Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2022 – 12:21 AM EDT

PDB ID	:	4NBC
Title	:	Oxygenase with Phe275 replaced by Trp and ferredoxin complex of carbazole 1,9a-dioxygenase (form1)
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 (i) 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 (i)) were used in the production of this report:

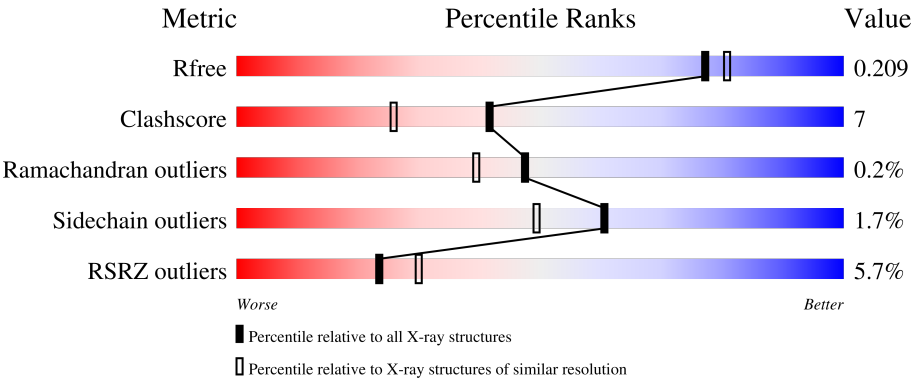
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	3% 83% 16% ·
1	B	392	4% 80% 18% ··
1	C	392	3% 82% 16% ··
2	D	115	27% 72% 17% · 10%
2	E	115	5% 79% 13% 8%

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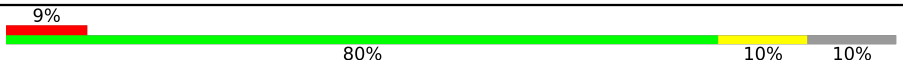
Mol	Chain	Length	Quality of chain
2	F	115	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12980 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	388	Total	C	N	O	S	0	0	0
			3131	2001	535	582	13			
1	B	388	Total	C	N	O	S	0	0	0
			3131	2001	535	582	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	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			
2	E	106	Total	C	N	O	S	0	0	0
			785	494	132	152	7			
2	F	103	Total	C	N	O	S	0	0	0
			759	477	127	148	7			

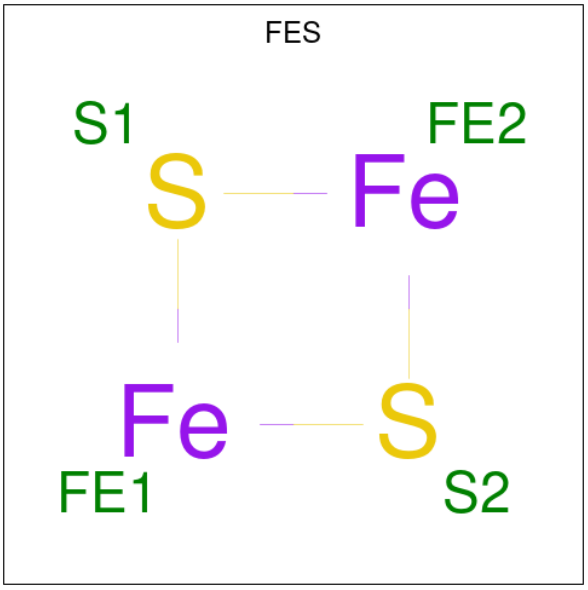
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	expression tag	UNP Q8GI16
D	109	GLU	-	expression tag	UNP Q8GI16
D	110	HIS	-	expression tag	UNP Q8GI16
D	111	HIS	-	expression tag	UNP Q8GI16
D	112	HIS	-	expression tag	UNP Q8GI16
D	113	HIS	-	expression tag	UNP Q8GI16
D	114	HIS	-	expression tag	UNP Q8GI16
D	115	HIS	-	expression tag	UNP Q8GI16
E	108	LEU	-	expression tag	UNP Q8GI16
E	109	GLU	-	expression tag	UNP Q8GI16
E	110	HIS	-	expression tag	UNP Q8GI16
E	111	HIS	-	expression tag	UNP Q8GI16
E	112	HIS	-	expression tag	UNP Q8GI16
E	113	HIS	-	expression tag	UNP Q8GI16
E	114	HIS	-	expression tag	UNP Q8GI16
E	115	HIS	-	expression tag	UNP Q8GI16
F	108	LEU	-	expression tag	UNP Q8GI16
F	109	GLU	-	expression tag	UNP Q8GI16
F	110	HIS	-	expression tag	UNP Q8GI16
F	111	HIS	-	expression tag	UNP Q8GI16
F	112	HIS	-	expression tag	UNP Q8GI16
F	113	HIS	-	expression tag	UNP Q8GI16
F	114	HIS	-	expression tag	UNP Q8GI16
F	115	HIS	-	expression tag	UNP Q8GI16

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

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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_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
4	F	1	Total Fe S 4 2 2	0	0

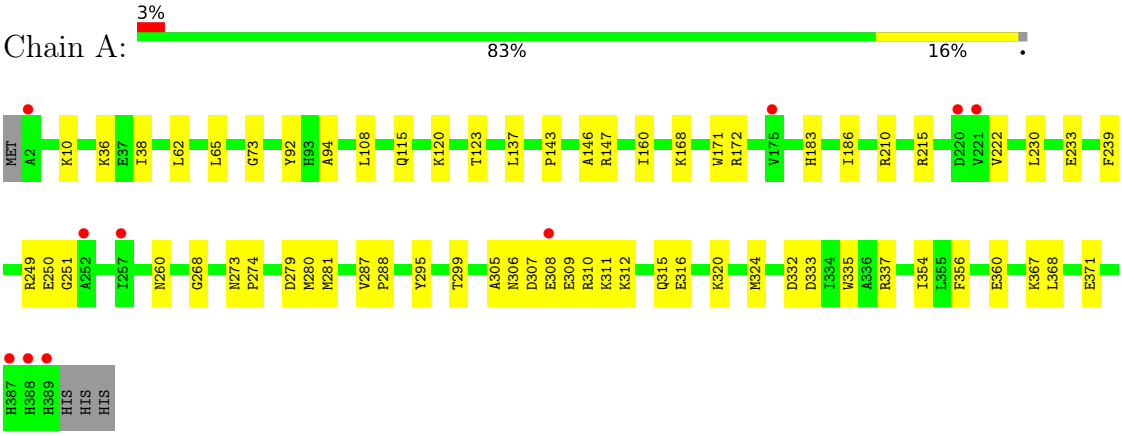
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	355	Total O 355 355	0	0
5	B	340	Total O 340 340	0	0
5	C	365	Total O 365 365	0	0
5	D	44	Total O 44 44	0	0
5	E	73	Total O 73 73	0	0
5	F	71	Total O 71 71	0	0

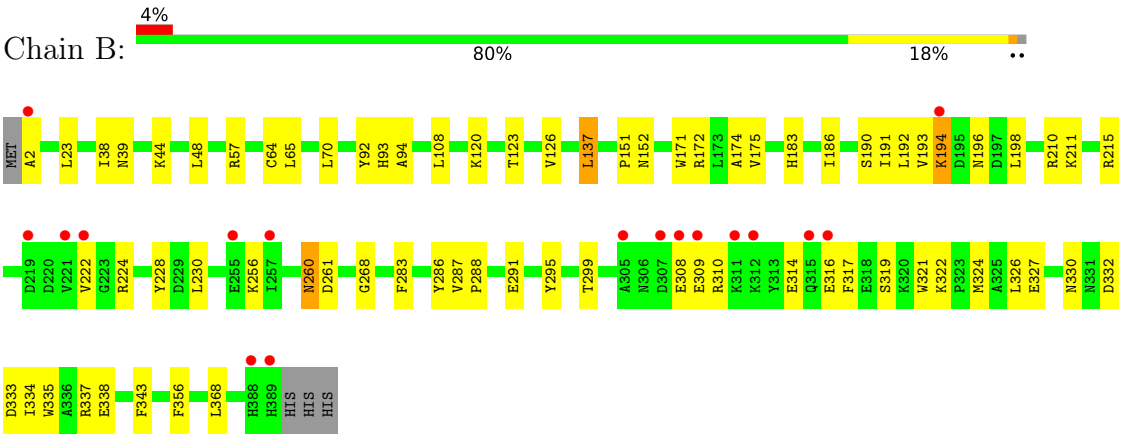
3 Residue-property plots (i)

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.

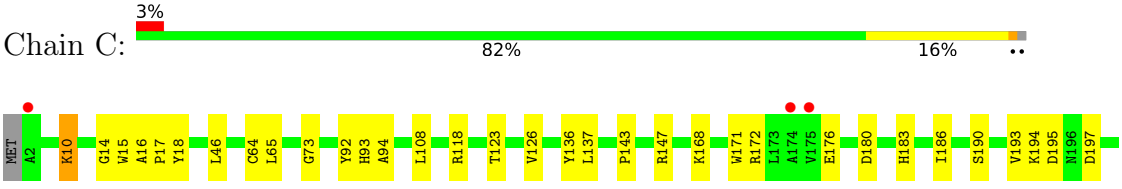
• Molecule 1: Terminal oxygenase component of carbazole

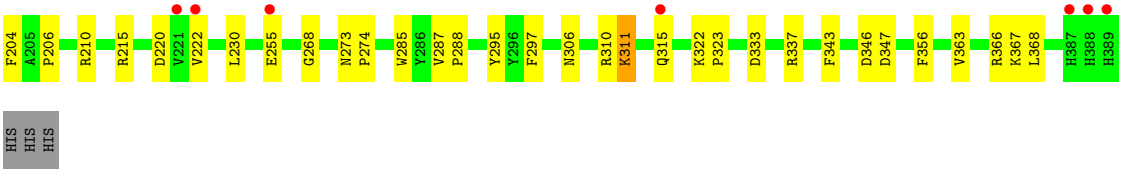


• Molecule 1: Terminal oxygenase component of carbazole

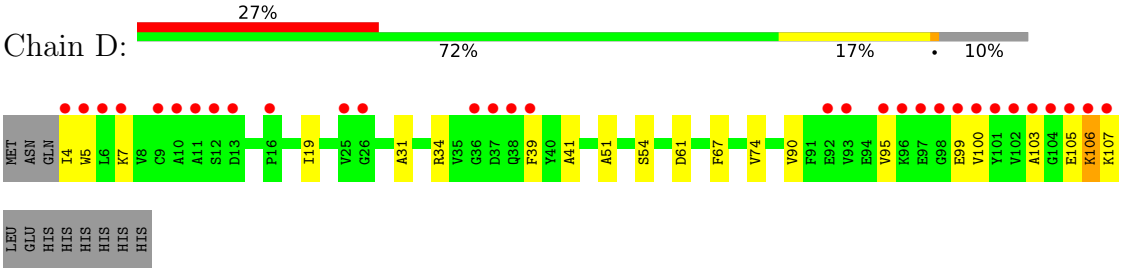


• Molecule 1: Terminal oxygenase component of carbazole

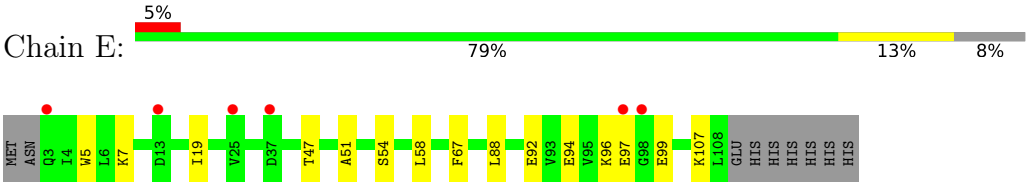




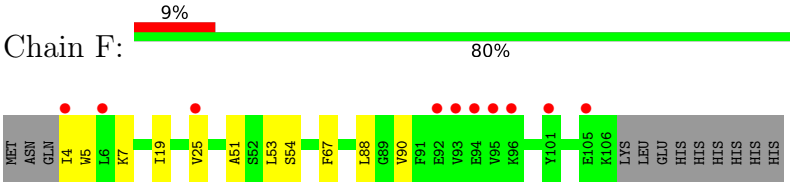
• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.50Å 90.08Å 105.38Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	39.28 – 1.95 39.28 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.28-1.95) 99.0 (39.28-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.215 0.183 , 0.209	Depositor DCC
R_{free} test set	6491 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12980	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

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	0/3217	0.61	0/4369
1	B	0.30	0/3217	0.60	0/4369
1	C	0.31	0/3217	0.60	0/4369
2	D	0.29	0/784	0.58	0/1066
2	E	0.31	0/801	0.60	0/1089
2	F	0.32	0/775	0.61	0/1055
All	All	0.31	0/12011	0.60	0/16317

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3131	0	3031	41	0
1	B	3131	0	3031	56	0
1	C	3131	0	3031	40	0
2	D	768	0	745	12	0
2	E	785	0	764	8	0
2	F	759	0	732	7	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	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
4	F	4	0	0	0	0
5	A	355	0	0	2	0
5	B	340	0	0	7	0
5	C	365	0	0	2	0
5	D	44	0	0	0	0
5	E	73	0	0	0	0
5	F	71	0	0	3	0
All	All	12980	0	11334	161	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 7.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:HG3	5:A:945:HOH:O	1.43	1.17
2:E:92:GLU:HB2	2:E:107:LYS:HE3	1.41	1.01
1:B:308:GLU:O	1:B:309:GLU:HG2	1.69	0.93
2:D:106:LYS:HE2	2:D:107:LYS:N	1.98	0.77
1:A:146:ALA:HB3	1:A:222:VAL:HG21	1.66	0.77
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.67	0.75
2:D:106:LYS:HE2	2:D:107:LYS:H	1.51	0.74
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.70	0.74
1:A:230:LEU:HB3	1:A:233:GLU:HG3	1.67	0.74
1:C:311:LYS:HA	1:C:311:LYS:HE2	1.69	0.74
1:C:194:LYS:HG3	1:C:195:ASP:H	1.54	0.72
1:C:194:LYS:HG3	1:C:195:ASP:N	2.05	0.72
1:C:220:ASP:OD1	1:C:222:VAL:HG22	1.92	0.68
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.77	0.67
1:C:118:ARG:NH2	5:C:660:HOH:O	2.30	0.64
2:D:90:VAL:HG23	2:D:107:LYS:HD2	1.79	0.64
1:B:39:ASN:H	1:B:44:LYS:HZ3	1.44	0.64
1:A:312:LYS:O	1:A:316:GLU:HG3	1.98	0.62
1:B:38:ILE:HD12	1:B:44:LYS:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:SER:HB3	1:B:193:VAL:HG23	1.81	0.61
1:B:191:ILE:HA	1:B:194:LYS:HE2	1.81	0.61
1:B:38:ILE:CD1	1:B:44:LYS:HD3	2.32	0.60
1:B:308:GLU:C	1:B:310:ARG:H	2.04	0.60
1:C:306:ASN:O	1:C:310:ARG:HG3	2.02	0.59
1:A:146:ALA:CB	1:A:222:VAL:HG21	2.32	0.59
1:B:2:ALA:HB2	5:B:918:HOH:O	2.03	0.58
1:C:197:ASP:OD2	1:C:255:GLU:HB2	2.03	0.58
1:A:249:ARG:HG3	1:A:250:GLU:N	2.19	0.57
1:B:310:ARG:O	1:B:314:GLU:HG3	2.04	0.57
1:B:38:ILE:HG23	1:B:57:ARG:HH21	1.70	0.57
1:C:10:LYS:HA	1:C:10:LYS:HE3	1.86	0.57
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.85	0.57
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.35	0.56
1:A:306:ASN:OD1	1:A:308:GLU:HB2	2.06	0.56
1:A:239:PHE:O	1:A:251:GLY:N	2.35	0.56
2:D:19:ILE:HG21	2:D:54:SER:HA	1.88	0.56
1:C:311:LYS:NZ	1:C:315:GLN:HG3	2.22	0.55
1:B:333:ASP:O	1:B:337:ARG:HG3	2.08	0.54
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.43	0.54
2:F:19:ILE:HG21	2:F:54:SER:HA	1.90	0.54
1:B:191:ILE:HA	1:B:194:LYS:CE	2.38	0.54
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.91	0.53
1:A:311:LYS:HE2	1:A:315:GLN:HE22	1.73	0.53
1:B:260:ASN:HD22	1:B:261:ASP:N	2.07	0.53
1:C:168:LYS:HE3	5:C:950:HOH:O	2.09	0.53
2:D:4:ILE:HG23	2:D:5:TRP:CD1	2.44	0.53
1:C:333:ASP:O	1:C:337:ARG:HG3	2.08	0.53
2:E:19:ILE:HG21	2:E:54:SER:HA	1.91	0.52
1:A:222:VAL:HG22	1:A:222:VAL:O	2.09	0.52
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.92	0.52
1:A:307:ASP:HA	1:A:310:ARG:HG2	1.92	0.52
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.92	0.51
1:B:120:LYS:HE3	5:B:614:HOH:O	2.09	0.51
1:B:2:ALA:HB3	5:B:649:HOH:O	2.10	0.51
1:B:190:SER:O	1:B:194:LYS:HD3	2.10	0.51
1:B:326:LEU:O	1:B:330:ASN:HB2	2.10	0.50
1:C:210:ARG:HH11	1:C:210:ARG:HG2	1.77	0.50
1:A:38:ILE:HD13	1:A:62:LEU:HD22	1.94	0.50
1:B:23:LEU:HD22	5:B:624:HOH:O	2.12	0.49
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HD3	1:B:194:LYS:H	1.77	0.49
1:B:196:ASN:O	1:B:256:LYS:HD2	2.12	0.49
2:F:4:ILE:HG23	2:F:5:TRP:CD1	2.48	0.49
1:C:194:LYS:HE3	1:C:195:ASP:OD1	2.13	0.49
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.48	0.49
2:E:7:LYS:HE3	2:E:99:GLU:HG2	1.95	0.48
1:B:283:PHE:HB2	1:B:299:THR:OG1	2.13	0.48
1:C:183:HIS:O	1:C:186:ILE:HG12	2.13	0.48
1:B:260:ASN:HD22	1:B:260:ASN:C	2.16	0.48
2:D:7:LYS:HE2	2:D:99:GLU:OE2	2.14	0.48
1:A:260:ASN:OD1	1:A:274:PRO:HD3	2.14	0.48
1:A:320:LYS:HE2	1:A:324:MET:HE1	1.96	0.48
1:B:196:ASN:HD22	1:B:198:LEU:HD21	1.78	0.48
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.95	0.48
1:A:273:ASN:HB2	1:A:281:MET:HG2	1.96	0.48
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.95	0.48
1:B:64:CYS:HB2	1:B:126:VAL:CG2	2.43	0.48
1:B:324:MET:HB2	5:B:834:HOH:O	2.13	0.47
1:C:93:HIS:HB2	4:C:502:FES:S1	2.54	0.47
2:F:25:VAL:HG23	5:F:344:HOH:O	2.14	0.47
1:A:120:LYS:HZ3	1:A:123:THR:H	1.60	0.47
1:B:64:CYS:HB2	1:B:126:VAL:HG21	1.96	0.47
1:A:168:LYS:HE2	5:A:946:HOH:O	2.15	0.47
1:B:215:ARG:HB3	1:B:228:TYR:HB2	1.96	0.47
1:B:308:GLU:C	1:B:310:ARG:N	2.68	0.47
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.44	0.47
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.45	0.47
1:B:171:TRP:CG	1:B:288:PRO:HG3	2.50	0.47
1:B:343:PHE:CG	1:C:73:GLY:HA3	2.50	0.46
1:B:93:HIS:HB2	4:B:502:FES:S1	2.55	0.46
1:B:322:LYS:O	1:B:327:GLU:HG3	2.14	0.46
1:C:215:ARG:HB2	1:C:230:LEU:HD11	1.97	0.46
2:D:31:ALA:O	2:D:41:ALA:HA	2.16	0.46
2:F:53:LEU:CD1	2:F:88:LEU:HD11	2.46	0.46
1:A:307:ASP:HA	1:A:310:ARG:CG	2.45	0.46
1:C:190:SER:HB3	1:C:193:VAL:HG23	1.97	0.46
2:F:90:VAL:HG13	5:F:337:HOH:O	2.15	0.46
1:A:307:ASP:HA	1:A:310:ARG:HD2	1.98	0.46
1:C:15:TRP:CZ3	1:C:363:VAL:HG13	2.51	0.46
1:C:363:VAL:CG1	1:C:367:LYS:HE3	2.46	0.46
2:E:92:GLU:OE1	2:E:107:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.51	0.46
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.46	0.45
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.97	0.45
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.50	0.45
2:D:103:ALA:C	2:D:105:GLU:N	2.69	0.45
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.52	0.45
1:B:308:GLU:O	1:B:310:ARG:N	2.42	0.45
1:A:367:LYS:O	1:A:371:GLU:HG3	2.17	0.44
1:B:308:GLU:O	1:B:309:GLU:CG	2.54	0.44
1:B:291:GLU:HG2	5:B:672:HOH:O	2.16	0.44
2:E:5:TRP:CZ3	2:E:94:GLU:HG2	2.52	0.44
1:C:311:LYS:HZ1	1:C:315:GLN:HG3	1.81	0.44
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.82	0.44
2:F:51:ALA:HB2	2:F:67:PHE:CG	2.52	0.44
1:B:39:ASN:H	1:B:44:LYS:NZ	2.13	0.44
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.48	0.44
1:A:10:LYS:HE2	1:A:10:LYS:HB2	1.88	0.44
1:C:171:TRP:CG	1:C:288:PRO:HG3	2.53	0.43
1:B:316:GLU:HA	1:B:319:SER:HG	1.83	0.43
2:D:61:ASP:O	2:D:74:VAL:HG22	2.18	0.43
1:B:151:PRO:O	1:B:152:ASN:HB2	2.19	0.43
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.33	0.43
1:B:222:VAL:O	1:B:222:VAL:CG1	2.67	0.43
1:B:215:ARG:HB2	1:B:230:LEU:HD11	2.01	0.43
1:A:279:ASP:OD1	1:A:280:MET:HG3	2.19	0.43
1:C:346:ASP:O	1:C:347:ASP:HB2	2.19	0.43
1:A:354:ILE:HD12	1:B:70:LEU:HB3	2.01	0.43
1:C:14:GLY:HA3	5:F:318:HOH:O	2.19	0.42
2:F:7:LYS:HB2	2:F:7:LYS:NZ	2.33	0.42
1:A:115:GLN:HA	1:A:115:GLN:OE1	2.19	0.42
1:A:210:ARG:HG3	1:A:360:GLU:CD	2.39	0.42
1:B:334:ILE:O	1:B:338:GLU:HG3	2.19	0.42
1:B:192:LEU:HD12	1:B:324:MET:SD	2.60	0.42
1:C:273:ASN:HA	1:C:274:PRO:HA	1.92	0.42
1:C:16:ALA:HB3	1:C:17:PRO:HD3	2.01	0.42
1:B:175:VAL:HG22	1:B:286:TYR:CD2	2.54	0.42
1:A:320:LYS:CE	1:A:324:MET:HE1	2.50	0.42
2:D:95:VAL:HG22	2:D:100:VAL:HG22	2.02	0.42
1:B:48:LEU:HD23	1:B:137:LEU:HD23	2.01	0.41
1:B:224:ARG:NH2	5:B:832:HOH:O	2.53	0.41
1:C:136:TYR:CE1	1:C:143:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:VAL:HA	1:A:288:PRO:HD3	1.92	0.41
1:A:307:ASP:HA	1:A:310:ARG:CD	2.49	0.41
1:B:174:ALA:HB1	1:B:286:TYR:CD1	2.55	0.41
1:C:322:LYS:HB3	1:C:323:PRO:CD	2.51	0.41
2:E:96:LYS:O	2:E:97:GLU:HB2	2.20	0.41
1:A:160:ILE:HG23	1:A:299:THR:HB	2.01	0.41
2:E:47:THR:HG23	2:E:88:LEU:HD23	2.03	0.41
1:C:64:CYS:HB2	1:C:126:VAL:CG2	2.50	0.41
1:A:305:ALA:HB3	1:A:309:GLU:OE2	2.20	0.41
1:C:204:PHE:O	1:C:206:PRO:HD3	2.21	0.41
1:A:73:GLY:HA3	1:C:343:PHE:CG	2.56	0.41
1:A:183:HIS:O	1:A:186:ILE:HG12	2.20	0.41
1:A:332:ASP:HA	1:A:335:TRP:NE1	2.36	0.41
1:A:333:ASP:O	1:A:337:ARG:HG3	2.21	0.41
2:D:34:ARG:HD2	2:D:39:PHE:CZ	2.56	0.41
1:B:183:HIS:O	1:B:186:ILE:HG12	2.22	0.41
1:B:317:PHE:HA	1:B:321:TRP:HB2	2.03	0.41
1:C:176:GLU:O	1:C:180:ASP:HB2	2.21	0.40
1:C:285:TRP:HB2	1:C:297:PHE:HB3	2.04	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	386/392 (98%)	370 (96%)	15 (4%)	1 (0%)	41	32
1	B	386/392 (98%)	366 (95%)	19 (5%)	1 (0%)	41	32
1	C	386/392 (98%)	364 (94%)	21 (5%)	1 (0%)	41	32
2	D	102/115 (89%)	95 (93%)	7 (7%)	0	100	100
2	E	104/115 (90%)	101 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	101/115 (88%)	97 (96%)	4 (4%)	0	100 100
All	All	1465/1521 (96%)	1393 (95%)	69 (5%)	3 (0%)	47 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	A	268	GLY
1	C	268	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	335/339 (99%)	330 (98%)	5 (2%)	65 56
1	B	335/339 (99%)	328 (98%)	7 (2%)	53 41
1	C	335/339 (99%)	328 (98%)	7 (2%)	53 41
2	D	82/93 (88%)	81 (99%)	1 (1%)	71 64
2	E	84/93 (90%)	83 (99%)	1 (1%)	71 64
2	F	81/93 (87%)	81 (100%)	0	100 100
All	All	1252/1296 (97%)	1231 (98%)	21 (2%)	60 49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	92	TYR
1	A	137	LEU
1	A	356	PHE
1	A	368	LEU
1	B	92	TYR
1	B	137	LEU
1	B	194	LYS

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Mol	Chain	Res	Type
1	B	211	LYS
1	B	260	ASN
1	B	356	PHE
1	B	368	LEU
1	C	10	LYS
1	C	46	LEU
1	C	92	TYR
1	C	137	LEU
1	C	311	LYS
1	C	356	PHE
1	C	368	LEU
2	D	106	LYS
2	E	58	LEU

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	165	GLN
1	A	196	ASN
1	A	315	GLN
1	B	165	GLN
1	B	260	ASN
1	C	165	GLN
1	C	388	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	-	-	-		
4	FES	D	201	2	0,4,4	-	-	-		
4	FES	F	201	2	0,4,4	-	-	-		
4	FES	E	201	2	0,4,4	-	-	-		
4	FES	B	502	1	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
4	FES	A	502	1	-	-	0/1/1/1
4	FES	D	201	2	-	-	0/1/1/1
4	FES	F	201	2	-	-	0/1/1/1
4	FES	E	201	2	-	-	0/1/1/1
4	FES	B	502	1	-	-	0/1/1/1
4	FES	C	502	1	-	-	0/1/1/1

There are no bond length outliers.

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	B	502	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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^{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	388/392 (98%)	-0.00	10 (2%) 56 63	13, 21, 37, 42	0
1	B	388/392 (98%)	0.08	17 (4%) 34 41	13, 25, 40, 44	0
1	C	388/392 (98%)	-0.02	10 (2%) 56 63	15, 24, 36, 41	0
2	D	104/115 (90%)	1.20	31 (29%) 0 0	17, 33, 42, 46	0
2	E	106/115 (92%)	0.21	6 (5%) 23 30	19, 29, 37, 41	0
2	F	103/115 (89%)	0.42	10 (9%) 7 11	19, 30, 38, 43	0
All	All	1477/1521 (97%)	0.15	84 (5%) 23 30	13, 25, 39, 46	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	VAL	10.0
1	A	221	VAL	6.0
2	D	4	ILE	5.8
2	F	4	ILE	5.6
1	B	2	ALA	5.3
1	B	305	ALA	4.8
2	F	25	VAL	4.8
1	C	388	HIS	4.6
2	D	25	VAL	4.5
1	A	389	HIS	4.4
2	D	93	VAL	4.4
1	B	222	VAL	4.3
2	D	104	GLY	4.3
2	D	101	TYR	4.3
2	D	92	GLU	4.3
2	D	98	GLY	4.1
2	D	96	LYS	4.1
2	D	95	VAL	4.1
2	D	5	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	105	GLU	4.0
1	C	389	HIS	3.9
2	D	37	ASP	3.9
2	D	97	GLU	3.8
2	D	99	GLU	3.8
1	B	309	GLU	3.8
2	D	6	LEU	3.7
2	F	101	TYR	3.6
2	F	105	GLU	3.6
2	D	12	SER	3.5
2	D	26	GLY	3.5
2	E	3	GLN	3.4
2	D	7	LYS	3.3
2	E	37	ASP	3.3
2	F	6	LEU	3.2
1	C	221	VAL	3.2
1	B	389	HIS	3.1
1	B	308	GLU	3.1
2	D	11	ALA	3.1
1	A	257	ILE	3.0
2	E	25	VAL	3.0
2	F	93	VAL	3.0
2	F	95	VAL	3.0
1	A	388	HIS	3.0
1	B	194	LYS	2.9
2	D	107	LYS	2.9
2	E	97	GLU	2.9
2	D	38	GLN	2.9
1	A	252	ALA	2.9
1	A	220	ASP	2.8
2	F	92	GLU	2.8
1	B	219	ASP	2.8
2	F	96	LYS	2.8
1	C	174	ALA	2.7
1	C	387	HIS	2.7
1	C	255	GLU	2.7
2	F	94	GLU	2.7
1	B	257	ILE	2.6
1	C	2	ALA	2.6
2	D	106	LYS	2.6
1	B	388	HIS	2.6
2	D	102	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	16	PRO	2.5
1	B	315	GLN	2.5
2	D	36	GLY	2.5
2	D	9	CYS	2.5
1	B	312	LYS	2.5
2	D	100	VAL	2.5
1	B	255	GLU	2.4
1	A	2	ALA	2.4
1	A	308	GLU	2.4
1	C	175	VAL	2.4
1	B	316	GLU	2.3
2	D	103	ALA	2.3
1	C	315	GLN	2.3
1	B	307	ASP	2.3
1	B	311	LYS	2.2
2	D	13	ASP	2.2
2	D	39	PHE	2.2
2	D	10	ALA	2.2
1	A	175	VAL	2.2
1	A	387	HIS	2.1
1	C	222	VAL	2.1
2	E	98	GLY	2.1
2	E	13	ASP	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE2	A	501	1/1	0.99	0.07	28,28,28,28	0
3	FE2	B	501	1/1	0.99	0.04	35,35,35,35	0
4	FES	C	502	4/4	0.99	0.10	19,20,21,22	0
4	FES	E	201	4/4	0.99	0.11	20,20,21,22	0
4	FES	B	502	4/4	1.00	0.13	14,17,18,18	0
3	FE2	C	501	1/1	1.00	0.04	32,32,32,32	0
4	FES	D	201	4/4	1.00	0.09	19,20,20,21	0
4	FES	A	502	4/4	1.00	0.13	16,17,19,19	0
4	FES	F	201	4/4	1.00	0.08	19,19,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.