



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 10:15 PM EDT

PDB ID : 4NBD  
Title : Carbazole-bound oxygenase with Phe275 replaced by Trp and ferredoxin complex of carbazole 1,9a-dioxygenase (form2)  
Authors : Ashikawa, Y.; Usami, Y.; Inoue, K.; Nojiri, H.  
Deposited on : 2013-10-23  
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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.29  
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) : 2.29

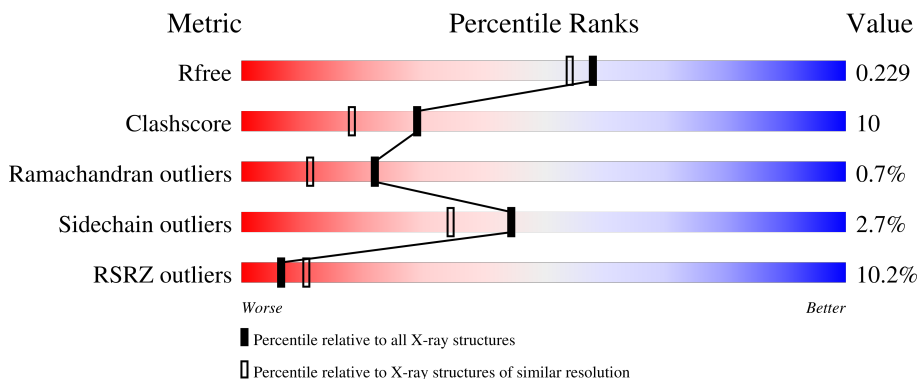
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	A	392	 4% 80% 17% ..
1	B	392	 15% 68% 28% ..
1	C	392	 5% 85% 13% ..
2	D	115	 34% 72% 17% • 10%
2	E	115	 7% 77% 16% 7%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11827 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
			Total	C	N	O	S			
1	A	384	3092	1978	525	576	13	0	0	0
1	B	384	3092	1978	525	576	13	0	0	0
1	C	388	3131	2001	535	582	13	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	TRP	PHE	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	275	TRP	PHE	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	275	TRP	PHE	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	103	Total	C	N	O	S	0	0	0
			759	477	127	148	7			
2	E	107	Total	C	N	O	S	0	0	0
			794	499	133	155	7			

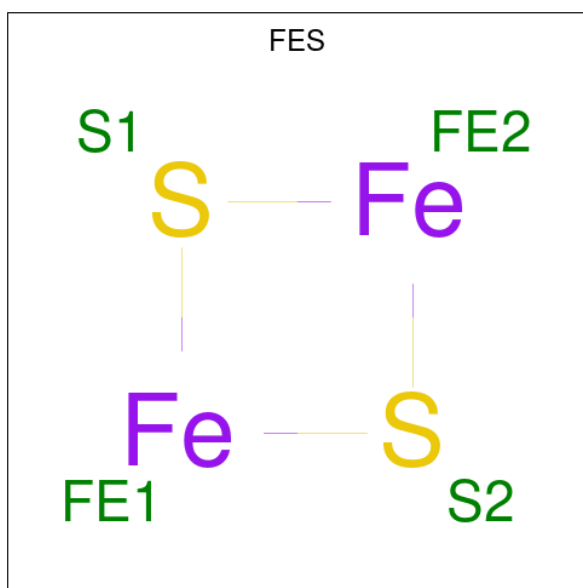
There are 16 discrepancies between the modelled and reference sequences:

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

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

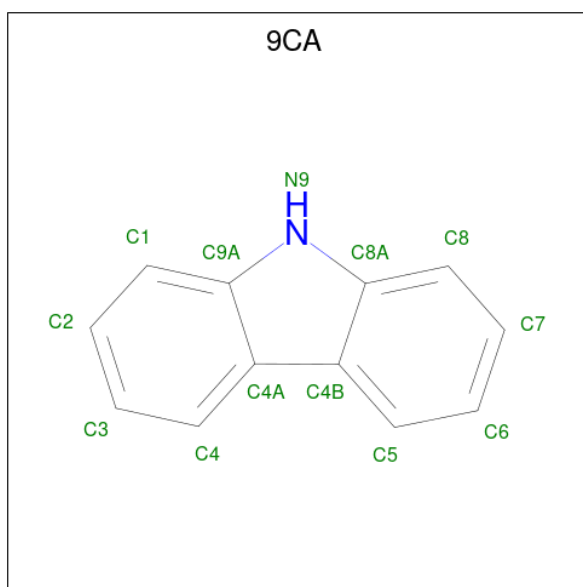
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- 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		

- 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	A	1	Total	C	N	0	0
			13	12	1		
5	B	1	Total	C	N	0	0
			13	12	1		
5	C	1	Total	C	N	0	0
			13	12	1		

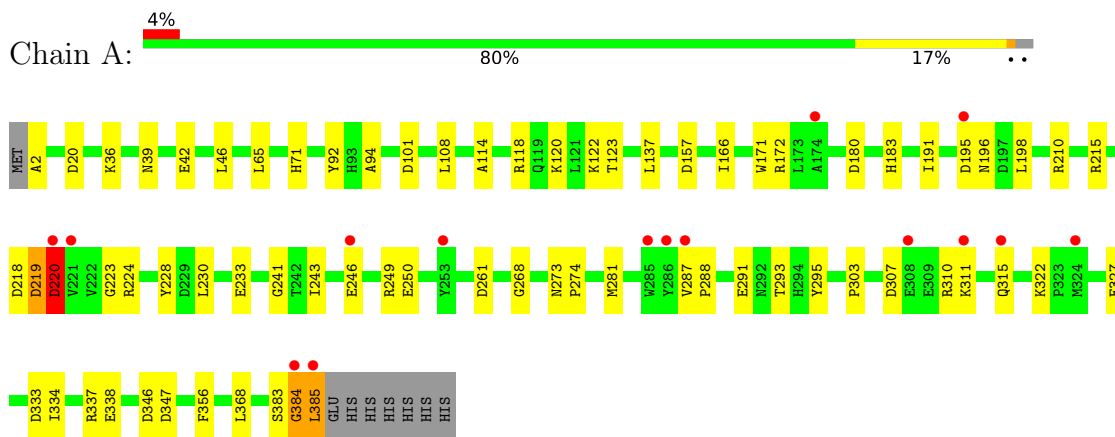
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total	O	0	0
			287	287		
6	B	196	Total	O	0	0
			196	196		
6	C	335	Total	O	0	0
			335	335		
6	D	37	Total	O	0	0
			37	37		
6	E	42	Total	O	0	0
			42	42		

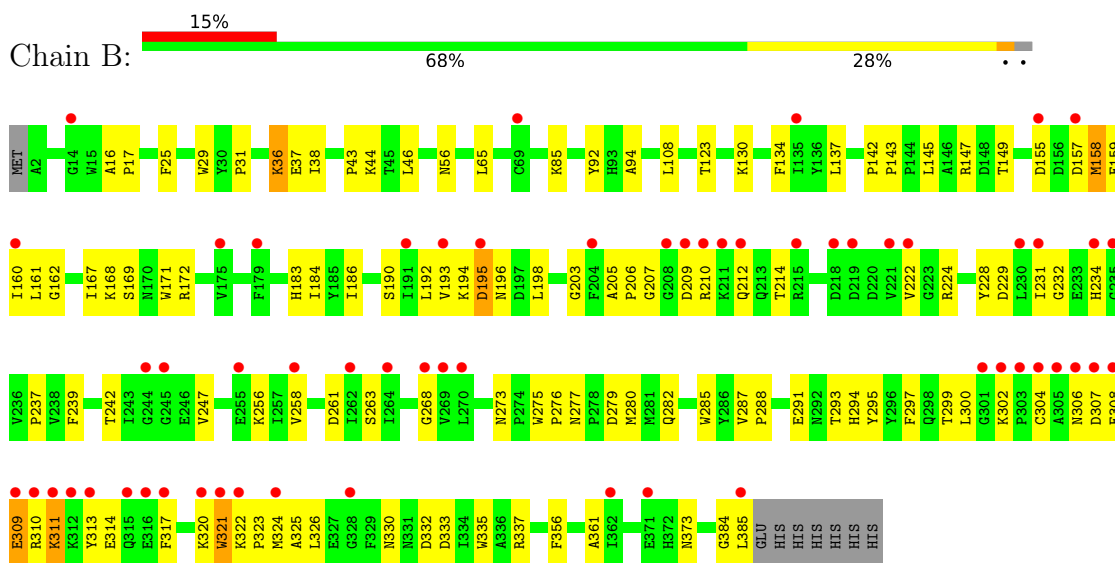
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

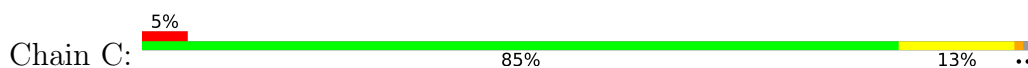
- Molecule 1: Terminal oxygenase component of carbazole

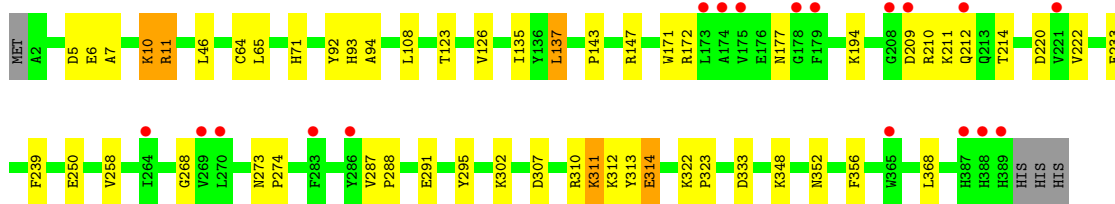


- Molecule 1: Terminal oxygenase component of carbazole

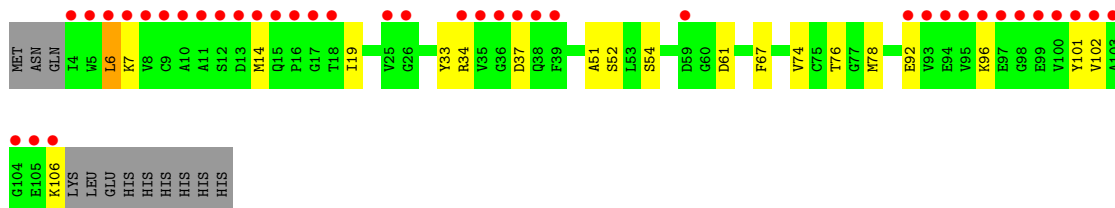


- Molecule 1: Terminal oxygenase component of carbazole

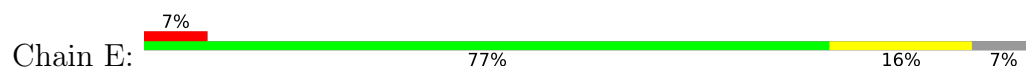




● Molecule 2: Ferredoxin CarAc



● Molecule 2: Ferredoxin CarAc





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.34Å 88.20Å 108.11Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	32.63 – 1.95 32.78 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.63-1.95) 99.1 (32.78-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.37 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.232 0.200 , 0.229	Depositor DCC
$R_{free}$ test set	6398 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: FES, FE2, 9CA

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	0.32	0/3175	0.62	1/4312 (0.0%)
1	B	0.28	0/3175	0.55	0/4312
1	C	0.34	0/3217	0.62	0/4369
2	D	0.29	0/775	0.55	0/1055
2	E	0.28	0/810	0.56	0/1101
All	All	0.31	0/11152	0.59	1/15149 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	N-CA-C	-5.13	97.15	111.00

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	3092	0	3004	49	0
1	B	3092	0	3004	91	0
1	C	3131	0	3031	46	0
2	D	759	0	732	14	0
2	E	794	0	770	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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	1	0
5	A	13	0	9	0	0
5	B	13	0	9	0	0
5	C	13	0	9	0	0
6	A	287	0	0	3	0
6	B	196	0	0	3	0
6	C	335	0	0	5	0
6	D	37	0	0	1	0
6	E	42	0	0	0	0
All	All	11827	0	10568	206	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 10.

All (206) 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:C:11:ARG:HH11	1:C:11:ARG:HB3	1.24	1.01
1:B:308:GLU:HG2	1:B:309:GLU:H	1.26	0.98
1:B:311:LYS:HE3	1:B:311:LYS:HA	1.54	0.89
1:C:233:GLU:HG2	6:C:622:HOH:O	1.75	0.86
1:B:306:ASN:ND2	1:B:308:GLU:HB3	1.94	0.82
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.65	0.78
1:B:308:GLU:HG2	1:B:309:GLU:N	2.00	0.77
1:B:384:GLY:O	1:B:385:LEU:HB3	1.85	0.77
1:A:230:LEU:HB3	1:A:233:GLU:HG3	1.68	0.76
1:C:310:ARG:O	1:C:314:GLU:HG2	1.87	0.75
1:A:210:ARG:HH22	2:D:52:SER:HB2	1.54	0.72
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.71	0.72
1:C:10:LYS:HA	1:C:10:LYS:HE3	1.71	0.71
1:A:385:LEU:HD12	1:C:348:LYS:HE3	1.74	0.70
1:B:229:ASP:OD2	1:B:361:ALA:HB2	1.92	0.69
1:A:385:LEU:H	1:A:385:LEU:HD13	1.58	0.69
1:A:2:ALA:HA	6:A:796:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:O	1:A:120:LYS:HE2	1.96	0.66
1:C:11:ARG:HB3	1:C:11:ARG:NH1	2.05	0.66
1:B:317:PHE:HA	1:B:321:TRP:HB2	1.77	0.66
1:C:93:HIS:HB2	4:C:502:FES:S1	2.37	0.65
1:B:196:ASN:O	1:B:256:LYS:HD2	1.97	0.65
1:C:311:LYS:HE3	1:C:311:LYS:HA	1.78	0.65
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.78	0.64
1:B:210:ARG:O	1:B:214:THR:HG22	1.98	0.64
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.80	0.63
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.78	0.63
1:A:210:ARG:NH2	2:D:52:SER:HB2	2.13	0.62
1:A:219:ASP:OD1	1:A:223:GLY:HA2	2.01	0.61
2:E:7:LYS:HE2	2:E:99:GLU:OE2	2.01	0.60
1:B:308:GLU:O	1:B:310:ARG:HG3	2.01	0.60
2:D:96:LYS:HG2	6:D:336:HOH:O	2.02	0.60
1:B:157:ASP:HB2	1:B:304:CYS:O	2.02	0.59
1:C:11:ARG:HH11	1:C:11:ARG:CB	2.06	0.59
1:B:190:SER:HB3	1:B:193:VAL:HG23	1.83	0.59
1:A:385:LEU:H	1:A:385:LEU:CD1	2.16	0.59
1:B:311:LYS:HA	1:B:311:LYS:CE	2.32	0.59
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.85	0.59
1:B:306:ASN:HD21	1:B:308:GLU:HB3	1.65	0.58
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.38	0.58
1:A:385:LEU:O	1:A:385:LEU:HD22	2.03	0.58
1:B:310:ARG:HG2	1:B:310:ARG:HH11	1.68	0.57
1:C:64:CYS:HB2	1:C:126:VAL:HG21	1.84	0.57
1:B:384:GLY:O	1:B:385:LEU:CB	2.53	0.57
1:B:385:LEU:O	1:B:385:LEU:HG	2.05	0.57
1:A:210:ARG:HH22	2:D:52:SER:CB	2.18	0.57
1:C:209:ASP:OD2	1:C:212:GLN:HG3	2.05	0.56
1:C:6:GLU:O	1:C:10:LYS:HG2	2.06	0.56
1:C:291:GLU:HG2	6:C:639:HOH:O	2.06	0.56
1:A:385:LEU:HA	1:C:352:ASN:OD1	2.07	0.55
1:C:211:LYS:N	1:C:211:LYS:HE2	2.21	0.55
1:B:261:ASP:HB3	1:B:273:ASN:O	2.07	0.55
1:B:192:LEU:O	1:B:196:ASN:HB3	2.07	0.54
1:B:159:GLU:HG2	1:B:313:TYR:HD2	1.73	0.54
1:B:228:TYR:CD1	1:B:263:SER:HB3	2.42	0.54
1:B:280:MET:HE1	1:B:321:TRP:CD1	2.43	0.54
1:A:249:ARG:HG3	1:A:250:GLU:N	2.23	0.54
1:B:37:GLU:O	1:B:44:LYS:HE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.89	0.53
1:B:36:LYS:O	1:B:36:LYS:HD2	2.08	0.53
1:A:385:LEU:HD12	1:C:348:LYS:CE	2.39	0.53
1:C:126:VAL:HG22	1:C:135:ILE:HG12	1.90	0.53
1:A:218:ASP:O	1:A:219:ASP:HB2	2.09	0.53
1:B:326:LEU:O	1:B:330:ASN:HB2	2.08	0.53
1:C:5:ASP:OD2	1:C:7:ALA:HB3	2.09	0.53
1:C:312:LYS:HE2	6:C:798:HOH:O	2.09	0.53
1:B:307:ASP:HA	1:B:310:ARG:HE	1.72	0.53
1:C:220:ASP:OD1	1:C:222:VAL:HG22	2.08	0.53
2:D:19:ILE:HG21	2:D:54:SER:HA	1.91	0.52
2:E:10:ALA:HA	2:E:99:GLU:OE1	2.09	0.52
1:B:145:LEU:O	1:B:149:THR:HG23	2.09	0.52
1:C:302:LYS:HD3	1:C:313:TYR:CD1	2.44	0.52
1:B:198:LEU:HD22	1:B:258:VAL:CG2	2.39	0.52
2:D:6:LEU:HD23	2:D:102:VAL:O	2.09	0.52
2:D:92:GLU:OE1	2:D:106:LYS:HE2	2.10	0.52
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.44	0.52
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.92	0.52
2:E:91:PHE:CZ	2:E:106:LYS:HB3	2.45	0.52
1:B:237:PRO:HB2	1:B:239:PHE:CE1	2.44	0.52
1:B:212:GLN:HG3	1:B:234:HIS:CD2	2.45	0.51
1:B:158:MET:HE3	1:B:158:MET:HA	1.90	0.51
1:B:159:GLU:HG2	1:B:313:TYR:CD2	2.46	0.51
2:D:51:ALA:HB2	2:D:67:PHE:CD2	2.46	0.51
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.45	0.51
1:C:311:LYS:HE3	1:C:314:GLU:HG3	1.92	0.51
1:A:243:ILE:O	1:A:246:GLU:HG2	2.10	0.51
2:D:61:ASP:O	2:D:74:VAL:HG22	2.10	0.51
1:B:184:ILE:HD11	1:B:203:GLY:HA2	1.92	0.50
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.93	0.50
1:A:39:ASN:HB2	1:A:42:GLU:OE1	2.12	0.50
1:B:198:LEU:HD22	1:B:258:VAL:HG21	1.94	0.50
1:A:333:ASP:O	1:A:337:ARG:HG3	2.12	0.49
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.46	0.49
1:B:308:GLU:CG	1:B:309:GLU:H	2.10	0.49
1:B:229:ASP:OD1	1:B:231:ILE:HG23	2.12	0.49
1:C:210:ARG:HD2	1:C:214:THR:OG1	2.13	0.49
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.94	0.49
1:A:241:GLY:HA2	6:B:662:HOH:O	2.13	0.49
1:B:276:PRO:HD3	1:B:300:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.27	0.49
2:D:6:LEU:HD23	2:D:6:LEU:N	2.27	0.49
1:A:122:LYS:HD2	6:A:815:HOH:O	2.12	0.48
1:A:261:ASP:HB3	1:A:273:ASN:O	2.13	0.48
1:B:321:TRP:HA	1:B:321:TRP:CE3	2.48	0.48
1:B:209:ASP:CG	1:B:212:GLN:HB2	2.34	0.48
2:E:99:GLU:OE1	2:E:99:GLU:HA	2.14	0.48
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.49	0.48
1:B:192:LEU:HD22	1:B:325:ALA:HA	1.95	0.48
1:B:167:ILE:HB	1:B:294:HIS:CE1	2.49	0.48
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.44	0.47
1:A:218:ASP:O	1:A:218:ASP:OD1	2.31	0.47
1:B:282:GLN:HG3	1:B:300:LEU:HD23	1.97	0.47
1:B:168:LYS:HA	1:B:293:THR:HG22	1.94	0.47
1:B:205:ALA:HB1	1:B:206:PRO:HD2	1.96	0.47
1:B:275:TRP:CG	1:B:276:PRO:HA	2.50	0.47
2:E:7:LYS:HE3	2:E:99:GLU:HG2	1.96	0.47
1:B:130:LYS:HB3	1:B:160:ILE:HB	1.96	0.47
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.95	0.46
1:B:155:ASP:HB2	1:B:158:MET:CG	2.45	0.46
1:B:160:ILE:O	1:B:161:LEU:HD23	2.15	0.46
1:A:196:ASN:HD22	1:A:198:LEU:HD21	1.80	0.46
1:A:385:LEU:CD1	1:A:385:LEU:N	2.78	0.46
1:B:322:LYS:N	1:B:323:PRO:HD2	2.31	0.46
1:A:334:ILE:O	1:A:338:GLU:HG3	2.16	0.45
1:C:64:CYS:HB2	1:C:126:VAL:CG2	2.46	0.45
1:A:180:ASP:HB3	1:A:183:HIS:HB3	1.98	0.45
1:B:321:TRP:HA	1:B:321:TRP:HE3	1.81	0.45
1:A:322:LYS:O	1:A:327:GLU:HG3	2.16	0.45
2:E:6:LEU:HD23	2:E:7:LYS:N	2.31	0.45
1:A:273:ASN:HB2	1:A:281:MET:HG2	1.97	0.45
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.47	0.45
1:C:307:ASP:HA	1:C:310:ARG:NH1	2.32	0.45
1:A:2:ALA:HB1	1:A:20:ASP:OD1	2.17	0.45
1:B:162:GLY:HA3	1:B:299:THR:HA	1.99	0.45
1:B:171:TRP:CG	1:B:288:PRO:HG3	2.52	0.44
1:B:285:TRP:HB2	1:B:297:PHE:HB3	1.98	0.44
1:B:333:ASP:O	1:B:337:ARG:HG3	2.17	0.44
1:C:322:LYS:HB3	1:C:323:PRO:CD	2.47	0.44
1:A:191:ILE:HG22	1:A:195:ASP:OD2	2.18	0.44
1:B:31:PRO:HB3	1:B:134:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLU:HG2	6:B:626:HOH:O	2.17	0.44
1:A:291:GLU:HG2	6:A:663:HOH:O	2.18	0.44
1:B:85:LYS:NZ	6:B:675:HOH:O	2.44	0.44
1:A:114:ALA:O	1:A:118:ARG:HD2	2.16	0.44
1:A:346:ASP:O	1:A:347:ASP:HB2	2.18	0.44
1:B:310:ARG:O	1:B:314:GLU:HG3	2.17	0.44
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.47	0.44
1:B:155:ASP:HB2	1:B:158:MET:HG3	1.99	0.44
2:E:95:VAL:HA	2:E:99:GLU:O	2.16	0.44
1:A:307:ASP:N	1:A:310:ARG:HH21	2.16	0.44
1:B:196:ASN:ND2	1:B:198:LEU:HD21	2.33	0.44
1:A:383:SER:HB3	6:C:794:HOH:O	2.17	0.43
1:C:258:VAL:HA	1:C:274:PRO:HG2	2.00	0.43
1:C:287:VAL:HA	1:C:288:PRO:HD3	1.91	0.43
2:D:7:LYS:HB3	2:D:101:TYR:CE1	2.52	0.43
1:A:166:ILE:HG23	1:A:293:THR:CG2	2.48	0.43
1:B:25:PHE:CD1	1:B:373:ASN:HB2	2.53	0.43
2:E:11:ALA:O	2:E:34:ARG:NH1	2.52	0.43
1:B:277:ASN:HB3	1:B:279:ASP:OD1	2.19	0.43
1:C:194:LYS:HB2	6:C:803:HOH:O	2.19	0.43
1:B:196:ASN:HD22	1:B:198:LEU:CG	2.32	0.43
2:E:68:HIS:HB2	4:E:201:FES:S2	2.58	0.43
2:E:90:VAL:HG23	2:E:107:LYS:HB3	2.00	0.43
1:B:36:LYS:HD2	1:B:36:LYS:C	2.39	0.43
2:E:96:LYS:O	2:E:97:GLU:HB2	2.19	0.43
1:B:194:LYS:C	1:B:196:ASN:H	2.22	0.43
1:B:242:THR:HG22	1:B:247:VAL:HA	2.01	0.43
1:C:307:ASP:HA	1:C:310:ARG:HH11	1.84	0.43
1:B:300:LEU:HG	1:B:326:LEU:HD21	2.00	0.43
1:A:311:LYS:O	1:A:315:GLN:HG3	2.18	0.42
1:B:222:VAL:O	1:B:222:VAL:HG12	2.19	0.42
1:B:321:TRP:CE3	1:B:321:TRP:CA	3.03	0.42
1:A:220:ASP:HB2	1:A:224:ARG:HG2	2.02	0.42
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.46	0.42
1:C:211:LYS:HE2	1:C:211:LYS:CA	2.49	0.42
1:B:279:ASP:OD2	1:B:302:LYS:HE2	2.20	0.42
1:A:171:TRP:CG	1:A:288:PRO:HG3	2.55	0.42
1:A:215:ARG:HB3	1:A:228:TYR:HB2	2.01	0.42
1:B:38:ILE:HG23	1:B:38:ILE:O	2.19	0.42
1:B:143:PRO:HG3	1:B:147:ARG:CZ	2.50	0.41
1:C:108:LEU:N	1:C:108:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LYS:HB3	1:C:323:PRO:HD3	2.01	0.41
2:D:76:THR:OG1	2:D:78:MET:HG2	2.19	0.41
1:A:273:ASN:HA	1:A:274:PRO:HA	1.87	0.41
1:B:29:TRP:CZ2	1:B:142:PRO:HB2	2.55	0.41
1:B:307:ASP:HA	1:B:310:ARG:NE	2.35	0.41
2:D:14:MET:O	2:D:34:ARG:NH1	2.50	0.41
1:B:231:ILE:HG13	1:B:232:GLY:N	2.34	0.41
1:B:304:CYS:HA	1:B:309:GLU:OE2	2.20	0.41
1:C:137:LEU:HD22	1:C:137:LEU:HA	1.97	0.41
1:C:273:ASN:HA	1:C:274:PRO:HA	1.90	0.41
1:B:161:LEU:HD11	1:B:314:GLU:HG2	2.03	0.41
1:B:196:ASN:HD22	1:B:198:LEU:HG	1.85	0.41
1:C:239:PHE:O	1:C:250:GLU:HA	2.20	0.41
1:C:177:ASN:HD21	1:C:333:ASP:HB3	1.85	0.41
1:A:157:ASP:OD2	1:A:303:PRO:HB3	2.20	0.41
1:B:43:PRO:HG3	1:B:56:ASN:CG	2.41	0.41
1:B:209:ASP:OD1	1:B:212:GLN:HB2	2.21	0.41
2:E:109:GLU:HG2	2:E:109:GLU:O	2.21	0.41
1:B:310:ARG:HG2	1:B:310:ARG:NH1	2.36	0.40
1:C:311:LYS:HE3	1:C:311:LYS:CA	2.50	0.40
1:B:183:HIS:O	1:B:186:ILE:HG12	2.22	0.40
1:C:307:ASP:OD1	1:C:310:ARG:NH1	2.54	0.40
1:B:222:VAL:HG11	1:B:224:ARG:HH12	1.86	0.40
1:A:384:GLY:O	1:C:352:ASN:ND2	2.55	0.40
1:B:320:LYS:O	1:B:324:MET:HB3	2.22	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	382/392 (97%)	361 (94%)	17 (4%)	4 (1%)	15 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	382/392 (97%)	344 (90%)	34 (9%)	4 (1%)	15	6
1	C	386/392 (98%)	369 (96%)	15 (4%)	2 (0%)	29	17
2	D	101/115 (88%)	92 (91%)	9 (9%)	0	100	100
2	E	105/115 (91%)	100 (95%)	5 (5%)	0	100	100
All	All	1356/1406 (96%)	1266 (93%)	80 (6%)	10 (1%)	22	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	C	268	GLY
1	A	268	GLY
1	B	195	ASP
1	B	309	GLU
1	A	71	HIS
1	A	384	GLY
1	C	71	HIS
1	A	219	ASP
1	B	207	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/339 (98%)	323 (98%)	8 (2%)	49	40
1	B	331/339 (98%)	321 (97%)	10 (3%)	41	30
1	C	335/339 (99%)	326 (97%)	9 (3%)	44	34
2	D	81/93 (87%)	78 (96%)	3 (4%)	34	22
2	E	85/93 (91%)	84 (99%)	1 (1%)	71	68
All	All	1163/1203 (97%)	1132 (97%)	31 (3%)	44	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	46	LEU
1	A	92	TYR
1	A	137	LEU
1	A	220	ASP
1	A	356	PHE
1	A	368	LEU
1	A	385	LEU
1	B	36	LYS
1	B	46	LEU
1	B	92	TYR
1	B	137	LEU
1	B	158	MET
1	B	169	SER
1	B	195	ASP
1	B	311	LYS
1	B	321	TRP
1	B	356	PHE
1	C	10	LYS
1	C	11	ARG
1	C	46	LEU
1	C	92	TYR
1	C	137	LEU
1	C	311	LYS
1	C	314	GLU
1	C	356	PHE
1	C	368	LEU
2	D	6	LEU
2	D	33	TYR
2	D	37	ASP
2	E	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	196	ASN
1	A	379	GLN
1	B	234	HIS
1	B	298	GLN
1	B	372	HIS
1	C	177	ASN
1	C	234	HIS

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Mol	Chain	Res	Type
1	C	260	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	A	503	-	15,15,15	1.27	1 (6%)	21,21,21	0.70	0
4	FES	E	201	2	0,4,4	-	-	-	-	-
5	9CA	B	503	-	15,15,15	1.27	1 (6%)	21,21,21	0.69	0
4	FES	A	502	1	0,4,4	-	-	-	-	-
5	9CA	C	503	-	15,15,15	1.27	1 (6%)	21,21,21	0.67	0
4	FES	B	502	1	0,4,4	-	-	-	-	-
4	FES	D	201	2	0,4,4	-	-	-	-	-
4	FES	C	502	1	0,4,4	-	-	-	-	-

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	A	503	-	-	-	0/3/3/3
4	FES	E	201	2	-	-	0/1/1/1
5	9CA	B	503	-	-	-	0/3/3/3
4	FES	A	502	1	-	-	0/1/1/1
5	9CA	C	503	-	-	-	0/3/3/3
4	FES	B	502	1	-	-	0/1/1/1
4	FES	D	201	2	-	-	0/1/1/1
4	FES	C	502	1	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	9CA	C4B-C4A	-2.19	1.39	1.45
5	A	503	9CA	C4B-C4A	-2.18	1.39	1.45
5	C	503	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	201	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	384/392 (97%)	0.18	15 (3%) 39 49	24, 34, 57, 65	0
1	B	384/392 (97%)	0.86	59 (15%) 2 3	27, 48, 66, 71	0
1	C	388/392 (98%)	0.07	18 (4%) 32 42	22, 33, 48, 66	0
2	D	103/115 (89%)	1.55	39 (37%) 0 0	33, 54, 66, 69	0
2	E	107/115 (93%)	0.42	8 (7%) 14 22	34, 50, 61, 69	0
All	All	1366/1406 (97%)	0.46	139 (10%) 6 11	22, 40, 64, 71	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	LEU	9.3
2	D	5	TRP	8.5
1	B	385	LEU	8.4
1	B	305	ALA	7.1
2	D	95	VAL	7.1
1	B	221	VAL	7.0
1	B	321	TRP	6.9
1	B	210	ARG	6.8
2	D	4	ILE	6.0
2	D	96	LYS	5.6
1	B	324	MET	5.5
1	B	211	LYS	5.5
2	D	12	SER	5.4
1	B	317	PHE	5.4
1	B	304	CYS	5.3
2	D	101	TYR	5.3
1	B	312	LYS	4.9
2	D	97	GLU	4.8
1	B	315	GLN	4.8
2	D	103	ALA	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	308	GLU	4.5
2	D	11	ALA	4.5
2	D	6	LEU	4.5
1	B	313	TYR	4.5
1	B	316	GLU	4.4
1	B	306	ASN	4.4
1	C	270	LEU	4.4
1	B	307	ASP	4.3
2	D	36	GLY	4.3
2	D	39	PHE	4.3
1	B	209	ASP	4.3
2	E	25	VAL	4.1
1	B	301	GLY	4.1
2	D	13	ASP	4.1
2	D	8	VAL	4.0
1	B	219	ASP	4.0
1	C	389	HIS	4.0
2	D	7	LYS	4.0
2	D	98	GLY	4.0
2	D	25	VAL	4.0
2	D	94	GLU	4.0
2	E	109	GLU	3.9
1	A	384	GLY	3.9
1	C	175	VAL	3.9
2	D	35	VAL	3.9
2	D	100	VAL	3.9
1	C	178	GLY	3.8
1	C	388	HIS	3.8
2	D	15	GLN	3.8
1	C	221	VAL	3.8
1	B	311	LYS	3.7
1	A	221	VAL	3.7
1	B	222	VAL	3.6
2	D	9	CYS	3.6
1	C	208	GLY	3.5
2	D	93	VAL	3.4
1	B	191	ILE	3.4
2	E	97	GLU	3.3
2	D	10	ALA	3.3
1	C	387	HIS	3.3
1	B	244	GLY	3.3
1	B	303	PRO	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	209	ASP	3.3
2	E	98	GLY	3.3
1	A	253	TYR	3.3
1	B	208	GLY	3.2
1	B	212	GLN	3.2
2	D	14	MET	3.2
1	B	179	PHE	3.1
1	B	270	LEU	3.1
1	B	175	VAL	3.1
1	B	160	ILE	3.1
1	B	245	GLY	3.1
1	B	269	VAL	3.0
1	C	269	VAL	3.0
1	B	235	GLY	2.9
2	D	26	GLY	2.9
2	D	99	GLU	2.9
1	C	179	PHE	2.9
1	B	157	ASP	2.9
2	D	18	THR	2.9
2	E	26	GLY	2.7
2	D	102	VAL	2.7
1	B	362	ILE	2.7
1	A	308	GLU	2.6
1	B	309	GLU	2.6
1	C	174	ALA	2.6
2	D	16	PRO	2.6
1	B	322	LYS	2.6
2	E	6	LEU	2.6
1	B	14	GLY	2.6
1	B	193	VAL	2.5
2	D	106	LYS	2.5
1	B	262	ILE	2.5
1	A	287	VAL	2.5
1	A	311	LYS	2.5
1	B	302	LYS	2.5
2	D	105	GLU	2.5
1	B	328	GLY	2.4
1	C	264	ILE	2.4
1	B	258	VAL	2.4
1	B	320	LYS	2.4
1	A	220	ASP	2.3
2	D	37	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	286	TYR	2.3
1	A	174	ALA	2.3
2	D	17	GLY	2.3
2	D	104	GLY	2.3
2	E	101	TYR	2.3
1	C	173	LEU	2.3
1	B	69	CYS	2.3
1	B	218	ASP	2.3
1	A	195	ASP	2.2
1	B	155	ASP	2.2
1	B	268	GLY	2.2
2	D	59	ASP	2.2
1	B	255	GLU	2.2
1	C	212	GLN	2.2
1	B	310	ARG	2.2
1	A	285	TRP	2.2
1	B	231	ILE	2.1
1	B	234	HIS	2.1
1	A	324	MET	2.1
1	B	264	ILE	2.1
1	B	230	LEU	2.1
1	A	315	GLN	2.1
2	D	92	GLU	2.1
1	B	215	ARG	2.1
2	E	37	ASP	2.1
1	A	246	GLU	2.1
2	D	38	GLN	2.1
1	B	135	ILE	2.1
1	B	204	PHE	2.1
1	B	195	ASP	2.1
1	B	371	GLU	2.1
1	C	283	PHE	2.0
1	C	365	TRP	2.0
1	A	286	TYR	2.0
2	D	34	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	9CA	A	503	13/13	0.85	0.16	52,55,56,56	0
5	9CA	B	503	13/13	0.88	0.14	55,57,59,59	0
5	9CA	C	503	13/13	0.97	0.18	23,26,27,28	0
3	FE2	C	501	1/1	0.98	0.06	33,33,33,33	0
3	FE2	B	501	1/1	0.98	0.08	70,70,70,70	0
4	FES	D	201	4/4	0.99	0.06	34,38,38,40	0
4	FES	E	201	4/4	0.99	0.11	35,36,37,38	0
3	FE2	A	501	1/1	0.99	0.05	44,44,44,44	0
4	FES	A	502	4/4	0.99	0.14	25,25,26,29	0
4	FES	C	502	4/4	0.99	0.12	33,34,36,36	0
4	FES	B	502	4/4	1.00	0.13	27,27,31,31	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.