LEU:HD11	2.32	0.59
2:D:7:LYS:HG2	2:D:101:TYR:HE1	1.68	0.58
2:D:90:VAL:HG23	2:D:107:LYS:HG2	1.85	0.58
1:B:48:LEU:HD13	1:B:137:LEU:HD23	1.86	0.58
2:D:10:ALA:HB3	2:D:13:ASP:OD2	2.05	0.56
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.40	0.56
1:C:360:GLU:HG3	7:C:625:HOH:O	2.04	0.56
1:A:114:ALA:O	1:A:118:ARG:HD3	2.06	0.56
1:C:220:ASP:OD1	1:C:222:VAL:HG22	2.05	0.55
2:F:106:LYS:O	2:F:107:LYS:HB3	2.06	0.55
1:A:39:ASN:HB2	1:A:42:GLU:OE1	2.07	0.54
1:B:334:ILE:O	1:B:338:GLU:HG3	2.08	0.54
1:B:167:ILE:HD12	1:B:334:ILE:HG23	1.91	0.53
1:B:273:ASN:OD1	1:B:281:MET:HG2	2.09	0.52
2:F:19:ILE:HG21	2:F:54:SER:HA	1.92	0.52
1:C:64:CYS:HB2	1:C:126:VAL:HG21	1.92	0.52
1:C:93:HIS:HB2	4:C:502:FES:S1	2.50	0.52
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.90	0.52
2:E:47:THR:HG23	2:E:88:LEU:HD23	1.92	0.52
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.26	0.51
1:A:220:ASP:OD1	1:A:221:VAL:N	2.38	0.51
1:A:93:HIS:HB2	4:A:502:FES:S1	2.50	0.51
2:D:4:ILE:HG13	2:D:5:TRP:CD1	2.44	0.51
2:F:51:ALA:HB2	2:F:67:PHE:CG	2.45	0.51
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.93	0.51
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.93	0.51
1:B:333:ASP:O	1:B:337:ARG:HG3	2.10	0.51
1:A:312:LYS:O	1:A:316:GLU:HG3	2.11	0.51
1:B:196:ASN:O	1:B:256:LYS:HD2	2.11	0.50
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.47	0.50
2:F:6:LEU:HD23	2:F:7:LYS:N	2.26	0.50
1:C:333:ASP:O	1:C:337:ARG:HG3	2.12	0.50
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.46	0.50
1:A:184:ILE:HD11	1:A:200:LEU:CD1	2.42	0.49
1:C:176:GLU:O	1:C:180:ASP:HB2	2.12	0.49
1:C:38:ILE:HG23	1:C:57:ARG:HH21	1.76	0.49
1:A:209:ASP:OD1	1:A:211:LYS:HG2	2.13	0.49
1:C:283:PHE:HB2	1:C:299:THR:OG1	2.13	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)
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.47	0.49
2:D:94:GLU:CD	2:D:96:LYS:HE3	2.33	0.49
1:C:285:TRP:HB2	1:C:297:PHE:HB3	1.95	0.48
1:B:176:GLU:O	1:B:180:ASP:HB2	2.12	0.48
1:A:241:GLY:HA2	7:B:767:HOH:O	2.13	0.48
2:E:5:TRP:CZ3	2:E:94:GLU:HG2	2.48	0.48
1:B:260:ASN:C	1:B:260:ASN:HD22	2.16	0.48
2:F:4:ILE:HG13	2:F:5:TRP:N	2.29	0.48
1:A:220:ASP:HB2	1:A:224:ARG:HB2	1.95	0.47
1:B:326:LEU:O	1:B:330:ASN:HB2	2.15	0.47
2:D:6:LEU:HD13	2:D:7:LYS:N	2.28	0.47
1:B:260:ASN:HD22	1:B:261:ASP:N	2.12	0.47
1:C:107:ILE:HG13	1:C:116:ILE:HG12	1.97	0.47
1:B:38:ILE:HG23	1:B:57:ARG:HH21	1.79	0.47
2:D:34:ARG:HH11	2:D:34:ARG:HG3	1.79	0.47
1:B:260:ASN:ND2	1:B:274:PRO:HD3	2.30	0.47
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.44	0.47
1:C:306:ASN:OD1	1:C:308:GLU:HB2	2.15	0.47
1:C:167:ILE:HB	1:C:294:HIS:CE1	2.49	0.46
1:C:48:LEU:HD23	1:C:137:LEU:HD23	1.96	0.46
1:A:222:VAL:HG23	1:A:224:ARG:HG3	1.96	0.46
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.96	0.46
1:A:36:LYS:NZ	7:A:832:HOH:O	2.48	0.46
2:F:99:GLU:HB3	2:F:101:TYR:HE1	1.81	0.46
1:C:183:HIS:O	1:C:186:ILE:HG12	2.16	0.46
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.98	0.46
1:A:65:LEU:CD2	1:A:123:THR:HG22	2.43	0.45
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.82	0.45
1:A:38:ILE:HD13	1:A:62:LEU:HD22	1.99	0.45
2:E:10:ALA:HB3	2:E:13:ASP:OD2	2.17	0.45
1:B:287:VAL:HA	1:B:288:PRO:HD3	1.88	0.45
1:C:215:ARG:HB2	1:C:230:LEU:HD11	1.99	0.45
1:B:206:PRO:HG2	1:B:357:GLU:HB3	1.99	0.44
1:A:322:LYS:HB3	1:A:323:PRO:CD	2.47	0.44
2:F:53:LEU:HD11	2:F:88:LEU:HD11	1.99	0.44
1:C:204:PHE:O	1:C:206:PRO:HD3	2.16	0.44
1:B:317:PHE:HA	1:B:321:TRP:HB2	1.99	0.44
1:C:184:ILE:HD11	1:C:200:LEU:CD1	2.48	0.44
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.47	0.44
2:E:20:ARG:HE	2:E:20:ARG:HB2	1.62	0.44
1:B:320:LYS:HG3	1:B:324:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:HIS:O	1:B:186:ILE:HG12	2.18	0.44
1:A:322:LYS:HB3	1:A:323:PRO:HD3	2.00	0.44
1:B:260:ASN:HD21	1:B:274:PRO:HD3	1.84	0.43
2:F:4:ILE:HG13	2:F:5:TRP:H	1.82	0.43
1:A:354:ILE:HD12	1:B:70:LEU:HB3	2.00	0.43
1:C:16:ALA:HB3	1:C:17:PRO:HD3	2.00	0.43
1:A:175:VAL:HG11	1:A:365:TRP:CE2	2.53	0.43
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.48	0.43
1:B:209:ASP:OD1	1:B:212:GLN:HG3	2.18	0.43
2:D:61:ASP:O	2:D:74:VAL:HG22	2.18	0.43
1:B:228:TYR:CD1	1:B:263:SER:HB3	2.52	0.43
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.53	0.43
2:D:39:PHE:HB2	2:D:93:VAL:HG11	2.01	0.43
1:B:306:ASN:OD1	1:B:309:GLU:HG3	2.18	0.43
1:A:118:ARG:HD2	7:A:757:HOH:O	2.19	0.43
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.49	0.43
1:B:214:THR:HG21	1:B:361:ALA:HA	2.01	0.43
1:A:167:ILE:HB	1:A:294:HIS:CE1	2.54	0.43
1:C:175:VAL:HG22	1:C:286:TYR:HD2	1.83	0.42
1:A:16:ALA:HB3	1:A:17:PRO:HD3	2.01	0.42
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.49	0.42
1:C:231:ILE:HG23	1:C:232:GLY:N	2.33	0.42
2:E:4:ILE:N	2:E:4:ILE:HD12	2.34	0.42
1:B:322:LYS:O	1:B:327:GLU:HG3	2.19	0.42
2:D:94:GLU:OE2	2:D:96:LYS:HE3	2.20	0.42
1:A:215:ARG:HB2	1:A:230:LEU:HD11	2.02	0.42
1:A:64:CYS:HB2	1:A:126:VAL:HG21	2.00	0.42
1:A:287:VAL:HA	1:A:288:PRO:HD3	1.92	0.42
1:A:108:LEU:N	1:A:108:LEU:HD12	2.35	0.42
1:C:380:ALA:HB3	7:C:761:HOH:O	2.18	0.42
1:C:230:LEU:HA	7:C:649:HOH:O	2.20	0.42
1:A:218:ASP:O	1:A:225:LYS:HD3	2.19	0.41
1:A:5:ASP:HB3	1:A:8:ILE:HD12	2.01	0.41
1:C:291:GLU:HG3	1:C:292:ASN:OD1	2.20	0.41
1:C:214:THR:HG21	1:C:361:ALA:HA	2.02	0.41
1:A:249:ARG:HG3	1:A:250:GLU:N	2.36	0.41
1:C:346:ASP:O	1:C:347:ASP:HB2	2.21	0.41
1:C:308:GLU:N	1:C:308:GLU:OE1	2.54	0.41
2:E:95:VAL:HA	2:E:99:GLU:O	2.20	0.41
2:E:96:LYS:HB3	2:E:96:LYS:HZ3	1.82	0.41
1:A:174:ALA:HB1	1:A:286:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HG23	1:A:299:THR:HB	2.02	0.41
1:C:273:ASN:HA	1:C:274:PRO:HA	1.85	0.41
1:B:202:LEU:O	1:C:109:THR:HG22	2.21	0.41
2:E:86:VAL:HA	2:E:87:PRO:HD3	1.93	0.40
2:F:73:ASN:OD1	2:F:75:CYS:HB2	2.22	0.40
2:E:17:GLY:HA2	7:E:330:HOH:O	2.21	0.40
1:C:262:VAL:CG1	1:C:270:LEU:HD11	2.51	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	385/392 (98%)	368 (96%)	16 (4%)	1 (0%)	46	36
1	B	385/392 (98%)	364 (94%)	20 (5%)	1 (0%)	46	36
1	C	386/392 (98%)	366 (95%)	19 (5%)	1 (0%)	46	36
2	D	102/115 (89%)	96 (94%)	6 (6%)	0	100	100
2	E	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
2	F	102/115 (89%)	97 (95%)	3 (3%)	2 (2%)	9	2
All	All	1472/1521 (97%)	1399 (95%)	68 (5%)	5 (0%)	46	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	C	268	GLY
1	A	268	GLY
2	F	5	TRP
2	F	106	LYS

### 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	334/339 (98%)	326 (98%)	8 (2%)	57	50
1	B	334/339 (98%)	327 (98%)	7 (2%)	61	56
1	C	335/339 (99%)	330 (98%)	5 (2%)	72	70
2	D	82/93 (88%)	79 (96%)	3 (4%)	41	32
2	E	92/93 (99%)	89 (97%)	3 (3%)	45	37
2	F	82/93 (88%)	81 (99%)	1 (1%)	78	76
All	All	1259/1296 (97%)	1232 (98%)	27 (2%)	61	56

All (27) 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	211	LYS
1	A	233	GLU
1	A	314	GLU
1	A	356	PHE
1	A	368	LEU
1	B	48	LEU
1	B	92	TYR
1	B	137	LEU
1	B	260	ASN
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	356	PHE
1	C	368	LEU
2	D	6	LEU
2	D	38	GLN

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Mol	Chain	Res	Type
2	D	105	GLU
2	E	2	ASN
2	E	6	LEU
2	E	37	ASP
2	F	105	GLU

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	A	379	GLN
1	B	260	ASN
1	B	388	HIS
1	C	379	GLN
1	C	388	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 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	-
5	OXY	A	503	3	1,1,1	0.92	0	0,0,0	0.00	-
4	FES	B	502	1	0,4,4	0.00	-	0,4,4	0.00	-
5	OXY	B	503	3	1,1,1	0.92	0	0,0,0	0.00	-
6	9CA	B	504	-	15,15,15	1.25	1 (6%)	20,21,21	0.43	0
4	FES	C	502	1	0,4,4	0.00	-	0,4,4	0.00	-
5	OXY	C	503	3	1,1,1	0.93	0	0,0,0	0.00	-
6	9CA	C	504	-	15,15,15	1.25	1 (6%)	20,21,21	0.44	0
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
5	OXY	A	503	3	-	0/0/0/0	0/0/0/0
4	FES	B	502	1	-	0/0/4/4	0/1/1/1
5	OXY	B	503	3	-	0/0/0/0	0/0/0/0
6	9CA	B	504	-	-	0/0/0/0	0/3/3/3
4	FES	C	502	1	-	0/0/4/4	0/1/1/1
5	OXY	C	503	3	-	0/0/0/0	0/0/0/0
6	9CA	C	504	-	-	0/0/0/0	0/3/3/3
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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	9CA	C4B-C4A	-2.13	1.39	1.45
6	C	504	9CA	C4B-C4A	-2.09	1.39	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	FES	1	0
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	387/392 (98%)	0.34	31 (8%) 15 17	23, 35, 50, 56	0
1	B	387/392 (98%)	0.33	22 (5%) 27 31	25, 38, 53, 58	0
1	C	388/392 (98%)	0.35	29 (7%) 17 20	28, 38, 52, 57	0
2	D	104/115 (90%)	1.32	37 (35%) 0 0	30, 48, 57, 61	0
2	E	114/115 (99%)	0.52	14 (12%) 5 5	31, 42, 54, 57	0
2	F	104/115 (90%)	1.34	30 (28%) 1 0	33, 47, 54, 57	0
All	All	1484/1521 (97%)	0.49	163 (10%) 7 8	23, 38, 53, 61	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	25	VAL	6.7
1	B	305	ALA	5.9
2	E	115	HIS	5.7
2	D	37	ASP	5.7
2	D	11	ALA	5.6
1	C	2	ALA	5.4
1	B	221	VAL	5.3
2	F	95	VAL	5.2
2	D	98	GLY	5.2
2	E	2	ASN	5.2
1	A	221	VAL	5.2
1	A	387	HIS	5.0
2	D	97	GLU	5.0
2	D	36	GLY	4.9
1	C	388	HIS	4.5
2	D	95	VAL	4.5
2	F	4	ILE	4.5
2	D	12	SER	4.5
2	D	104	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	F	93	VAL	4.5
2	F	101	TYR	4.2
2	F	105	GLU	4.1
2	D	92	GLU	4.1
2	D	25	VAL	4.1
1	A	388	HIS	4.0
1	C	389	HIS	4.0
2	F	6	LEU	4.0
1	B	308	GLU	4.0
2	D	93	VAL	4.0
2	D	101	TYR	4.0
2	F	27	ALA	3.9
1	C	315	GLN	3.9
1	A	175	VAL	3.9
2	D	5	TRP	3.9
2	E	37	ASP	3.8
1	A	362	ILE	3.8
2	E	113	HIS	3.8
1	B	208	GLY	3.8
2	D	105	GLU	3.7
2	F	92	GLU	3.7
1	A	2	ALA	3.7
2	F	97	GLU	3.7
2	D	99	GLU	3.7
1	C	221	VAL	3.7
2	E	97	GLU	3.6
1	B	235	GLY	3.6
2	E	112	HIS	3.6
1	C	235	GLY	3.6
2	F	5	TRP	3.6
1	C	362	ILE	3.5
2	D	7	LYS	3.4
2	D	4	ILE	3.4
1	B	234	HIS	3.4
1	C	179	PHE	3.3
2	F	28	ALA	3.3
1	B	355	LEU	3.3
1	C	178	GLY	3.3
2	F	9	CYS	3.3
1	A	308	GLU	3.3
1	C	175	VAL	3.3
1	C	387	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	100	VAL	3.2
2	F	96	LYS	3.2
2	D	40	TYR	3.1
2	F	94	GLU	3.1
1	C	174	ALA	3.1
1	C	307	ASP	3.1
1	C	234	HIS	3.1
2	D	38	GLN	3.0
2	D	13	ASP	3.0
2	F	75	CYS	3.0
1	C	236	VAL	3.0
2	D	100	VAL	3.0
1	B	230	LEU	3.0
2	D	6	LEU	3.0
2	D	15	GLN	3.0
2	F	103	ALA	3.0
1	B	209	ASP	3.0
2	D	35	VAL	2.9
2	F	23	ASN	2.9
2	F	26	GLY	2.9
2	D	39	PHE	2.9
1	B	236	VAL	2.9
1	C	209	ASP	2.9
2	E	114	HIS	2.8
2	D	16	PRO	2.8
1	A	269	VAL	2.8
2	D	94	GLU	2.8
1	B	219	ASP	2.8
1	A	361	ALA	2.7
2	D	107	LYS	2.7
2	D	17	GLY	2.7
1	A	285	TRP	2.7
1	B	222	VAL	2.7
1	B	388	HIS	2.7
1	A	286	TYR	2.7
1	A	179	PHE	2.7
1	A	264	ILE	2.6
1	A	305	ALA	2.6
2	D	103	ALA	2.6
1	C	218	ASP	2.6
1	A	355	LEU	2.6
2	E	98	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	222	VAL	2.6
1	B	306	ASN	2.6
2	F	107	LYS	2.6
2	F	38	GLN	2.6
2	D	9	CYS	2.5
1	A	270	LEU	2.5
1	B	363	VAL	2.5
2	F	40	TYR	2.5
1	B	312	LYS	2.5
1	A	72	ARG	2.5
2	D	34	ARG	2.5
2	E	25	VAL	2.5
1	C	308	GLU	2.4
1	C	231	ILE	2.4
1	C	269	VAL	2.4
1	A	178	GLY	2.4
1	C	255	GLU	2.4
2	E	27	ALA	2.4
1	C	157	ASP	2.4
1	C	177	ASN	2.4
1	A	220	ASP	2.4
1	C	311	LYS	2.4
1	B	232	GLY	2.4
1	A	177	ASN	2.4
1	A	92	TYR	2.4
2	F	76	THR	2.3
2	E	110	HIS	2.3
1	A	356	PHE	2.3
2	F	91	PHE	2.3
1	C	210	ARG	2.3
2	D	18	THR	2.2
1	A	174	ALA	2.2
1	B	205	ALA	2.2
1	B	211	LYS	2.2
1	C	363	VAL	2.2
2	F	90	VAL	2.2
1	A	194	LYS	2.2
1	B	354	ILE	2.2
1	A	365	TRP	2.2
2	F	35	VAL	2.2
1	C	70	LEU	2.2
2	E	50	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	14	MET	2.1
1	A	173	LEU	2.1
2	D	91	PHE	2.1
1	A	181	PRO	2.1
1	A	180	ASP	2.1
1	A	182	SER	2.1
2	E	11	ALA	2.1
2	F	7	LYS	2.1
1	C	355	LEU	2.1
1	B	307	ASP	2.1
2	F	59	ASP	2.1
1	A	354	ILE	2.1
1	B	311	LYS	2.1
2	D	96	LYS	2.1
2	E	7	LYS	2.1
2	D	10	ALA	2.0
1	A	218	ASP	2.0
2	F	106	LYS	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(Å <sup>2</sup> )	Q<0.9
6	9CA	B	504	13/13	0.82	0.25	5.10	48,50,51,51	0
5	OXY	A	503	2/2	0.98	0.30	1.99	41,41,41,45	0
6	9CA	C	504	13/13	0.85	0.19	0.10	46,48,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FES	E	201	4/4	0.99	0.13	-0.22	23,30,30,32	0
3	FE2	A	501	1/1	0.99	0.15	-0.34	32,32,32,32	0
4	FES	B	502	4/4	0.99	0.17	-0.50	25,27,29,32	0
4	FES	C	502	4/4	0.99	0.13	-0.51	33,35,35,36	0
4	FES	D	201	4/4	0.99	0.10	-0.68	30,30,31,31	0
5	OXY	C	503	2/2	0.98	0.13	-0.98	52,52,52,55	0
4	FES	A	502	4/4	0.99	0.14	-1.02	27,27,29,29	0
5	OXY	B	503	2/2	0.95	0.10	-1.09	59,59,59,60	0
3	FE2	B	501	1/1	0.99	0.09	-1.56	48,48,48,48	0
3	FE2	C	501	1/1	0.99	0.09	-1.81	39,39,39,39	0
4	FES	F	201	4/4	0.99	0.04	-1.96	31,33,34,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.