



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:19 am BST

PDB ID : 3VMG  
Title : Reduced carbazole-bound complex between oxygenase and ferredoxin in carbazole 1,9a-dioxygenase  
Authors : Ashikawa, Y.; Nojiri, H.  
Deposited on : 2011-12-12  
Resolution : 1.95 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	:	2.11
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)	:	2.11

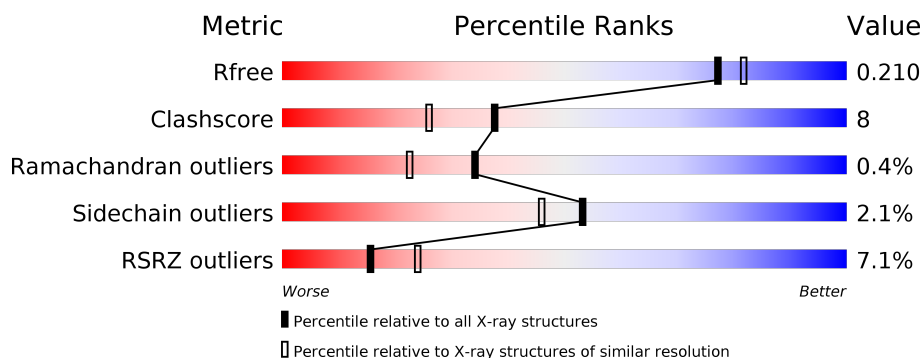
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	392	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	392	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>..</div> </div> </div>
2	D	115	<div> <div>32%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
2	E	115	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>7%</div> </div> </div>
2	F	115	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>10%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	9CA	C	2002	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12864 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	389	Total	C	N	O	S	0	0	0
			3136	2004	535	583	14			
1	B	389	Total	C	N	O	S	0	0	0
			3136	2004	535	583	14			
1	C	389	Total	C	N	O	S	0	0	0
			3136	2004	535	583	14			

There are 24 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Ferredoxin component of carbazole.

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	107	Total	C	N	O	S	0	0	0
			794	499	133	155	7			
2	F	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			

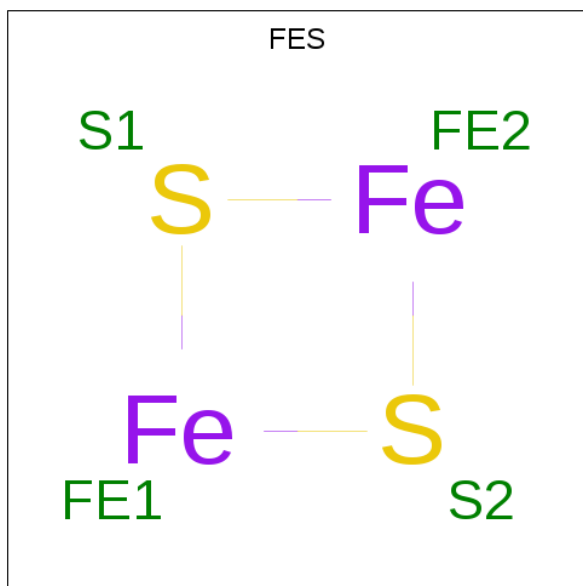
There are 24 discrepancies between the modelled and reference sequences:

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).

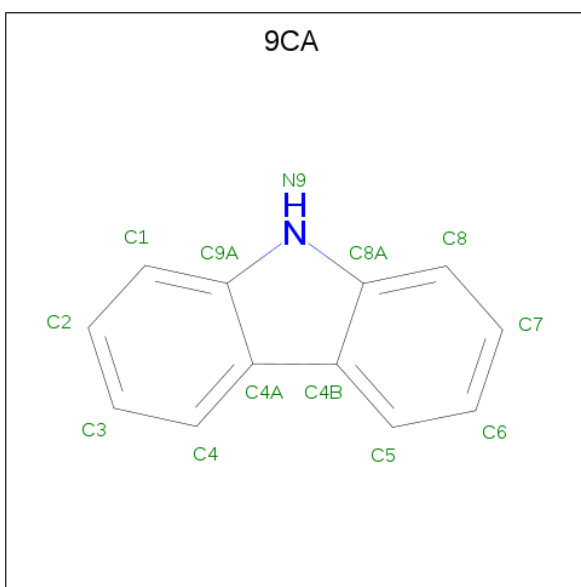
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- 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 4 2 2	0	0
4	B	1	Total Fe S 4 2 2	0	0
4	C	1	Total Fe S 4 2 2	0	0
4	D	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	F	1	Total Fe S 4 2 2	0	0

- Molecule 5 is 9H-CARBAZOLE (three-letter code: 9CA) (formula: C<sub>12</sub>H<sub>9</sub>N).



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

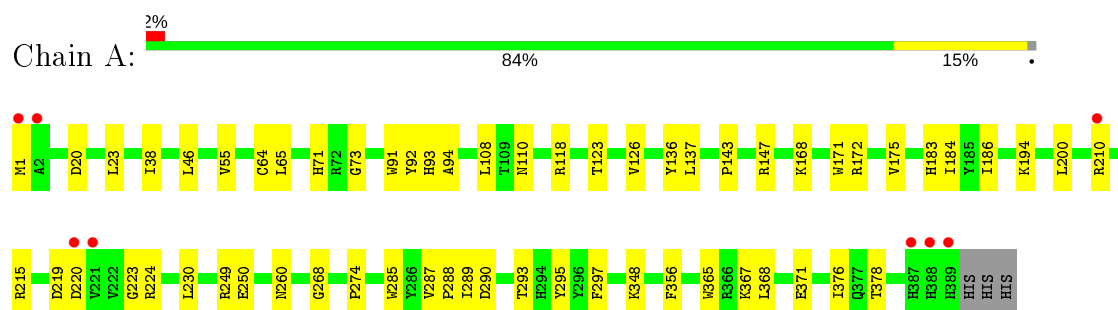
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	291	Total	O	0	0
			291	291		
6	C	299	Total	O	0	0
			299	299		
6	D	39	Total	O	0	0
			39	39		
6	E	45	Total	O	0	0
			45	45		
6	F	60	Total	O	0	0
			60	60		

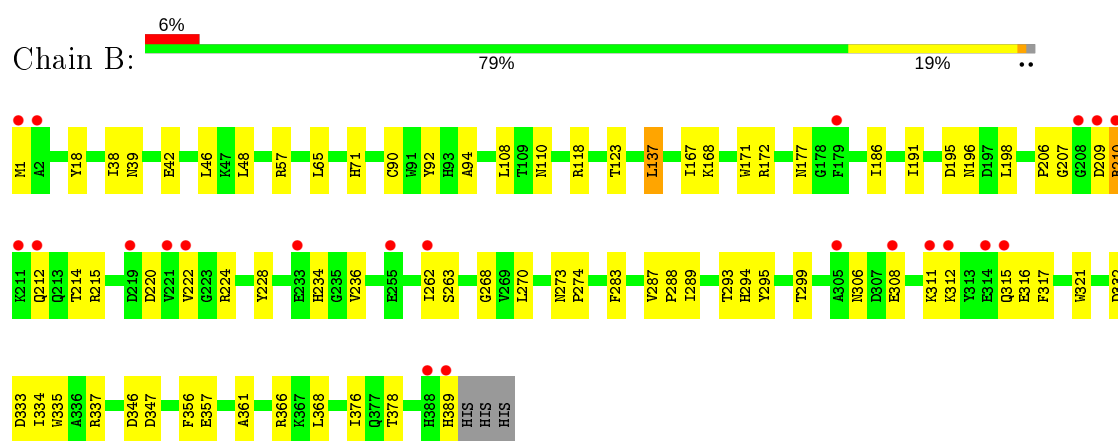
### 3 Residue-property plots [i](#)

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

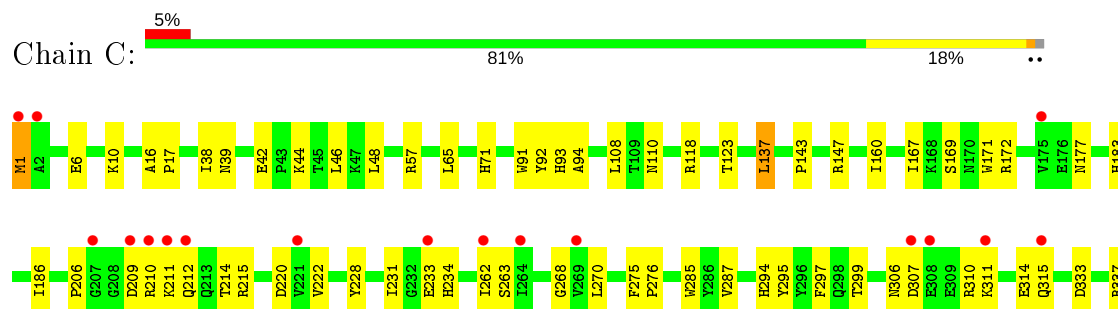
- Molecule 1: Terminal oxygenase component of carbazole



- Molecule 1: Terminal oxygenase component of carbazole



- Molecule 1: Terminal oxygenase component of carbazole







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.16 Å   89.84 Å   105.21 Å 90.00°   104.40°   90.00°	Depositor
Resolution (Å)	40.62 – 1.95 40.61 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.62-1.95) 99.5 (40.61-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.96 (at 1.95 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.198   ,   0.219 0.190   ,   0.210	Depositor DCC
$R_{free}$ test set	6437 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: 9CA, 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	0.33	0/3221	0.62	0/4372
1	B	0.31	0/3221	0.60	0/4372
1	C	0.31	0/3221	0.59	0/4372
2	D	0.31	0/784	0.55	0/1066
2	E	0.30	0/810	0.58	0/1101
2	F	0.30	0/784	0.61	0/1066
All	All	0.31	0/12041	0.60	0/16349

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ARG	Sidechain

### 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	3136	0	3042	40	0
1	B	3136	0	3042	51	0
1	C	3136	0	3042	54	0
2	D	768	0	745	9	0
2	E	794	0	770	20	0
2	F	768	0	745	7	0
3	A	1	0	0	0	0
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	1	0
4	E	4	0	0	1	0
4	F	4	0	0	0	0
5	B	13	0	9	1	0
5	C	13	0	9	6	0
6	A	339	0	0	3	0
6	B	291	0	0	4	0
6	C	299	0	0	3	0
6	D	39	0	0	0	0
6	E	45	0	0	0	0
6	F	60	0	0	1	0
All	All	12864	0	11404	178	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 (178) 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:1:MET:H2	1:A:378:THR:HG22	1.34	0.90
2:E:92:GLU:HB2	2:E:107:LYS:HE3	1.55	0.87
1:A:289:ILE:HB	1:A:293:THR:HG23	1.57	0.86
1:C:262:ILE:HD11	5:C:2002:9CA:C7	2.12	0.79
1:C:262:ILE:HG23	1:C:270:LEU:HD11	1.67	0.77
1:C:262:ILE:CG2	1:C:270:LEU:HD11	2.19	0.72
1:A:290:ASP:OD1	1:A:293:THR:HG22	1.90	0.71
1:A:1:MET:H1	1:A:376:ILE:CG2	2.03	0.71
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:LEU:O	2:E:109:GLU:HB3	1.92	0.70
1:A:1:MET:N	1:A:378:THR:HG22	2.04	0.70
1:A:184:ILE:HD11	1:A:200:LEU:CD1	2.20	0.70
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.74	0.70
1:C:6:GLU:O	1:C:10:LYS:HG2	1.92	0.69
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.73	0.69
2:D:7:LYS:HD2	2:D:99:GLU:OE2	1.92	0.69
1:B:1:MET:HG3	1:B:376:ILE:HB	1.75	0.68
1:A:194:LYS:HB2	6:A:547:HOH:O	1.95	0.66
1:C:210:ARG:HG2	6:C:932:HOH:O	1.96	0.66
1:B:209:ASP:OD2	1:B:212:GLN:HG3	1.97	0.65
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.79	0.65
2:D:90:VAL:HG23	2:D:107:LYS:HG2	1.79	0.65
2:D:19:ILE:HG21	2:D:54:SER:HA	1.79	0.65
1:C:262:ILE:CD1	5:C:2002:9CA:C7	2.75	0.64
1:B:311:LYS:O	1:B:315:GLN:HG3	1.98	0.63
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.81	0.63
1:B:206:PRO:HG2	1:B:357:GLU:HB3	1.81	0.62
1:A:184:ILE:HD11	1:A:200:LEU:HD11	1.80	0.62
1:C:1:MET:HB2	1:C:378:THR:HG21	1.81	0.62
1:C:233:GLU:HG2	6:C:918:HOH:O	2.00	0.62
1:B:1:MET:H3	1:B:376:ILE:HG21	1.65	0.61
1:A:1:MET:H1	1:A:376:ILE:HG21	1.62	0.61
1:C:306:ASN:O	1:C:310:ARG:HG3	1.99	0.61
1:B:317:PHE:HA	1:B:321:TRP:HB2	1.83	0.61
2:E:4:ILE:HG23	2:E:5:TRP:N	2.15	0.60
1:B:361:ALA:HB3	6:B:1067:HOH:O	2.02	0.60
1:B:1:MET:HB2	1:B:378:THR:CG2	2.31	0.60
2:E:96:LYS:NZ	2:E:96:LYS:HB3	2.16	0.59
1:B:262:ILE:CG2	1:B:270:LEU:HD11	2.33	0.59
1:C:177:ASN:HD22	1:C:337:ARG:HE	1.51	0.58
1:A:118:ARG:HG3	6:F:903:HOH:O	2.03	0.58
2:D:7:LYS:HG2	2:D:101:TYR:CE2	2.39	0.57
1:C:262:ILE:CD1	5:C:2002:9CA:C8	2.83	0.57
1:C:48:LEU:HD23	1:C:137:LEU:HD23	1.84	0.57
1:C:220:ASP:OD1	1:C:222:VAL:HG22	2.05	0.57
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.87	0.56
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.88	0.56
1:C:177:ASN:ND2	1:C:337:ARG:HE	2.04	0.56
1:B:186:ILE:HG22	1:C:91:TRP:O	2.06	0.55
1:C:177:ASN:HD21	1:C:333:ASP:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:ALA:HB3	2:D:13:ASP:OD2	2.06	0.54
1:A:367:LYS:O	1:A:371:GLU:HG3	2.07	0.54
2:F:53:LEU:CD1	2:F:88:LEU:HD11	2.38	0.54
1:C:262:ILE:HD13	5:C:2002:9CA:C8	2.37	0.54
1:C:210:ARG:O	1:C:214:THR:HG22	2.08	0.53
1:C:311:LYS:O	1:C:315:GLN:HG3	2.09	0.53
2:E:3:GLN:HG3	2:E:4:ILE:N	2.23	0.53
1:A:91:TRP:O	1:C:186:ILE:HG22	2.09	0.53
1:B:48:LEU:HD23	1:B:137:LEU:HD23	1.89	0.53
1:B:196:ASN:HD22	1:B:198:LEU:HD21	1.74	0.53
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.44	0.52
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.92	0.52
1:B:333:ASP:O	1:B:337:ARG:HG3	2.09	0.52
1:B:177:ASN:HD21	1:B:333:ASP:HB3	1.74	0.52
1:C:262:ILE:HD13	6:C:1073:HOH:O	2.09	0.52
1:C:38:ILE:HA	1:C:44:LYS:HZ3	1.75	0.51
2:F:7:LYS:HB2	2:F:7:LYS:NZ	2.25	0.51
1:C:38:ILE:HG23	1:C:57:ARG:HH21	1.74	0.51
1:B:191:ILE:O	1:B:195:ASP:HB2	2.11	0.50
1:C:231:ILE:HD13	1:C:262:ILE:HD12	1.92	0.50
1:B:312:LYS:HD3	1:B:312:LYS:O	2.11	0.50
2:E:4:ILE:CG2	2:E:5:TRP:N	2.75	0.50
1:B:118:ARG:NH2	6:B:931:HOH:O	2.45	0.50
1:C:210:ARG:HG3	1:C:211:LYS:N	2.27	0.50
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.47	0.49
1:B:210:ARG:O	1:B:214:THR:HG22	2.12	0.49
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.48	0.49
1:A:23:LEU:HD22	6:A:649:HOH:O	2.13	0.49
1:B:38:ILE:HG23	1:B:57:ARG:HH21	1.78	0.49
1:A:1:MET:N	1:A:378:THR:CG2	2.74	0.48
1:B:171:TRP:CG	1:B:288:PRO:HG3	2.48	0.48
1:C:167:ILE:HB	1:C:294:HIS:CE1	2.48	0.48
2:E:68:HIS:HB2	4:E:201:FES:S2	2.53	0.48
2:E:10:ALA:HB3	2:E:13:ASP:OD2	2.13	0.48
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.48	0.48
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.43	0.48
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.96	0.48
1:A:249:ARG:HG3	1:A:250:GLU:N	2.29	0.47
1:C:231:ILE:CD1	1:C:262:ILE:HD12	2.44	0.47
2:F:19:ILE:HG21	2:F:54:SER:HA	1.95	0.47
1:C:16:ALA:HB3	1:C:17:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ILE:HD11	5:C:2002:9CA:C8	2.44	0.47
2:D:68:HIS:HB2	4:D:201:FES:S2	2.54	0.47
1:A:184:ILE:HD11	1:A:200:LEU:HD12	1.96	0.47
1:A:260:ASN:HD22	1:A:274:PRO:HD2	1.79	0.47
1:A:290:ASP:CG	1:A:293:THR:HG22	2.35	0.47
1:B:1:MET:N	1:B:376:ILE:HG21	2.30	0.47
2:E:96:LYS:HB3	2:E:96:LYS:HZ2	1.79	0.47
1:B:90:CYS:O	1:B:94:ALA:HA	2.14	0.47
2:F:51:ALA:HB2	2:F:67:PHE:CG	2.49	0.47
1:C:93:HIS:HB2	4:C:401:FES:S1	2.55	0.47
2:E:108:LEU:O	2:E:109:GLU:CB	2.62	0.47
1:A:183:HIS:O	1:A:186:ILE:HG12	2.14	0.46
1:C:233:GLU:HG3	1:C:234:HIS:CD2	2.50	0.46
2:E:47:THR:HG23	2:E:88:LEU:HD23	1.97	0.46
1:C:262:ILE:HD11	5:C:2002:9CA:C6	2.46	0.46
1:A:220:ASP:HB2	1:A:224:ARG:HB2	1.97	0.46
1:C:311:LYS:HE3	1:C:314:GLU:OE1	2.15	0.46
2:F:4:ILE:HG13	2:F:5:TRP:H	1.80	0.46
1:C:209:ASP:CG	1:C:212:GLN:HE21	2.19	0.46
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.30	0.45
1:C:285:TRP:HB2	1:C:297:PHE:HB3	1.99	0.45
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.51	0.45
1:B:273:ASN:HA	1:B:274:PRO:HA	1.84	0.45
1:A:64:CYS:HB2	1:A:126:VAL:HG21	1.97	0.45
1:A:168:LYS:HE2	6:A:864:HOH:O	2.16	0.45
2:D:31:ALA:O	2:D:41:ALA:HA	2.17	0.45
1:B:1:MET:HB2	1:B:378:THR:HG21	1.97	0.45
2:E:4:ILE:HG23	2:E:5:TRP:CD1	2.52	0.45
1:B:220:ASP:OD1	1:B:222:VAL:N	2.48	0.45
1:B:224:ARG:NH2	6:B:976:HOH:O	2.49	0.44
1:B:167:ILE:HB	1:B:294:HIS:CE1	2.52	0.44
2:E:92:GLU:OE1	2:E:107:LYS:NZ	2.50	0.44
1:B:167:ILE:HD12	1:B:334:ILE:HG23	1.98	0.44
1:C:275:PHE:CG	1:C:276:PRO:HA	2.53	0.44
1:B:289:ILE:HB	1:B:293:THR:OG1	2.18	0.43
1:A:175:VAL:HG11	1:A:365:TRP:CE2	2.53	0.43
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.83	0.43
1:A:93:HIS:HB2	4:A:401:FES:S1	2.58	0.43
1:B:321:TRP:HA	1:B:321:TRP:CE3	2.54	0.43
1:A:287:VAL:HA	1:A:288:PRO:HD3	1.88	0.43
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:O	1:B:316:GLU:HG3	2.18	0.43
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.48	0.43
1:B:177:ASN:HD22	1:B:337:ARG:HE	1.65	0.43
1:B:283:PHE:HB2	1:B:299:THR:OG1	2.19	0.43
1:B:228:TYR:CD1	1:B:263:SER:HB3	2.54	0.43
1:A:136:TYR:CE1	1:A:143:PRO:HD2	2.54	0.43
1:C:333:ASP:O	1:C:337:ARG:HG3	2.19	0.43
2:E:25:VAL:HG13	2:E:25:VAL:O	2.19	0.43
1:B:94:ALA:HB1	1:B:108:LEU:HB2	2.01	0.42
1:B:207:GLY:HA3	1:B:234:HIS:O	2.19	0.42
1:B:312:LYS:HD2	1:B:316:GLU:OE2	2.18	0.42
1:C:160:ILE:HG23	1:C:299:THR:HB	2.01	0.42
1:A:285:TRP:HB2	1:A:297:PHE:HB3	2.01	0.42
1:B:306:ASN:OD1	1:B:308:GLU:HB2	2.19	0.42
1:C:206:PRO:HG2	1:C:357:GLU:HB3	2.01	0.42
1:C:39:ASN:HB2	1:C:42:GLU:OE2	2.19	0.42
1:A:1:MET:HA	1:A:20:ASP:OD2	2.18	0.42
1:C:183:HIS:O	1:C:186:ILE:HG12	2.19	0.42
1:C:228:TYR:CD1	1:C:263:SER:HB3	2.54	0.42
1:B:1:MET:H3	1:B:376:ILE:CG2	2.30	0.42
2:F:4:ILE:HG13	2:F:5:TRP:CD1	2.54	0.42
2:E:99:GLU:OE1	2:E:99:GLU:HA	2.18	0.42
1:B:168:LYS:HE2	6:B:906:HOH:O	2.18	0.42
2:E:3:GLN:HG3	2:E:4:ILE:H	1.83	0.42
1:C:39:ASN:HB2	1:C:42:GLU:CD	2.40	0.42
2:E:19:ILE:HG21	2:E:54:SER:HA	2.02	0.42
1:A:64:CYS:HB2	1:A:126:VAL:CG2	2.50	0.42
1:B:207:GLY:HA2	1:B:236:VAL:HG23	2.01	0.41
1:C:346:ASP:O	1:C:347:ASP:HB2	2.20	0.41
1:A:260:ASN:HD22	1:A:274:PRO:CD	2.34	0.41
1:C:209:ASP:CG	1:C:212:GLN:HG3	2.40	0.41
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.47	0.41
2:F:5:TRP:CH2	2:F:92:GLU:HG3	2.56	0.41
1:B:346:ASP:O	1:B:347:ASP:HB2	2.21	0.41
1:C:215:ARG:HB3	1:C:228:TYR:HB2	2.02	0.41
1:A:219:ASP:OD1	1:A:223:GLY:HA2	2.20	0.41
1:B:39:ASN:HB2	1:B:42:GLU:OE1	2.20	0.41
2:E:5:TRP:CZ3	2:E:94:GLU:HG2	2.57	0.40
1:A:38:ILE:CD1	1:A:55:VAL:HG12	2.52	0.40
1:B:215:ARG:HB3	1:B:228:TYR:HB2	2.03	0.40
1:B:18:TYR:CE2	1:B:366:ARG:HG2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:HA3	1:C:343:PHE:CG	2.56	0.40
2:D:99:GLU:HB3	2:D:101:TYR:CE1	2.57	0.40
2:E:91:PHE:N	2:E:91:PHE:CD1	2.88	0.40
1:B:262:ILE:HD13	5:B:2001:9CA:C8	2.52	0.40
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.52	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	387/392 (99%)	372 (96%)	13 (3%)	2 (0%)	29	17
1	B	387/392 (99%)	366 (95%)	19 (5%)	2 (0%)	29	17
1	C	387/392 (99%)	366 (95%)	19 (5%)	2 (0%)	29	17
2	D	102/115 (89%)	98 (96%)	4 (4%)	0	100	100
2	E	105/115 (91%)	100 (95%)	5 (5%)	0	100	100
2	F	102/115 (89%)	101 (99%)	1 (1%)	0	100	100
All	All	1470/1521 (97%)	1403 (95%)	61 (4%)	6 (0%)	34	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	268	GLY
1	A	71	HIS
1	A	268	GLY
1	B	268	GLY
1	C	71	HIS
1	B	71	HIS

### 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	336/339 (99%)	329 (98%)	7 (2%)	53	46
1	B	336/339 (99%)	328 (98%)	8 (2%)	49	40
1	C	336/339 (99%)	327 (97%)	9 (3%)	44	34
2	D	82/93 (88%)	82 (100%)	0	100	100
2	E	85/93 (91%)	83 (98%)	2 (2%)	49	40
2	F	82/93 (88%)	81 (99%)	1 (1%)	71	68
All	All	1257/1296 (97%)	1230 (98%)	27 (2%)	53	46

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	110	ASN
1	A	137	LEU
1	A	348	LYS
1	A	356	PHE
1	A	368	LEU
1	B	46	LEU
1	B	92	TYR
1	B	110	ASN
1	B	137	LEU
1	B	210	ARG
1	B	356	PHE
1	B	368	LEU
1	B	389	HIS
1	C	1	MET
1	C	46	LEU
1	C	92	TYR
1	C	110	ASN
1	C	137	LEU
1	C	169	SER
1	C	307	ASP

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Mol	Chain	Res	Type
1	C	356	PHE
1	C	368	LEU
2	E	6	LEU
2	E	96	LYS
2	F	37	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	165	GLN
1	A	260	ASN
1	B	110	ASN
1	B	177	ASN
1	C	110	ASN
1	C	165	GLN
1	C	177	ASN
1	C	212	GLN
1	C	234	HIS
1	C	388	HIS
2	E	3	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z  > 2$
5	9CA	B	2001	-	15,15,15	1.27	1 (6%)	21,21,21	0.70	0
4	FES	B	401	1	0,4,4	0.00	-	-		
4	FES	E	201	2	0,4,4	0.00	-	-		
4	FES	A	401	1	0,4,4	0.00	-	-		
4	FES	D	201	2	0,4,4	0.00	-	-		
4	FES	C	401	1	0,4,4	0.00	-	-		
4	FES	F	201	2	0,4,4	0.00	-	-		
5	9CA	C	2002	-	15,15,15	1.27	1 (6%)	21,21,21	0.70	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
5	9CA	B	2001	-	-	-	0/3/3/3
4	FES	B	401	1	-	-	0/1/1/1
4	FES	E	201	2	-	-	0/1/1/1
4	FES	A	401	1	-	-	0/1/1/1
4	FES	D	201	2	-	-	0/1/1/1
4	FES	C	401	1	-	-	0/1/1/1
4	FES	F	201	2	-	-	0/1/1/1
5	9CA	C	2002	-	-	-	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2002	9CA	C4B-C4A	-2.16	1.39	1.45
5	B	2001	9CA	C4B-C4A	-2.15	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.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	9CA	1	0
4	E	201	FES	1	0
4	A	401	FES	1	0
4	D	201	FES	1	0
4	C	401	FES	1	0
5	C	2002	9CA	6	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	389/392 (99%)	0.08	8 (2%) 63 72	15, 23, 39, 47	0
1	B	389/392 (99%)	0.28	22 (5%) 23 32	15, 27, 43, 49	0
1	C	389/392 (99%)	0.16	20 (5%) 28 37	18, 27, 40, 49	0
2	D	104/115 (90%)	1.37	37 (35%) 0 0	20, 37, 46, 48	0
2	E	107/115 (93%)	0.35	10 (9%) 8 14	22, 33, 42, 47	0
2	F	104/115 (90%)	0.48	8 (7%) 13 21	23, 34, 41, 45	0
All	All	1482/1521 (97%)	0.29	105 (7%) 16 24	15, 27, 43, 49	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	11.9
1	A	1	MET	8.9
1	B	1	MET	8.5
1	A	221	VAL	7.0
1	B	221	VAL	5.9
2	D	98	GLY	5.2
1	A	389	HIS	5.1
1	B	222	VAL	5.1
1	C	221	VAL	5.0
1	A	2	ALA	5.0
2	F	25	VAL	5.0
1	B	211	LYS	4.9
2	D	5	TRP	4.8
2	D	95	VAL	4.6
2	D	4	ILE	4.6
1	B	209	ASP	4.5
2	D	92	GLU	4.5
2	D	97	GLU	4.5
1	C	209	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	308	GLU	4.3
2	D	101	TYR	4.2
2	D	6	LEU	4.2
2	D	37	ASP	4.2
2	D	25	VAL	4.1
2	D	35	VAL	4.1
1	B	210	ARG	4.0
2	D	13	ASP	4.0
1	B	305	ALA	3.9
2	D	11	ALA	3.8
2	D	93	VAL	3.8
2	D	104	GLY	3.8
2	D	99	GLU	3.8
2	D	105	GLU	3.7
1	C	388	HIS	3.6
1	A	388	HIS	3.5
2	D	12	SER	3.5
1	C	211	LYS	3.5
2	F	4	ILE	3.5
1	B	389	HIS	3.4
1	B	212	GLN	3.4
2	D	39	PHE	3.4
2	F	107	LYS	3.3
2	E	97	GLU	3.3
1	B	208	GLY	3.3
2	D	40	TYR	3.2
2	D	107	LYS	3.2
1	C	389	HIS	3.2
2	D	8	VAL	3.2
2	D	38	GLN	3.2
1	B	312	LYS	3.1
1	C	308	GLU	3.1
2	F	105	GLU	3.1
2	E	27	ALA	3.1
2	D	96	LYS	3.0
1	A	387	HIS	2.9
2	E	11	ALA	2.9
2	D	9	CYS	2.9
2	D	7	LYS	2.9
2	D	16	PRO	2.9
1	A	220	ASP	2.9
1	C	262	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	307	ASP	2.8
1	C	2	ALA	2.8
1	B	219	ASP	2.8
1	C	264	ILE	2.8
2	E	3	GLN	2.8
2	E	25	VAL	2.7
2	F	106	LYS	2.7
1	C	210	ARG	2.7
1	A	210	ARG	2.6
1	C	233	GLU	2.6
2	D	94	GLU	2.6
2	E	37	ASP	2.5
2	D	36	GLY	2.5
1	C	212	GLN	2.4
1	B	315	GLN	2.4
2	F	90	VAL	2.4
2	D	103	ALA	2.4
2	D	15	GLN	2.4
1	B	388	HIS	2.4
1	B	262	ILE	2.4
1	B	2	ALA	2.3
1	C	315	GLN	2.3
1	C	269	VAL	2.3
2	D	10	ALA	2.3
2	D	17	GLY	2.2
2	D	100	VAL	2.2
1	B	255	GLU	2.2
1	B	314	GLU	2.2
2	E	7	LYS	2.2
2	D	34	ARG	2.2
1	C	387	HIS	2.2
2	E	98	GLY	2.1
1	B	311	LYS	2.1
2	E	26	GLY	2.1
2	F	97	GLU	2.1
2	E	109	GLU	2.1
1	C	175	VAL	2.1
2	D	22	VAL	2.1
1	C	207	GLY	2.0
2	F	92	GLU	2.0
2	D	106	LYS	2.0
1	B	179	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	311	LYS	2.0
1	B	233	GLU	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	9CA	C	2002	13/13	0.90	0.11	27,28,28,28	0
5	9CA	B	2001	13/13	0.94	0.10	29,29,29,29	0
4	FES	E	201	4/4	0.99	0.10	22,22,23,24	0
4	FES	A	401	4/4	0.99	0.11	20,20,20,21	0
4	FES	D	201	4/4	0.99	0.10	18,20,21,23	0
4	FES	C	401	4/4	0.99	0.09	21,22,24,24	0
4	FES	F	201	4/4	0.99	0.04	22,23,23,24	0
3	FE2	A	501	1/1	0.99	0.11	23,23,23,23	0
3	FE2	B	501	1/1	0.99	0.09	29,29,29,29	0
4	FES	B	401	4/4	1.00	0.12	18,19,21,21	0
3	FE2	C	501	1/1	1.00	0.06	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.