



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:45 PM UTC

PDB ID : 4NBD / pdb_00004nbd
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

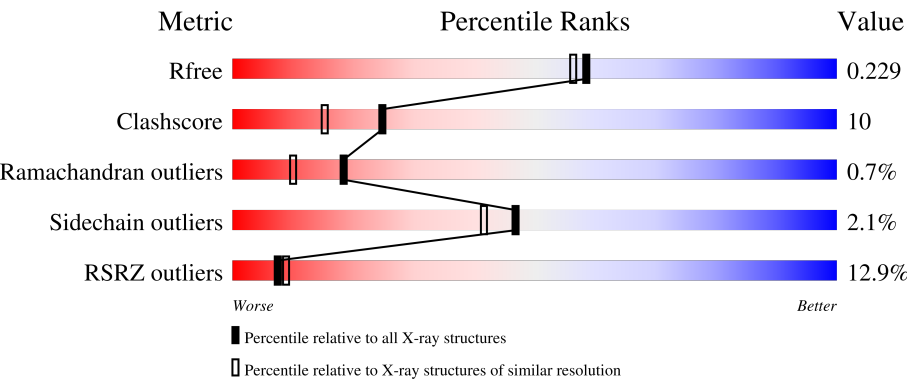
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 ≥ 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	6% 78% 19% ..
1	B	392	27% 66% 30% ..
1	C	392	3% 83% 14% ..
2	D	115	20% 72% 17% 10%
2	E	115	11% 75% 17% 7%

2 Entry composition

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
1	A	384	Total	C	N	O	S	0	0	0
			3092	1978	525	576	13			
1	B	384	Total	C	N	O	S	0	0	0
			3092	1978	525	576	13			
1	C	388	Total	C	N	O	S	0	0	0
			3131	2001	535	582	13			

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			

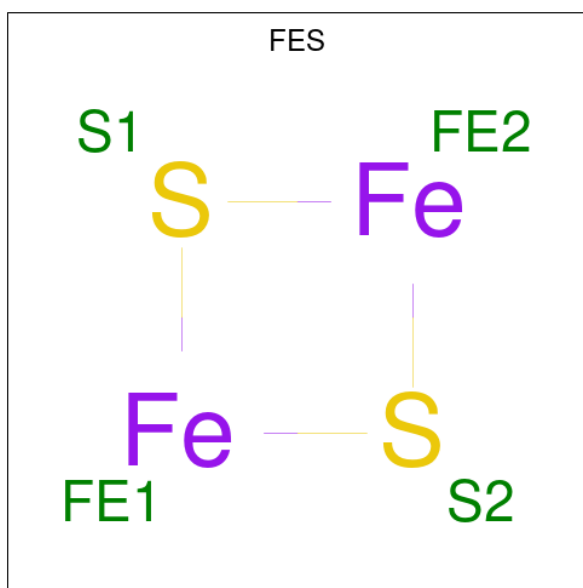
There are 16 discrepancies between the modelled and reference sequences:

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 (CCD ID: FE2) (formula: Fe).

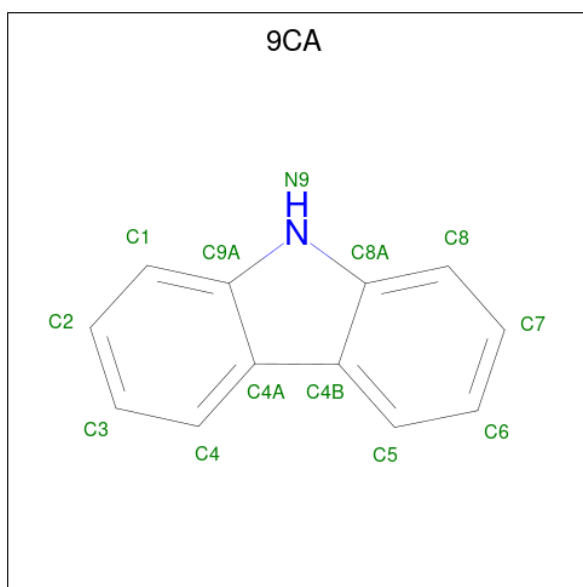
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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 (CCD ID: 9CA) (formula: $\text{C}_{12}\text{H}_9\text{N}$).



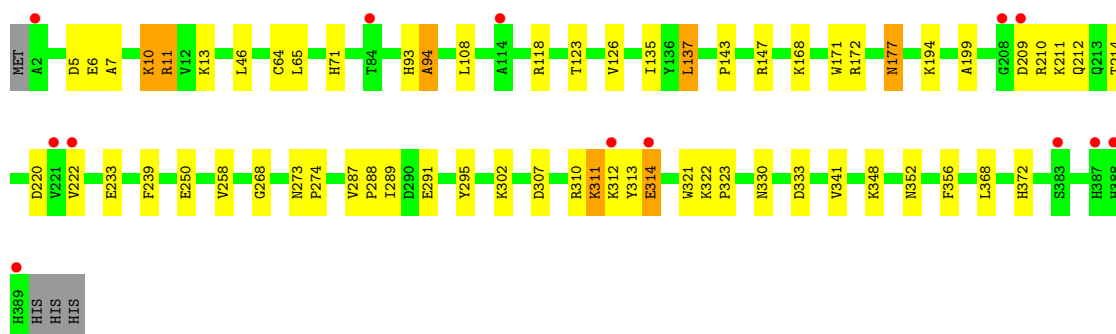
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			13	12	1		
5	B	1	Total	C	N	0	0
			13	12	1		
5	C	1	Total	C	N	0	0
			13	12	1		

- Molecule 6 is water.

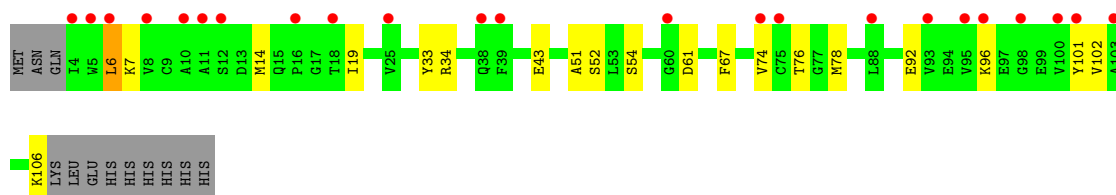
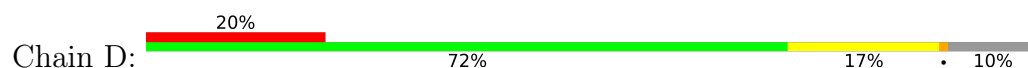
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total	O	0	0
			287	287		
6	B	196	Total	O	0	0
			196	196		
6	C	335	Total	O	0	0
			335	335		
6	D	37	Total	O	0	0
			37	37		
6	E	42	Total	O	0	0
			42	42		

- Molecule 1: Terminal oxygenase component of carbazole

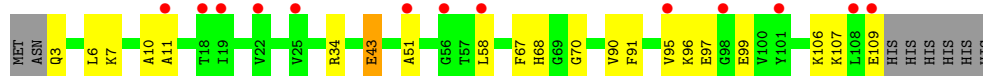
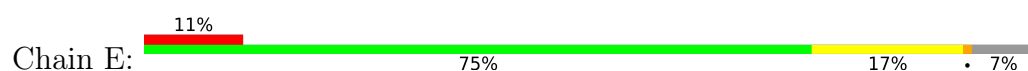




• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.34Å 88.20Å 108.11Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	32.63 – 1.95 32.63 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.63-1.95) 99.4 (32.63-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.37 (at 1.95Å)	Xtriage
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 ²)	34.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11827	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/3175	0.89	8/4312 (0.2%)
1	B	0.33	0/3175	0.85	6/4312 (0.1%)
1	C	0.39	0/3217	0.89	10/4369 (0.2%)
2	D	0.32	0/775	0.81	1/1055 (0.1%)
2	E	0.32	0/810	0.82	2/1101 (0.2%)
All	All	0.36	0/11152	0.86	27/15149 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	N-CA-C	-9.27	97.15	110.59
2	E	43	GLU	N-CA-C	-7.16	101.08	110.53
1	B	289	ILE	N-CA-C	-6.77	105.24	111.67
1	C	289	ILE	N-CA-C	-6.62	105.39	111.67
1	A	289	ILE	N-CA-C	-6.54	105.46	111.67
1	C	199	ALA	N-CA-C	-6.21	97.59	108.20
1	A	341	VAL	N-CA-C	6.20	116.87	110.36
1	A	94	ALA	N-CA-C	6.05	119.96	112.58
1	B	94	ALA	N-CA-C	5.89	119.78	112.24
1	C	372	HIS	N-CA-C	5.86	120.13	112.92
1	A	357	GLU	N-CA-C	5.70	120.77	111.37
1	B	95	TRP	N-CA-C	-5.65	101.49	109.96
1	B	110	ASN	CA-C-N	5.61	125.32	119.82
1	B	110	ASN	C-N-CA	5.61	125.32	119.82
1	A	168	LYS	N-CA-C	5.58	118.26	109.39
1	B	177	ASN	N-CA-C	-5.36	106.43	113.12
1	C	321	TRP	N-CA-C	5.33	117.09	111.28
1	A	160	ILE	N-CA-C	5.28	115.56	108.17
1	A	95	TRP	N-CA-C	-5.26	102.07	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	VAL	N-CA-C	5.26	115.88	110.36
1	C	13	LYS	N-CA-C	5.22	118.43	111.75
1	C	94	ALA	N-CA-C	5.16	119.53	113.23
1	C	330	ASN	N-CA-C	5.11	119.14	113.01
2	E	70	GLY	N-CA-C	-5.10	104.71	112.51
2	D	43	GLU	N-CA-C	-5.10	103.42	110.35
1	C	177	ASN	N-CA-C	-5.04	105.44	112.45
1	C	168	LYS	N-CA-C	5.01	117.24	108.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3092	0	3004	51	0
1	B	3092	0	3004	93	0
1	C	3131	0	3031	47	0
2	D	759	0	732	14	0
2	E	794	0	770	14	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11827	0	10568	211	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 (211) 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:HE3	1:C:10:LYS:HA	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:HD13	1:A:385:LEU:H	1.58	0.69
1:A:2:ALA:HA	6:A:796:HOH:O	1.94	0.68
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:158:MET:HE1	1:B:301:GLY:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:280:MET:HE3	1:A:313:TYR:HE1	1.67	0.58
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:HE2	1:C:211:LYS:N	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:37:GLU:O	1:B:44:LYS:HE2	2.08	0.54
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.89	0.53
1:B:36:LYS:HD2	1:B:36:LYS:O	2.08	0.53
1:B:209:ASP:CG	1:B:212:GLN:HB2	2.34	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:A:249:ARG:HG3	1:A:250:GLU:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:36:LYS:HD2	1:B:36:LYS:C	2.39	0.48
1:B:194:LYS:C	1:B:196:ASN:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:43:PRO:HG3	1:B:56:ASN:CG	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:280:MET:HE1	1:B:321:TRP:CD1	2.54	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
2:E:96:LYS:O	2:E:97:GLU:HB2	2.19	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:C:118:ARG:HH12	2:E:43:GLU:CD	2.27	0.42
1:B:222:VAL:HG12	1:B:222:VAL:O	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:O	1:B:38:ILE:HG23	2.19	0.42
1:A:280:MET:HE3	1:A:313:TYR:CE1	2.52	0.41
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
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:B:271:LYS:NZ	6:B:688:HOH:O	2.52	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:O	1:B:197:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:152:ASN:HB3	1:B:281:MET:HE1	2.02	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%)	12	5
1	B	382/392 (97%)	344 (90%)	34 (9%)	4 (1%)	12	5
1	C	386/392 (98%)	369 (96%)	15 (4%)	2 (0%)	24	16
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%)	18	10

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 ⓘ

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%)	325 (98%)	6 (2%)	51	47
1	B	331/339 (98%)	324 (98%)	7 (2%)	47	41
1	C	335/339 (99%)	327 (98%)	8 (2%)	43	36
2	D	81/93 (87%)	79 (98%)	2 (2%)	42	34
2	E	85/93 (91%)	83 (98%)	2 (2%)	43	36
All	All	1163/1203 (97%)	1138 (98%)	25 (2%)	47	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	46	LEU
1	A	137	LEU
1	A	356	PHE
1	A	368	LEU
1	A	385	LEU
1	B	46	LEU
1	B	137	LEU
1	B	158	MET
1	B	169	SER

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Mol	Chain	Res	Type
1	B	311	LYS
1	B	321	TRP
1	B	360	GLU
1	C	10	LYS
1	C	11	ARG
1	C	46	LEU
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	E	3	GLN
2	E	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	213	GLN
1	A	234	HIS
1	A	298	GLN
1	A	379	GLN
1	B	196	ASN
1	B	212	GLN
1	B	234	HIS
1	B	277	ASN
1	B	298	GLN
1	B	372	HIS
1	C	127	GLN
1	C	177	ASN
1	C	234	HIS
1	C	315	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	503	-	15,15,15	1.37	3 (20%)	21,21,21	0.98	0
4	FES	B	502	1	0,4,4	-	-	-		
4	FES	C	502	1	0,4,4	-	-	-		
5	9CA	A	503	-	15,15,15	1.37	3 (20%)	21,21,21	1.00	0
4	FES	A	502	1	0,4,4	-	-	-		
4	FES	D	201	2	0,4,4	-	-	-		
5	9CA	C	503	-	15,15,15	1.36	3 (20%)	21,21,21	0.97	0
4	FES	E	201	2	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	B	503	-	-	-	0/3/3/3
4	FES	B	502	1	-	-	0/1/1/1
4	FES	C	502	1	-	-	0/1/1/1
5	9CA	A	503	-	-	-	0/3/3/3
4	FES	A	502	1	-	-	0/1/1/1
4	FES	D	201	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	9CA	C	503	-	-	-	0/3/3/3
4	FES	E	201	2	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	9CA	C4B-C4A	-2.85	1.39	1.46
5	A	503	9CA	C9A-N9	-2.83	1.33	1.38
5	A	503	9CA	C4B-C4A	-2.83	1.39	1.46
5	C	503	9CA	C4B-C4A	-2.80	1.39	1.46
5	B	503	9CA	C9A-N9	-2.78	1.33	1.38
5	A	503	9CA	C8A-N9	-2.78	1.33	1.38
5	C	503	9CA	C9A-N9	-2.76	1.33	1.38
5	C	503	9CA	C8A-N9	-2.75	1.33	1.38
5	B	503	9CA	C8A-N9	-2.75	1.33	1.38

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	C	502	FES	1	0
4	E	201	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/392 (97%)	0.33	23 (5%) 27 32	24, 34, 57, 65	0
1	B	384/392 (97%)	1.41	104 (27%) 1 1	27, 48, 66, 71	0
1	C	388/392 (98%)	0.23	13 (3%) 48 54	22, 33, 48, 66	0
2	D	103/115 (89%)	1.36	23 (22%) 2 2	33, 54, 66, 69	0
2	E	107/115 (93%)	1.01	13 (12%) 8 10	34, 50, 61, 69	0
All	All	1366/1406 (97%)	0.74	176 (12%) 7 9	22, 40, 64, 71	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	PHE	6.0
1	B	301	GLY	5.9
1	B	221	VAL	5.6
1	B	321	TRP	5.6
1	B	324	MET	5.2
1	A	385	LEU	5.1
1	B	384	GLY	5.0
1	B	385	LEU	4.8
1	B	230	LEU	4.5
1	A	384	GLY	4.4
1	B	191	ILE	4.4
2	D	4	ILE	4.2
1	B	315	GLN	4.1
1	B	258	VAL	4.1
1	B	238	VAL	4.0
1	B	303	PRO	4.0
1	B	275	TRP	4.0
1	A	221	VAL	4.0
1	A	246	GLU	3.9
1	B	205	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	3.8
1	B	325	ALA	3.8
2	D	95	VAL	3.8
1	B	305	ALA	3.7
1	B	211	LYS	3.7
1	B	236	VAL	3.7
2	D	5	TRP	3.7
1	A	220	ASP	3.6
1	B	304	CYS	3.6
1	A	253	TYR	3.6
1	B	160	ILE	3.6
1	B	316	GLU	3.5
1	C	388	HIS	3.5
2	D	39	PHE	3.5
1	B	272	VAL	3.5
1	B	204	PHE	3.5
1	B	154	LEU	3.5
1	B	223	GLY	3.5
2	D	6	LEU	3.4
1	B	208	GLY	3.4
1	B	222	VAL	3.4
1	B	227	VAL	3.3
1	B	210	ARG	3.3
2	D	101	TYR	3.2
1	A	218	ASP	3.2
1	B	158	MET	3.2
1	B	150	PRO	3.2
1	B	235	GLY	3.2
1	B	262	ILE	3.2
1	B	155	ASP	3.2
1	B	157	ASP	3.2
1	A	252	ALA	3.1
1	B	277	ASN	3.1
1	B	253	TYR	3.1
1	A	260	ASN	3.1
1	B	14	GLY	3.1
1	B	192	LEU	3.0
1	B	266	LEU	3.0
1	B	193	VAL	3.0
1	C	2	ALA	3.0
1	B	153	PHE	3.0
1	B	239	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	129	ALA	2.9
1	A	383	SER	2.9
1	B	312	LYS	2.9
2	D	25	VAL	2.9
2	E	98	GLY	2.9
1	C	222	VAL	2.8
1	B	323	PRO	2.8
1	B	259	ALA	2.8
1	B	206	PRO	2.8
1	B	132	CYS	2.8
2	E	58	LEU	2.8
2	E	18	THR	2.8
2	D	88	LEU	2.8
1	B	231	ILE	2.8
1	B	161	LEU	2.7
1	A	261	ASP	2.7
1	B	280	MET	2.7
2	D	98	GLY	2.7
1	B	299	THR	2.7
1	B	311	LYS	2.7
2	D	93	VAL	2.7
2	E	22	VAL	2.7
2	D	38	GLN	2.7
2	D	18	THR	2.6
1	B	308	GLU	2.6
1	B	232	GLY	2.6
2	E	108	LEU	2.6
2	E	25	VAL	2.6
1	B	234	HIS	2.5
1	B	146	ALA	2.5
2	D	10	ALA	2.5
2	E	101	TYR	2.5
1	C	389	HIS	2.5
1	A	2	ALA	2.5
1	B	2	ALA	2.5
1	B	274	PRO	2.5
1	B	229	ASP	2.5
1	B	261	ASP	2.5
1	B	254	GLY	2.5
1	B	215	ARG	2.5
2	D	11	ALA	2.5
1	C	221	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	283	PHE	2.4
1	B	257	ILE	2.4
1	C	209	ASP	2.4
1	B	328	GLY	2.4
1	B	300	LEU	2.4
1	C	114	ALA	2.4
1	B	269	VAL	2.4
1	C	312	LYS	2.4
1	B	209	ASP	2.4
1	B	329	PHE	2.4
1	B	126	VAL	2.4
1	B	133	VAL	2.4
1	A	324	MET	2.4
1	B	319	SER	2.4
1	B	60	GLY	2.3
1	B	226	GLY	2.3
1	B	216	VAL	2.3
1	B	145	LEU	2.3
1	B	326	LEU	2.3
1	A	245	GLY	2.3
2	D	96	LYS	2.3
1	C	383	SER	2.3
1	B	175	VAL	2.3
2	D	100	VAL	2.3
1	B	202	LEU	2.3
2	D	75	CYS	2.3
1	A	210	ARG	2.2
1	A	305	ALA	2.2
1	A	314	GLU	2.2
1	B	148	ASP	2.2
2	E	19	ILE	2.2
1	B	212	GLN	2.2
2	D	8	VAL	2.2
1	B	159	GLU	2.2
1	A	219	ASP	2.2
1	B	228	TYR	2.2
1	C	314	GLU	2.2
1	A	209	ASP	2.2
1	B	251	GLY	2.2
1	B	142	PRO	2.2
1	B	361	ALA	2.2
2	D	103	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	311	LYS	2.2
1	A	195	ASP	2.2
2	D	12	SER	2.2
1	B	207	GLY	2.2
2	D	60	GLY	2.2
1	B	380	ALA	2.2
1	B	310	ARG	2.2
2	E	109	GLU	2.1
2	D	74	VAL	2.1
2	E	56	GLY	2.1
2	E	95	VAL	2.1
1	B	322	LYS	2.1
1	B	278	PRO	2.1
1	B	306	ASN	2.1
1	C	84	THR	2.1
1	C	387	HIS	2.1
1	A	196	ASN	2.1
2	D	16	PRO	2.1
1	B	219	ASP	2.1
1	C	208	GLY	2.0
1	B	273	ASN	2.0
1	B	217	VAL	2.0
1	B	247	VAL	2.0
1	B	265	TRP	2.0
1	B	270	LEU	2.0
2	E	11	ALA	2.0
2	E	51	ALA	2.0
1	A	308	GLU	2.0
1	B	225	LYS	2.0
1	B	281	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	9CA	A	503	13/13	0.84	0.13	52,55,56,56	0
5	9CA	B	503	13/13	0.87	0.14	55,57,59,59	0
5	9CA	C	503	13/13	0.96	0.05	23,26,27,28	0
3	FE2	A	501	1/1	0.98	0.07	44,44,44,44	0
3	FE2	B	501	1/1	0.98	0.05	70,70,70,70	0
3	FE2	C	501	1/1	0.98	0.07	33,33,33,33	0
4	FES	D	201	4/4	0.99	0.04	34,38,38,40	0
4	FES	E	201	4/4	0.99	0.04	35,36,37,38	0
4	FES	A	502	4/4	0.99	0.04	25,25,26,29	0
4	FES	B	502	4/4	0.99	0.03	27,27,31,31	0
4	FES	C	502	4/4	0.99	0.04	33,34,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.