Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 06:18 PM EDT

PDB ID	:	4NBE
Title	:	Fluorene-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	:	2.10 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:

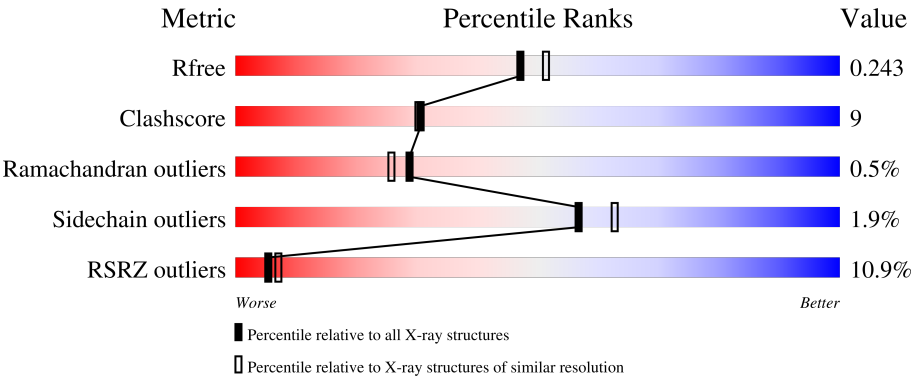
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	7% 83% 14% .
1	B	392	12% 66% 31% ..
1	C	392	7% 80% 18% ..
2	D	115	32% 69% 21% 10%
2	E	115	11% 83% 14% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11686 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	383	Total	C	N	O	S	0	0	0
			3084	1972	524	575	13			
1	B	385	Total	C	N	O	S	0	0	0
			3101	1983	526	579	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	111	Total	C	N	O	S	0	0	0
			834	523	145	159	7			

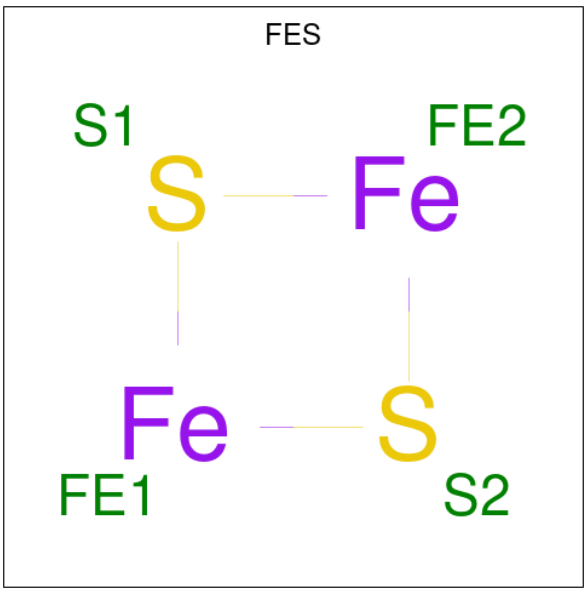
There are 16 discrepancies between the modelled and reference sequences:

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).

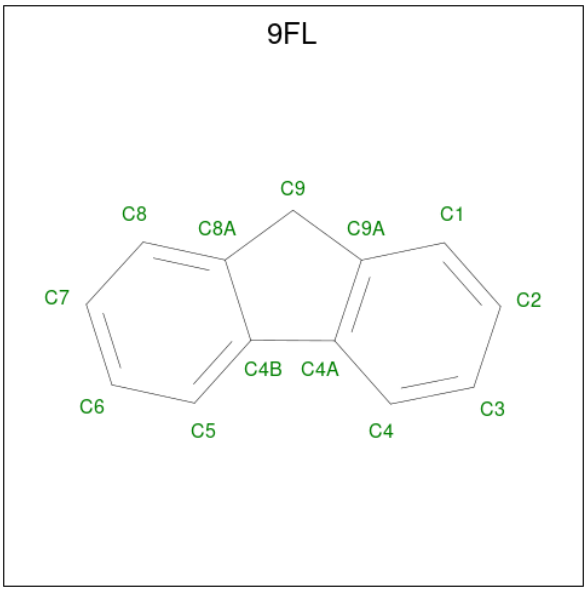
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 5 is 9H-fluorene (three-letter code: 9FL) (formula: $C_{13}H_{10}$).



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

- Molecule 6 is water.

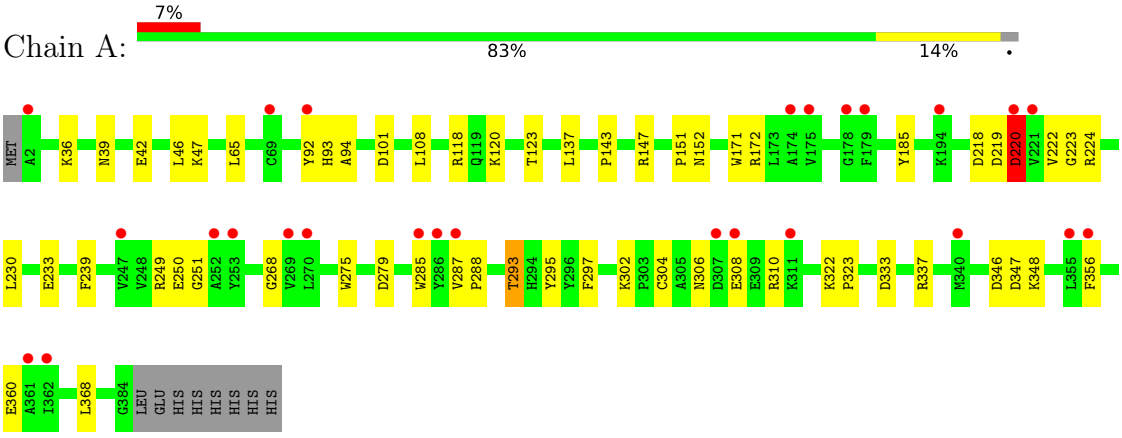
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	262	Total O 262 262	0	0
6	B	155	Total O 155 155	0	0
6	C	242	Total O 242 242	0	0
6	D	28	Total O 28 28	0	0
6	E	41	Total O 41 41	0	0

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.

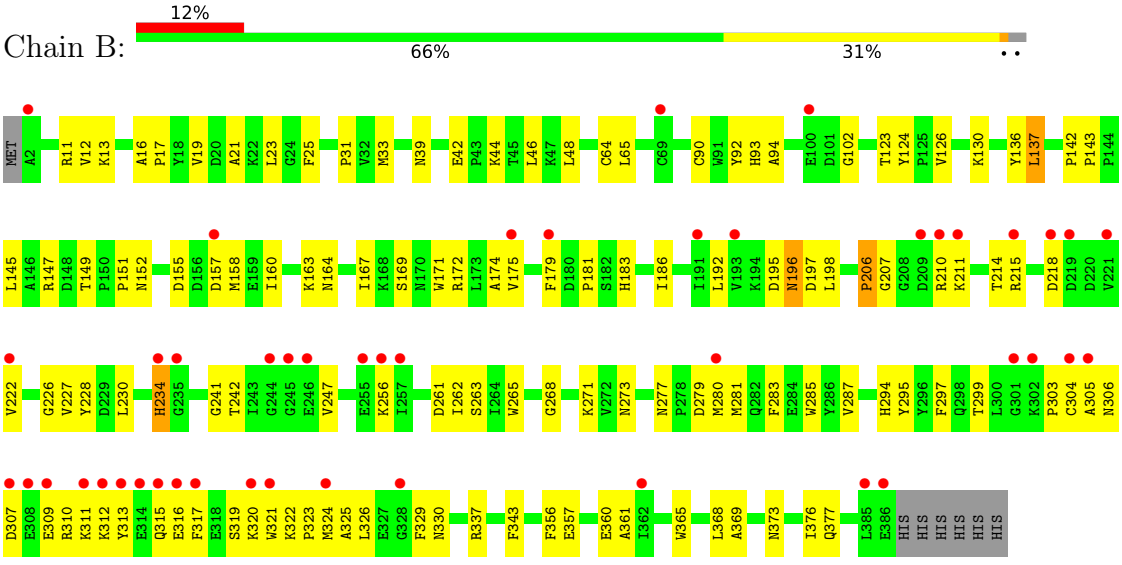
• Molecule 1: Terminal oxygenase component of carbazole

Chain A:



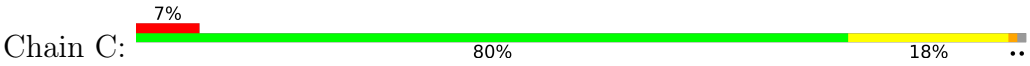
• Molecule 1: Terminal oxygenase component of carbazole

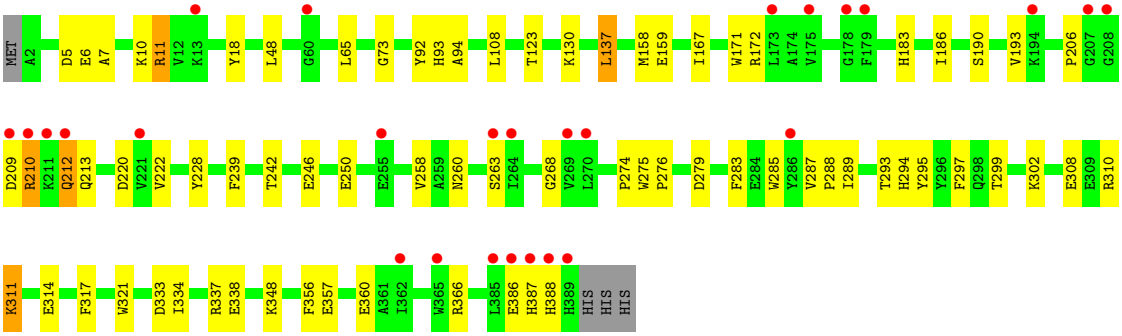
Chain B:



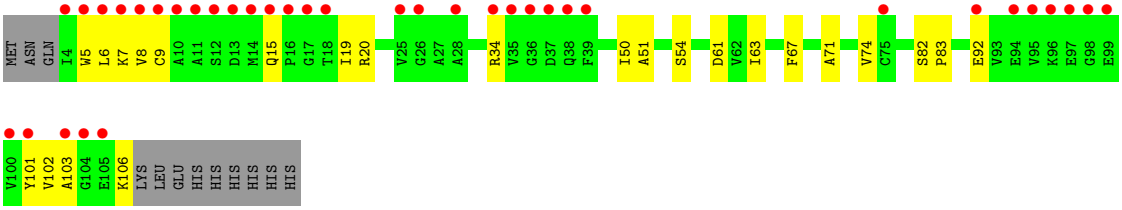
• Molecule 1: Terminal oxygenase component of carbazole

Chain C:

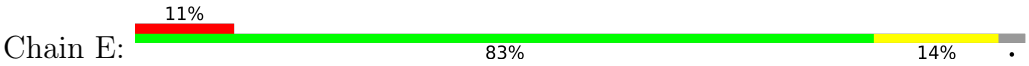


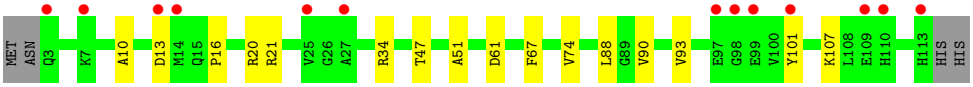


• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.45Å 88.26Å 108.62Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	33.75 – 2.10 33.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.75-2.10) 99.2 (33.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.20 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.252 0.211 , 0.243	Depositor DCC
R_{free} test set	5182 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11686	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 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FES, FE2, 9FL

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	0.35	0/3167	0.63	1/4301 (0.0%)
1	B	0.31	0/3184	0.58	0/4324
1	C	0.35	0/3217	0.61	0/4369
2	D	0.31	0/775	0.57	0/1055
2	E	0.32	0/854	0.61	0/1161
All	All	0.33	0/11197	0.60	1/15210 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ASP	N-CA-C	-6.08	94.58	111.00

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	3084	0	2993	33	0
1	B	3101	0	3010	89	0
1	C	3131	0	3031	53	0
2	D	759	0	732	18	0
2	E	834	0	798	10	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	1	0
4	B	4	0	0	1	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
5	A	13	0	10	2	0
5	C	13	0	10	0	0
6	A	262	0	0	5	0
6	B	155	0	0	1	0
6	C	242	0	0	2	0
6	D	28	0	0	1	0
6	E	41	0	0	1	0
All	All	11686	0	10584	198	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 9.

All (198) 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	1.16	1.10
1:A:230:LEU:HB3	1:A:233:GLU:HG3	1.51	0.92
1:C:357:GLU:O	1:C:360:GLU:HG2	1.75	0.87
1:C:11:ARG:HH11	1:C:11:ARG:CB	1.94	0.79
1:B:322:LYS:HB3	1:B:323:PRO:HD3	1.64	0.79
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.67	0.77
1:C:260:ASN:HB2	6:C:817:HOH:O	1.86	0.74
1:C:6:GLU:O	1:C:10:LYS:HD3	1.86	0.74
1:B:196:ASN:O	1:B:256:LYS:HD2	1.87	0.74
2:E:47:THR:HG23	2:E:88:LEU:HD23	1.71	0.73
1:B:192:LEU:HD13	1:B:324:MET:HB3	1.72	0.69
1:B:261:ASP:HB3	1:B:273:ASN:O	1.92	0.68
1:B:241:GLY:HA2	6:B:688:HOH:O	1.92	0.68
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.75	0.67
1:C:311:LYS:HE3	1:C:311:LYS:HA	1.77	0.67
1:B:311:LYS:O	1:B:315:GLN:HG3	1.95	0.66
1:C:209:ASP:HB3	1:C:212:GLN:NE2	2.11	0.66
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ALA:CB	1:B:337:ARG:HD3	2.27	0.64
1:C:220:ASP:OD1	1:C:222:VAL:HG22	1.97	0.64
1:C:386:GLU:HG2	1:C:387:HIS:N	2.12	0.63
1:A:220:ASP:HB2	1:A:224:ARG:HB2	1.81	0.62
1:B:277:ASN:HB3	1:B:279:ASP:OD1	2.00	0.62
2:D:20:ARG:HH11	2:D:20:ARG:HG2	1.65	0.62
1:C:11:ARG:HB3	1:C:11:ARG:NH1	2.01	0.62
1:B:227:VAL:HG23	1:B:368:LEU:HD22	1.81	0.62
1:C:209:ASP:HB3	1:C:212:GLN:CD	2.21	0.62
2:D:6:LEU:HD23	2:D:102:VAL:O	2.00	0.61
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.82	0.61
1:B:285:TRP:HB2	1:B:297:PHE:HB3	1.83	0.60
1:C:93:HIS:HB2	4:C:502:FES:S1	2.42	0.60
1:B:174:ALA:HB2	1:B:337:ARG:HD3	1.83	0.60
2:E:90:VAL:HG23	2:E:107:LYS:HB2	1.84	0.60
1:A:39:ASN:HB2	1:A:42:GLU:OE1	2.02	0.60
1:B:210:ARG:HH22	2:E:21:ARG:HH12	1.50	0.59
2:D:92:GLU:OE2	2:D:106:LYS:HE2	2.02	0.59
1:B:155:ASP:HB2	1:B:158:MET:HB2	1.83	0.59
1:B:206:PRO:HG2	1:B:357:GLU:HB3	1.84	0.59
2:D:7:LYS:HG2	2:D:101:TYR:HE1	1.67	0.58
1:B:11:ARG:HH21	1:C:388:HIS:CE1	2.22	0.58
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.85	0.57
1:B:167:ILE:HB	1:B:294:HIS:CE1	2.39	0.57
1:B:326:LEU:O	1:B:330:ASN:HB2	2.05	0.56
1:A:47:LYS:HE2	6:A:753:HOH:O	2.04	0.56
1:B:207:GLY:HA3	1:B:234:HIS:O	2.06	0.56
1:B:183:HIS:O	1:B:186:ILE:HG12	2.06	0.56
1:B:228:TYR:CD1	1:B:263:SER:HB3	2.40	0.56
1:A:249:ARG:HG3	1:A:250:GLU:N	2.21	0.56
1:B:12:VAL:HG21	1:B:19:VAL:HG21	1.87	0.56
1:B:21:ALA:HB2	1:B:376:ILE:HD12	1.88	0.55
1:B:304:CYS:HB3	1:B:309:GLU:HB3	1.88	0.55
1:B:305:ALA:HB3	1:B:309:GLU:OE1	2.05	0.55
1:B:280:MET:HE3	1:B:313:TYR:HE1	1.72	0.55
2:D:51:ALA:HB2	2:D:67:PHE:CD2	2.41	0.55
1:A:101:ASP:O	1:A:120:LYS:HE2	2.07	0.55
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.88	0.55
1:A:360:GLU:OE2	2:D:50:ILE:HD12	2.05	0.55
1:B:305:ALA:O	1:B:306:ASN:HB3	2.07	0.55
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ASP:O	2:D:74:VAL:HG22	2.07	0.54
1:B:175:VAL:HG11	1:B:365:TRP:CE2	2.43	0.54
6:A:754:HOH:O	1:C:348:LYS:HE3	2.08	0.54
1:C:130:LYS:NZ	1:C:158:MET:HB3	2.22	0.54
1:B:312:LYS:O	1:B:316:GLU:HG3	2.08	0.54
1:B:198:LEU:HD23	1:B:256:LYS:CB	2.38	0.53
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.90	0.53
2:D:103:ALA:HB1	6:D:310:HOH:O	2.07	0.53
1:B:198:LEU:HD23	1:B:256:LYS:HB2	1.90	0.53
1:A:304:CYS:CB	1:A:310:ARG:HG3	2.38	0.53
2:D:19:ILE:HG21	2:D:54:SER:HA	1.91	0.53
1:B:13:LYS:HE2	6:E:340:HOH:O	2.09	0.52
2:D:7:LYS:HG2	2:D:101:TYR:CE1	2.43	0.52
1:A:219:ASP:OD1	1:A:223:GLY:HA2	2.09	0.52
1:A:275:TRP:CZ3	5:A:503:9FL:H3	2.46	0.51
2:D:6:LEU:HD21	2:D:102:VAL:HG13	1.91	0.51
1:C:228:TYR:CD1	1:C:263:SER:HB3	2.46	0.51
1:B:65:LEU:HD21	1:B:102:GLY:HA2	1.91	0.51
1:C:310:ARG:O	1:C:314:GLU:HG3	2.09	0.51
1:C:311:LYS:HE3	1:C:311:LYS:CA	2.41	0.51
1:B:31:PRO:HB2	1:B:297:PHE:CE2	2.45	0.51
1:C:212:GLN:N	1:C:212:GLN:OE1	2.43	0.51
1:B:242:THR:HG22	1:B:247:VAL:HG22	1.93	0.51
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.44	0.51
1:C:48:LEU:HD23	1:C:137:LEU:HD23	1.93	0.50
1:C:258:VAL:HA	1:C:274:PRO:HG2	1.94	0.50
1:C:360:GLU:HG3	6:C:830:HOH:O	2.10	0.50
1:A:293:THR:HG21	6:A:736:HOH:O	2.11	0.50
1:B:25:PHE:CD1	1:B:373:ASN:HB2	2.46	0.50
1:B:33:MET:SD	1:B:44:LYS:HD3	2.51	0.50
1:B:48:LEU:HD23	1:B:137:LEU:HD23	1.94	0.50
1:B:130:LYS:HB3	1:B:160:ILE:HB	1.93	0.50
1:B:325:ALA:O	1:B:329:PHE:HB3	2.12	0.50
1:B:196:ASN:ND2	1:B:198:LEU:HD21	2.27	0.49
1:B:196:ASN:HD22	1:B:198:LEU:HD21	1.77	0.49
1:C:283:PHE:HB2	1:C:299:THR:OG1	2.13	0.49
1:C:183:HIS:O	1:C:186:ILE:HG12	2.12	0.49
2:E:61:ASP:O	2:E:74:VAL:HG22	2.12	0.49
1:A:93:HIS:HB2	4:A:502:FES:S1	2.52	0.49
1:B:214:THR:HG21	1:B:361:ALA:HA	1.94	0.48
1:B:210:ARG:NH2	2:E:21:ARG:HH12	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.95	0.48
1:C:333:ASP:O	1:C:337:ARG:HG3	2.13	0.48
1:B:215:ARG:HB3	1:B:228:TYR:HB2	1.94	0.48
1:B:215:ARG:HB2	1:B:230:LEU:HD11	1.95	0.48
1:C:279:ASP:OD2	1:C:302:LYS:HE3	2.13	0.48
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.48	0.48
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.48	0.48
1:C:5:ASP:OD2	1:C:7:ALA:HB3	2.13	0.48
2:E:16:PRO:HA	2:E:34:ARG:HG2	1.95	0.48
1:B:310:ARG:HG2	1:B:310:ARG:HH11	1.79	0.48
1:B:357:GLU:H	1:B:357:GLU:CD	2.17	0.47
1:C:210:ARG:HG2	1:C:210:ARG:O	2.15	0.47
1:A:239:PHE:O	1:A:251:GLY:N	2.47	0.47
5:A:503:9FL:H7	6:A:643:HOH:O	2.14	0.47
1:C:171:TRP:CG	1:C:288:PRO:HG3	2.49	0.47
1:A:348:LYS:HD2	6:A:821:HOH:O	2.15	0.47
1:C:239:PHE:O	1:C:250:GLU:HA	2.15	0.47
1:B:179:PHE:O	1:B:181:PRO:HD3	2.15	0.47
1:B:151:PRO:O	1:B:152:ASN:HB2	2.15	0.46
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.45	0.46
1:B:196:ASN:HD22	1:B:198:LEU:CG	2.28	0.46
2:E:20:ARG:HG2	2:E:20:ARG:HH11	1.81	0.46
1:B:317:PHE:HA	1:B:321:TRP:HB2	1.97	0.46
1:A:171:TRP:CG	1:A:288:PRO:HG3	2.51	0.46
1:A:304:CYS:HB3	1:A:310:ARG:HG3	1.97	0.46
1:A:322:LYS:HB3	1:A:323:PRO:CD	2.46	0.46
1:B:281:MET:HE3	1:B:283:PHE:CE2	2.51	0.46
1:B:316:GLU:HA	1:B:319:SER:OG	2.16	0.46
1:A:151:PRO:O	1:A:152:ASN:HB2	2.16	0.45
1:C:308:GLU:H	1:C:308:GLU:CD	2.20	0.45
2:D:15:GLN:C	2:D:34:ARG:HD3	2.37	0.45
1:B:369:ALA:O	1:B:373:ASN:HB3	2.16	0.45
1:B:157:ASP:OD1	1:B:303:PRO:HB3	2.16	0.45
1:C:11:ARG:HH11	1:C:11:ARG:CG	2.29	0.45
2:D:8:VAL:O	2:D:9:CYS:HB3	2.16	0.45
1:C:108:LEU:N	1:C:108:LEU:HD12	2.32	0.45
1:B:198:LEU:HA	1:B:256:LYS:HB2	1.99	0.45
1:B:281:MET:HE3	1:B:283:PHE:CZ	2.51	0.45
1:A:222:VAL:CG2	1:A:224:ARG:HG3	2.46	0.45
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.47	0.45
1:B:175:VAL:HG11	1:B:365:TRP:NE1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.47	0.44
1:B:136:TYR:CD2	1:B:142:PRO:HB3	2.52	0.44
1:B:218:ASP:O	1:B:218:ASP:OD1	2.34	0.44
1:A:218:ASP:O	1:A:219:ASP:HB2	2.16	0.44
1:B:39:ASN:HB2	1:B:42:GLU:OE1	2.17	0.44
2:D:92:GLU:HB2	2:D:103:ALA:HB3	1.99	0.44
1:A:279:ASP:OD2	1:A:302:LYS:HE3	2.18	0.44
1:B:64:CYS:HB3	1:B:124:TYR:O	2.18	0.44
1:B:163:LYS:HG2	1:B:164:ASN:N	2.33	0.44
1:B:143:PRO:HG3	1:B:147:ARG:CZ	2.48	0.43
1:A:306:ASN:OD1	1:A:308:GLU:HB2	2.19	0.43
1:C:190:SER:HB3	1:C:193:VAL:HG23	2.00	0.43
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.53	0.43
1:B:320:LYS:HG3	1:B:324:MET:HG3	1.99	0.43
1:C:285:TRP:HB2	1:C:297:PHE:HB3	2.00	0.43
1:C:334:ILE:O	1:C:338:GLU:HG3	2.18	0.43
1:A:346:ASP:O	1:A:347:ASP:HB2	2.19	0.43
1:B:23:LEU:HD23	1:B:377:GLN:HG3	2.01	0.43
1:B:283:PHE:HB2	1:B:299:THR:OG1	2.19	0.42
1:C:289:ILE:HB	1:C:293:THR:OG1	2.18	0.42
1:B:93:HIS:HB2	4:B:502:FES:S1	2.60	0.42
1:B:196:ASN:HD22	1:B:198:LEU:CD2	2.32	0.42
1:B:234:HIS:ND1	1:B:234:HIS:N	2.67	0.42
2:D:82:SER:HB2	2:D:83:PRO:HA	2.02	0.42
2:E:10:ALA:HB3	2:E:13:ASP:OD2	2.19	0.42
1:C:167:ILE:HB	1:C:294:HIS:CE1	2.55	0.42
2:D:63:ILE:O	2:D:71:ALA:HA	2.19	0.42
1:B:222:VAL:O	1:B:222:VAL:HG12	2.19	0.42
1:B:320:LYS:O	1:B:323:PRO:HD2	2.19	0.42
1:B:145:LEU:O	1:B:149:THR:HG23	2.20	0.42
1:A:118:ARG:HH11	1:A:118:ARG:HG2	1.85	0.41
1:A:333:ASP:O	1:A:337:ARG:HG3	2.20	0.41
1:B:211:LYS:HE3	1:B:211:LYS:HB3	1.89	0.41
1:B:228:TYR:CE1	1:B:263:SER:HB3	2.55	0.41
1:B:226:GLY:HA3	1:B:265:TRP:CE3	2.55	0.41
1:A:185:TYR:CZ	1:B:94:ALA:HB2	2.55	0.41
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.55	0.41
1:B:174:ALA:HA	1:B:337:ARG:HD3	2.02	0.41
1:B:262:ILE:HA	1:B:271:LYS:O	2.20	0.41
1:C:275:TRP:CG	1:C:276:PRO:HA	2.55	0.41
1:C:311:LYS:HE3	1:C:311:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:CYS:O	1:B:94:ALA:HA	2.20	0.41
1:C:159:GLU:OE1	1:C:310:ARG:HD3	2.21	0.41
1:C:167:ILE:HD12	1:C:334:ILE:HG23	2.03	0.41
1:B:196:ASN:O	1:B:197:ASP:C	2.59	0.41
1:B:287:VAL:O	1:B:294:HIS:HA	2.21	0.41
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.56	0.41
2:E:93:VAL:HG13	2:E:101:TYR:O	2.21	0.41
1:A:285:TRP:HB2	1:A:297:PHE:HB3	2.01	0.41
1:B:64:CYS:HB2	1:B:126:VAL:CG2	2.51	0.41
1:B:196:ASN:HD22	1:B:198:LEU:HG	1.86	0.41
1:C:283:PHE:HB2	1:C:299:THR:HG1	1.86	0.40
1:C:317:PHE:HA	1:C:321:TRP:HB2	2.03	0.40
1:B:343:PHE:CG	1:C:73:GLY:HA3	2.56	0.40
1:C:206:PRO:HA	1:C:213:GLN:HE22	1.86	0.40
2:D:5:TRP:CD2	2:D:103:ALA:HB2	2.57	0.40
1:C:242:THR:HA	1:C:246:GLU:O	2.21	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	381/392 (97%)	359 (94%)	21 (6%)	1 (0%)	41 41
1	B	383/392 (98%)	343 (90%)	36 (9%)	4 (1%)	15 11
1	C	386/392 (98%)	364 (94%)	20 (5%)	2 (0%)	29 26
2	D	101/115 (88%)	92 (91%)	9 (9%)	0	100 100
2	E	109/115 (95%)	106 (97%)	3 (3%)	0	100 100
All	All	1360/1406 (97%)	1264 (93%)	89 (6%)	7 (0%)	29 26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLY
1	B	268	GLY
1	C	268	GLY
1	C	210	ARG
1	B	195	ASP
1	B	196	ASN
1	B	206	PRO

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	330/339 (97%)	322 (98%)	8 (2%)	49	53
1	B	332/339 (98%)	324 (98%)	8 (2%)	49	53
1	C	335/339 (99%)	329 (98%)	6 (2%)	59	65
2	D	81/93 (87%)	81 (100%)	0	100	100
2	E	89/93 (96%)	89 (100%)	0	100	100
All	All	1167/1203 (97%)	1145 (98%)	22 (2%)	57	63

All (22) 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	293	THR
1	A	356	PHE
1	A	368	LEU
1	B	46	LEU
1	B	92	TYR
1	B	137	LEU
1	B	169	SER
1	B	234	HIS

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Mol	Chain	Res	Type
1	B	307	ASP
1	B	356	PHE
1	B	360	GLU
1	C	11	ARG
1	C	92	TYR
1	C	137	LEU
1	C	212	GLN
1	C	311	LYS
1	C	356	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	B	196	ASN
1	B	298	GLN
1	C	177	ASN
1	C	213	GLN
1	C	260	ASN
1	C	387	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FES	A	502	1	0,4,4	-	-	-		
5	9FL	A	503	-	15,15,15	3.14	9 (60%)	21,21,21	0.75	0
4	FES	D	201	2	0,4,4	-	-	-		
4	FES	E	201	2	0,4,4	-	-	-		
4	FES	C	502	1	0,4,4	-	-	-		
4	FES	B	502	1	0,4,4	-	-	-		
5	9FL	C	503	-	15,15,15	3.14	9 (60%)	21,21,21	0.75	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
4	FES	A	502	1	-	-	0/1/1/1
5	9FL	A	503	-	-	-	0/3/3/3
4	FES	D	201	2	-	-	0/1/1/1
4	FES	E	201	2	-	-	0/1/1/1
4	FES	C	502	1	-	-	0/1/1/1
4	FES	B	502	1	-	-	0/1/1/1
5	9FL	C	503	-	-	-	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	9FL	C4A-C4B	-5.32	1.33	1.46
5	C	503	9FL	C4A-C4B	-5.29	1.33	1.46
5	A	503	9FL	C9-C8A	-4.80	1.39	1.51
5	C	503	9FL	C9-C8A	-4.78	1.39	1.51
5	A	503	9FL	C9-C9A	-4.77	1.39	1.51
5	C	503	9FL	C9-C9A	-4.74	1.39	1.51
5	C	503	9FL	C5-C4B	-4.06	1.33	1.40
5	C	503	9FL	C4-C4A	-4.01	1.33	1.40
5	A	503	9FL	C5-C4B	-4.00	1.33	1.40
5	A	503	9FL	C4-C4A	-3.98	1.33	1.40
5	A	503	9FL	C1-C9A	-3.60	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	9FL	C1-C9A	-3.60	1.33	1.39
5	C	503	9FL	C8-C8A	-3.59	1.33	1.39
5	A	503	9FL	C8-C8A	-3.56	1.33	1.39
5	C	503	9FL	C4B-C8A	-2.77	1.33	1.40
5	A	503	9FL	C4B-C8A	-2.77	1.33	1.40
5	A	503	9FL	C4A-C9A	-2.73	1.33	1.40
5	C	503	9FL	C4A-C9A	-2.72	1.33	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	FES	1	0
5	A	503	9FL	2	0
4	C	502	FES	1	0
4	B	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^{th} 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	383/392 (97%)	0.44	26 (6%) 17 21	25, 37, 53, 59	0
1	B	385/392 (98%)	0.71	46 (11%) 4 5	30, 47, 59, 64	0
1	C	388/392 (98%)	0.38	27 (6%) 16 20	24, 38, 51, 60	0
2	D	103/115 (89%)	1.43	37 (35%) 0 0	38, 50, 60, 63	0
2	E	111/115 (96%)	0.50	13 (11%) 4 6	36, 47, 56, 59	0
All	All	1370/1406 (97%)	0.58	149 (10%) 5 7	24, 42, 58, 64	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	11	ALA	6.9
1	B	321	TRP	6.6
1	C	210	ARG	6.2
1	B	221	VAL	6.2
1	B	304	CYS	5.9
1	B	308	GLU	5.9
2	D	101	TYR	5.9
1	C	221	VAL	5.5
1	B	312	LYS	5.3
2	D	5	TRP	5.2
2	D	12	SER	5.1
2	D	96	LYS	5.0
2	D	95	VAL	4.8
2	E	113	HIS	4.6
1	C	178	GLY	4.4
1	C	175	VAL	4.4
2	D	9	CYS	4.4
1	B	316	GLU	4.3
1	C	209	ASP	4.3
1	A	2	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	36	GLY	4.3
1	C	179	PHE	4.3
1	C	264	ILE	4.3
2	D	4	ILE	4.2
1	C	270	LEU	4.2
1	C	208	GLY	4.1
1	B	210	ARG	4.1
2	E	25	VAL	4.1
1	A	252	ALA	4.0
1	B	307	ASP	4.0
1	B	219	ASP	4.0
1	B	385	LEU	4.0
2	D	25	VAL	3.8
1	B	317	PHE	3.8
2	D	103	ALA	3.8
2	D	10	ALA	3.7
2	D	97	GLU	3.7
1	C	388	HIS	3.7
2	D	7	LYS	3.7
1	A	221	VAL	3.7
1	C	269	VAL	3.6
1	A	253	TYR	3.6
2	D	35	VAL	3.6
2	D	26	GLY	3.6
1	B	311	LYS	3.5
2	D	15	GLN	3.5
1	C	211	LYS	3.4
1	C	389	HIS	3.4
1	A	308	GLU	3.4
2	D	104	GLY	3.4
1	B	245	GLY	3.4
2	D	34	ARG	3.4
1	A	175	VAL	3.4
2	D	14	MET	3.3
2	D	100	VAL	3.3
2	E	27	ALA	3.3
2	D	8	VAL	3.3
1	B	244	GLY	3.2
1	B	315	GLN	3.2
2	E	3	GLN	3.2
1	A	179	PHE	3.1
2	D	13	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	314	GLU	3.1
1	C	173	LEU	3.0
1	B	222	VAL	3.0
1	C	362	ILE	3.0
2	E	109	GLU	3.0
1	A	269	VAL	3.0
1	A	270	LEU	3.0
1	A	356	PHE	2.9
1	B	191	ILE	2.9
2	D	18	THR	2.9
1	B	386	GLU	2.9
2	E	110	HIS	2.9
1	A	286	TYR	2.9
1	B	255	GLU	2.8
1	B	175	VAL	2.8
1	B	313	TYR	2.8
1	B	2	ALA	2.7
1	B	324	MET	2.7
1	B	301	GLY	2.7
2	D	39	PHE	2.7
2	D	94	GLU	2.7
1	A	174	ALA	2.7
1	A	355	LEU	2.7
1	B	362	ILE	2.6
1	C	365	TRP	2.6
1	A	194	LYS	2.6
2	D	6	LEU	2.6
1	C	286	TYR	2.6
2	D	37	ASP	2.6
2	D	98	GLY	2.5
2	E	97	GLU	2.5
1	B	235	GLY	2.5
2	E	7	LYS	2.5
1	B	328	GLY	2.5
2	D	28	ALA	2.5
1	C	387	HIS	2.5
1	B	302	LYS	2.5
2	D	17	GLY	2.4
1	A	361	ALA	2.4
1	B	309	GLU	2.4
1	C	385	LEU	2.4
1	A	69	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	157	ASP	2.4
2	D	75	CYS	2.4
1	B	100	GLU	2.4
2	D	16	PRO	2.4
1	A	287	VAL	2.3
1	B	305	ALA	2.3
1	A	307	ASP	2.3
1	B	256	LYS	2.3
1	B	234	HIS	2.3
2	E	101	TYR	2.3
2	D	99	GLU	2.3
1	A	285	TRP	2.3
1	B	320	LYS	2.2
1	C	207	GLY	2.2
2	E	98	GLY	2.2
1	C	386	GLU	2.2
2	E	14	MET	2.2
1	B	69	CYS	2.2
1	B	179	PHE	2.2
1	B	209	ASP	2.2
2	D	38	GLN	2.2
1	C	255	GLU	2.2
1	A	178	GLY	2.2
1	B	218	ASP	2.2
1	C	263	SER	2.2
1	A	92	TYR	2.1
1	B	193	VAL	2.1
1	A	340	MET	2.1
1	A	362	ILE	2.1
1	C	194	LYS	2.1
2	D	105	GLU	2.1
1	A	311	LYS	2.1
2	E	13	ASP	2.1
1	C	13	LYS	2.1
1	C	60	GLY	2.1
1	B	257	ILE	2.1
1	A	247	VAL	2.1
2	D	92	GLU	2.1
2	E	99	GLU	2.1
1	A	220	ASP	2.0
1	B	280	MET	2.0
1	B	215	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	212	GLN	2.0
1	B	246	GLU	2.0
1	B	211	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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^{th} 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	9FL	A	503	13/13	0.81	0.22	50,52,53,53	0
5	9FL	C	503	13/13	0.91	0.23	41,43,44,45	0
3	FE2	C	501	1/1	0.97	0.07	42,42,42,42	0
3	FE2	A	501	1/1	0.98	0.07	43,43,43,43	0
4	FES	C	502	4/4	0.98	0.14	35,36,37,41	0
4	FES	D	201	4/4	0.99	0.10	34,37,38,40	0
4	FES	E	201	4/4	0.99	0.14	31,36,37,38	0
4	FES	B	502	4/4	0.99	0.16	30,32,37,43	0
3	FE2	B	501	1/1	0.99	0.02	61,61,61,61	0
4	FES	A	502	4/4	1.00	0.16	27,27,31,32	0

6.5 Other polymers (i)

There are no such residues in this entry.