



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:10 AM UTC

PDB ID : 4NB8 / pdb_00004nb8
Title : Oxygenase with Ile262 replaced by Leu and ferredoxin complex of carbazole
1,9a-dioxygenase
Authors : Ashikawa, Y.; Usami, Y.; Inoue, K.; Nojiri, H.
Deposited on : 2013-10-23
Resolution : 2.01 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

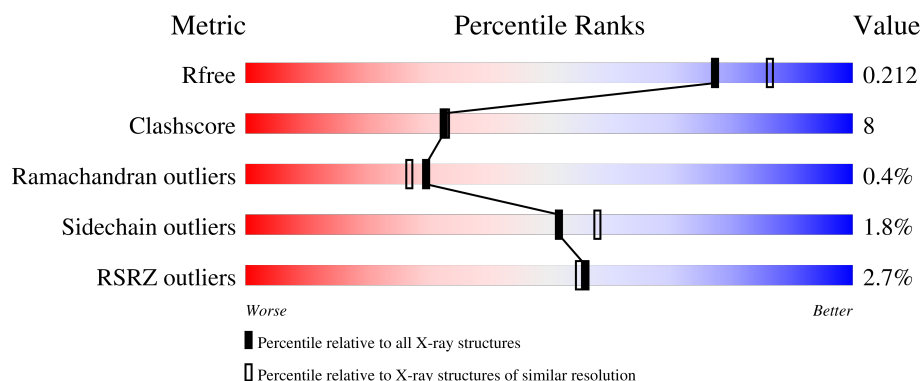
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	2% 82% 16% ..
1	B	392	2% 77% 21% ..
1	C	392	% 77% 21% ..
2	D	115	6% 80% 11% 9%
2	E	115	3% 80% 14% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	115	9% 75% 15% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12776 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
			3128	1999	534	582	13			
1	B	388	Total	C	N	O	S	0	0	0
			3128	1999	534	582	13			
1	C	388	Total	C	N	O	S	0	0	0
			3128	1999	534	582	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	LEU	ILE	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	262	LEU	ILE	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	262	LEU	ILE	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

Continued on next page...

Continued from previous page...

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	105	Total	C	N	O	S	0	0	0
			776	489	130	150	7			
2	E	110	Total	C	N	O	S	0	0	0
			822	515	141	159	7			
2	F	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			

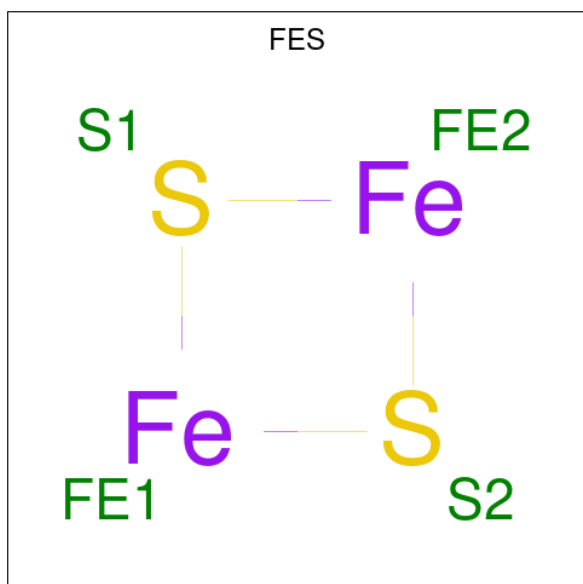
There are 24 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Fe 2	S 2	0	0
4	B	1	Total 4	Fe 2	S 2	0	0
4	C	1	Total 4	Fe 2	S 2	0	0
4	D	1	Total 4	Fe 2	S 2	0	0
4	E	1	Total 4	Fe 2	S 2	0	0
4	F	1	Total 4	Fe 2	S 2	0	0

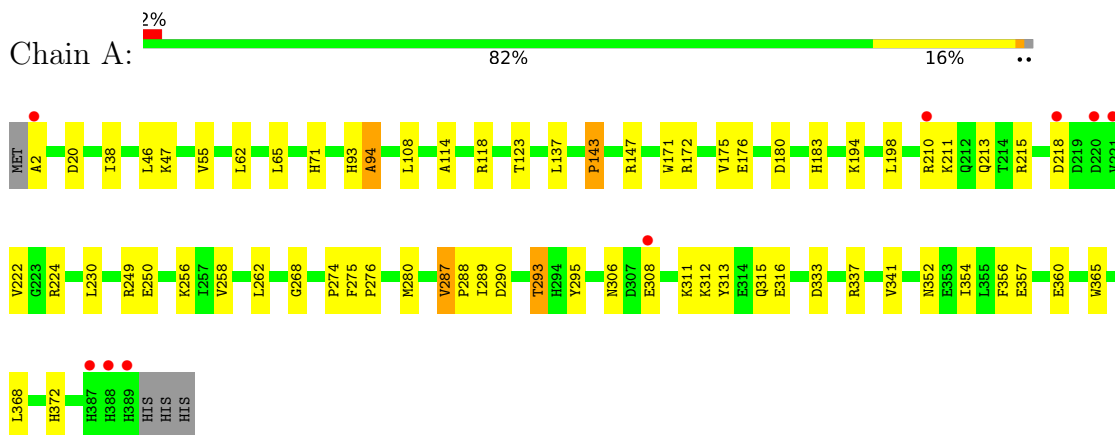
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	329	Total 329	O 329	0	0
5	B	290	Total 290	O 290	0	0
5	C	278	Total 278	O 278	0	0
5	D	26	Total 26	O 26	0	0
5	E	51	Total 51	O 51	0	0
5	F	25	Total 25	O 25	0	0

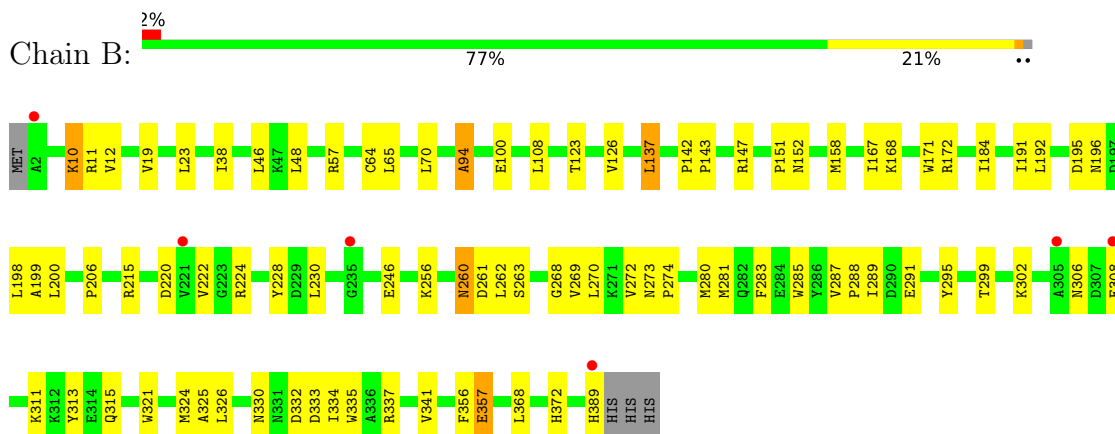
3 Residue-property plots

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.

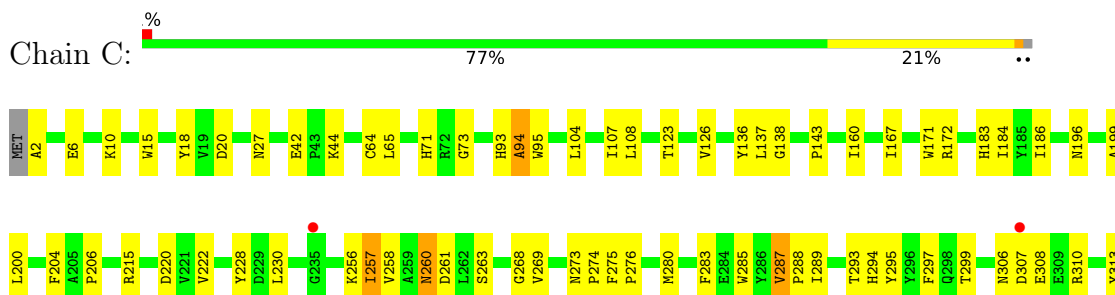
- Molecule 1: Terminal oxygenase component of carbazole



- Molecule 1: Terminal oxygenase component of carbazole

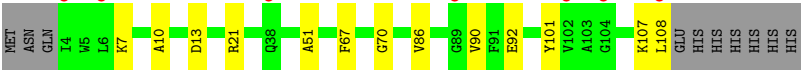
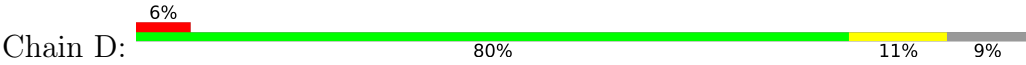


- Molecule 1: Terminal oxygenase component of carbazole

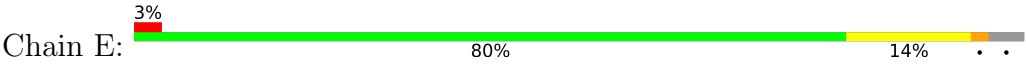




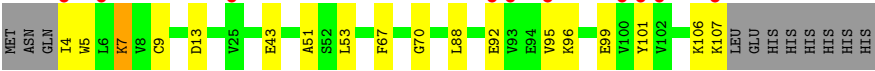
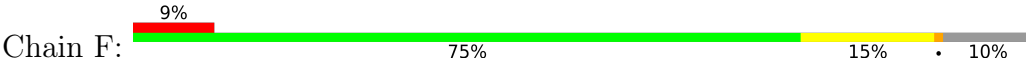
● Molecule 2: Ferredoxin CarAc



● Molecule 2: Ferredoxin CarAc



● Molecule 2: Ferredoxin CarAc



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.27Å 89.82Å 105.25Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	47.87 – 2.01 47.87 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.87-2.01) 99.6 (47.87-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.216 0.185 , 0.212	Depositor DCC
R_{free} test set	5907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12776	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: 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	0.39	0/3213	0.88	8/4362 (0.2%)
1	B	0.37	0/3213	0.88	8/4362 (0.2%)
1	C	0.37	0/3213	0.86	7/4362 (0.2%)
2	D	0.33	0/792	0.88	2/1077 (0.2%)
2	E	0.37	0/840	0.89	3/1142 (0.3%)
2	F	0.32	0/784	0.83	2/1066 (0.2%)
All	All	0.37	0/12055	0.87	30/16371 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-C	7.67	115.51	107.76
1	B	289	ILE	N-CA-C	-7.10	104.93	111.67
1	C	287	VAL	N-CA-C	6.86	114.53	108.63
2	E	43	GLU	N-CA-C	-6.86	100.83	110.50
1	B	341	VAL	N-CA-C	6.63	117.32	110.36
1	A	289	ILE	N-CA-C	-6.61	105.39	111.67
1	A	357	GLU	N-CA-C	6.50	122.09	111.37
1	A	341	VAL	N-CA-C	6.41	117.09	110.36
2	F	70	GLY	N-CA-C	-6.26	104.53	112.54
2	F	43	GLU	N-CA-C	-6.20	101.77	110.50
1	C	289	ILE	N-CA-C	-5.96	106.00	111.67
1	A	94	ALA	N-CA-C	5.88	119.77	112.24
2	E	4	ILE	N-CA-C	5.76	116.22	110.23
1	B	372	HIS	N-CA-C	5.75	120.30	112.88
1	C	199	ALA	N-CA-C	-5.74	99.89	109.24
1	B	142	PRO	N-CA-C	5.70	116.67	110.58
2	E	109	GLU	N-CA-C	5.68	122.91	110.80
1	B	94	ALA	N-CA-C	5.67	119.50	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	86	VAL	N-CA-C	5.63	113.45	107.76
1	C	94	ALA	N-CA-C	5.60	119.41	112.24
1	A	372	HIS	N-CA-C	5.49	120.68	112.94
1	C	95	TRP	N-CA-C	-5.43	101.81	109.96
1	B	357	GLU	N-CA-C	5.34	122.18	110.80
1	A	352	ASN	N-CA-C	5.25	119.53	113.18
1	B	199	ALA	N-CA-C	-5.23	100.21	108.73
1	C	73	GLY	N-CA-C	5.14	121.86	114.10
1	B	168	LYS	N-CA-C	5.10	117.50	109.39
2	D	70	GLY	N-CA-C	-5.09	106.02	112.54
1	A	143	PRO	N-CA-C	-5.08	104.50	110.70
1	C	160	ILE	N-CA-C	5.05	115.59	108.36

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	3128	0	3030	43	0
1	B	3128	0	3030	55	0
1	C	3128	0	3030	55	0
2	D	776	0	756	13	0
2	E	822	0	790	10	0
2	F	768	0	745	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	1	0
4	F	4	0	0	0	0
5	A	329	0	0	4	0
5	B	290	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	278	0	0	5	0
5	D	26	0	0	0	0
5	E	51	0	0	0	0
5	F	25	0	0	1	0
All	All	12776	0	11381	183	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (183) 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:6:GLU:O	1:C:10:LYS:HG2	1.71	0.90
1:C:360:GLU:HG3	5:C:782:HOH:O	1.80	0.80
1:B:11:ARG:HH21	1:C:388:HIS:CE1	2.01	0.78
1:A:114:ALA:O	1:A:118:ARG:HD3	1.85	0.76
1:A:210:ARG:NH2	2:D:21:ARG:HH12	1.83	0.76
1:A:290:ASP:OD1	1:A:293:THR:HG22	1.87	0.74
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.70	0.73
1:C:2:ALA:HB3	5:C:838:HOH:O	1.88	0.73
2:D:7:LYS:HG2	2:D:101:TYR:HE1	1.52	0.73
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.75	0.69
2:E:110:HIS:CD2	2:E:111:HIS:H	2.12	0.68
1:B:389:HIS:ND1	1:B:389:HIS:O	2.27	0.68
1:C:220:ASP:OD1	1:C:222:VAL:HG22	1.94	0.66
1:A:312:LYS:O	1:A:316:GLU:HG3	1.95	0.66
2:D:7:LYS:HG2	2:D:101:TYR:CE1	2.30	0.66
1:B:260:ASN:HD22	1:B:260:ASN:H	1.47	0.63
1:C:257:ILE:HD11	1:C:260:ASN:OD1	1.98	0.63
1:B:280:MET:HE3	1:B:313:TYR:HE1	1.64	0.63
1:A:38:ILE:HD13	1:A:62:LEU:HD22	1.82	0.62
2:D:92:GLU:HG2	2:D:107:LYS:HD3	1.82	0.61
1:A:118:ARG:HD2	5:A:751:HOH:O	2.01	0.60
1:B:306:ASN:OD1	1:B:308:GLU:HB2	2.00	0.60
1:B:10:LYS:HD3	1:B:10:LYS:O	2.02	0.60
1:B:260:ASN:H	1:B:260:ASN:ND2	1.99	0.59
1:C:260:ASN:C	1:C:260:ASN:HD22	2.11	0.58
1:C:2:ALA:HB1	1:C:20:ASP:OD1	2.04	0.58
1:A:312:LYS:HE2	1:A:316:GLU:OE2	2.03	0.58
1:C:306:ASN:O	1:C:310:ARG:HG3	2.05	0.57
1:A:210:ARG:HH21	2:D:21:ARG:HH12	1.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ALA:HB1	1:A:20:ASP:OD1	2.05	0.56
2:F:53:LEU:CD1	2:F:88:LEU:HD11	2.35	0.56
1:B:158:MET:CE	1:B:281:MET:HE2	2.35	0.55
1:B:262:LEU:HD11	1:B:272:VAL:HG13	1.88	0.55
1:B:326:LEU:O	1:B:330:ASN:HB2	2.06	0.55
1:C:333:ASP:O	1:C:337:ARG:HG3	2.06	0.55
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.42	0.55
2:F:4:ILE:HG13	2:F:5:TRP:N	2.22	0.54
1:B:158:MET:HE3	1:B:281:MET:HE2	1.89	0.54
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.89	0.54
1:C:261:ASP:HB3	1:C:273:ASN:O	2.08	0.54
1:B:220:ASP:OD1	1:B:222:VAL:HB	2.08	0.53
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.43	0.53
1:C:184:ILE:HD11	1:C:200:LEU:CD1	2.38	0.52
2:F:99:GLU:HB3	2:F:101:TYR:HE1	1.74	0.52
1:B:260:ASN:HD22	1:B:260:ASN:N	2.04	0.51
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.93	0.51
1:B:283:PHE:HB2	1:B:299:THR:OG1	2.09	0.51
1:B:196:ASN:O	1:B:256:LYS:HD2	2.11	0.51
1:C:260:ASN:HD22	1:C:261:ASP:N	2.08	0.51
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.41	0.51
1:B:184:ILE:HD11	1:B:200:LEU:CD1	2.41	0.51
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.46	0.51
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.92	0.50
1:B:167:ILE:HD12	1:B:334:ILE:HG23	1.92	0.50
2:F:7:LYS:HB2	2:F:7:LYS:NZ	2.26	0.50
1:B:38:ILE:HG23	1:B:57:ARG:HH21	1.75	0.50
1:B:215:ARG:HB3	1:B:228:TYR:HB2	1.94	0.50
1:A:280:MET:HE3	1:A:313:TYR:HE1	1.77	0.50
2:E:3:GLN:HG2	2:E:4:ILE:N	2.26	0.50
1:B:224:ARG:NH2	5:B:828:HOH:O	2.44	0.49
1:C:183:HIS:O	1:C:186:ILE:HG12	2.12	0.49
2:E:16:PRO:HA	2:E:34:ARG:HG2	1.93	0.49
2:F:4:ILE:HG13	2:F:5:TRP:CD1	2.47	0.49
2:F:51:ALA:HB2	2:F:67:PHE:CG	2.46	0.49
2:F:92:GLU:CD	2:F:107:LYS:HZ1	2.21	0.49
1:B:273:ASN:OD1	1:B:281:MET:HG2	2.11	0.49
1:B:100:GLU:HG2	5:B:675:HOH:O	2.13	0.49
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.95	0.49
1:B:261:ASP:HB3	1:B:273:ASN:O	2.13	0.49
2:F:4:ILE:HG13	2:F:5:TRP:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HE3	1:B:281:MET:CE	2.43	0.48
2:D:108:LEU:HD12	2:D:108:LEU:N	2.28	0.48
1:B:333:ASP:O	1:B:337:ARG:HG3	2.13	0.48
1:C:64:CYS:HB2	1:C:126:VAL:CG2	2.44	0.48
1:C:379:GLN:NE2	5:C:617:HOH:O	2.44	0.48
1:A:210:ARG:HD3	1:A:360:GLU:OE2	2.14	0.47
1:B:311:LYS:O	1:B:315:GLN:HG3	2.14	0.47
1:C:258:VAL:HB	1:C:274:PRO:O	2.14	0.47
1:A:198:LEU:HD23	1:A:256:LYS:HB2	1.97	0.47
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.96	0.47
1:A:306:ASN:OD1	1:A:308:GLU:HB2	2.13	0.47
1:B:196:ASN:HD22	1:B:198:LEU:HD21	1.80	0.47
1:B:260:ASN:HD22	1:B:261:ASP:N	2.13	0.47
1:C:27:ASN:HA	1:C:138:GLY:HA3	1.96	0.47
1:B:222:VAL:O	1:B:222:VAL:HG12	2.15	0.47
1:C:317:PHE:HA	1:C:321:TRP:HB2	1.97	0.47
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.45	0.46
2:E:110:HIS:CG	2:E:111:HIS:H	2.33	0.46
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.97	0.46
1:B:23:LEU:HD23	5:B:713:HOH:O	2.15	0.46
2:E:10:ALA:HB3	2:E:13:ASP:OD2	2.15	0.46
1:B:302:LYS:HD3	1:B:313:TYR:CD1	2.51	0.46
1:A:249:ARG:HG3	1:A:250:GLU:N	2.31	0.46
1:C:332:ASP:HA	1:C:335:TRP:NE1	2.30	0.46
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.98	0.45
2:F:95:VAL:HA	2:F:99:GLU:O	2.16	0.45
2:D:108:LEU:CD1	2:D:108:LEU:H	2.28	0.45
2:E:47:THR:HG23	2:E:88:LEU:HD23	1.98	0.45
1:A:93:HIS:HB2	4:A:502:FES:S1	2.56	0.45
1:A:215:ARG:HD3	5:A:867:HOH:O	2.17	0.45
1:A:311:LYS:O	1:A:315:GLN:HG3	2.17	0.45
1:C:346:ASP:O	1:C:347:ASP:HB2	2.17	0.45
1:C:379:GLN:HB2	5:C:614:HOH:O	2.17	0.45
1:C:285:TRP:HB2	1:C:297:PHE:HB3	1.99	0.45
2:D:108:LEU:HD12	2:D:108:LEU:H	1.81	0.45
1:C:306:ASN:OD1	1:C:308:GLU:HB2	2.17	0.45
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.51	0.45
2:F:106:LYS:NZ	5:F:323:HOH:O	2.49	0.45
1:A:180:ASP:HB3	1:A:183:HIS:HB3	1.98	0.44
1:C:171:TRP:CG	1:C:288:PRO:HG3	2.51	0.44
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HB	1:A:274:PRO:O	2.18	0.44
1:C:93:HIS:HB2	4:C:502:FES:S1	2.57	0.44
1:A:175:VAL:HG11	1:A:365:TRP:CE2	2.53	0.44
1:B:280:MET:HE3	1:B:313:TYR:CE1	2.48	0.44
1:C:257:ILE:HD13	1:C:257:ILE:O	2.17	0.44
1:A:38:ILE:CD1	1:A:55:VAL:HG12	2.49	0.43
1:C:2:ALA:HB1	1:C:20:ASP:CG	2.43	0.43
1:C:273:ASN:HA	1:C:274:PRO:HA	1.86	0.43
1:A:210:ARG:HA	1:A:213:GLN:HG2	1.99	0.43
1:B:215:ARG:HB2	1:B:230:LEU:HD11	2.00	0.43
1:C:42:GLU:HG2	1:C:44:LYS:HE3	2.01	0.43
1:C:283:PHE:HB2	1:C:299:THR:OG1	2.18	0.43
2:D:51:ALA:HB2	2:D:67:PHE:CD2	2.54	0.43
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.48	0.43
1:C:204:PHE:O	1:C:206:PRO:HD3	2.18	0.43
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.54	0.43
1:C:257:ILE:HD13	1:C:257:ILE:C	2.43	0.43
1:B:171:TRP:CG	1:B:288:PRO:HG3	2.53	0.43
1:A:215:ARG:CZ	5:A:759:HOH:O	2.67	0.43
1:B:65:LEU:HD23	1:B:123:THR:HG22	2.00	0.43
1:B:228:TYR:CD1	1:B:263:SER:HB3	2.53	0.43
1:A:354:ILE:HD12	1:B:70:LEU:HB3	2.00	0.43
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.34	0.43
2:E:4:ILE:HG22	2:E:5:TRP:CD1	2.54	0.43
1:C:64:CYS:HB2	1:C:126:VAL:HG21	2.01	0.43
1:B:321:TRP:O	1:B:325:ALA:HB3	2.19	0.42
1:C:228:TYR:CD1	1:C:263:SER:HB3	2.54	0.42
1:B:273:ASN:HA	1:B:274:PRO:HA	1.88	0.42
1:C:196:ASN:O	1:C:256:LYS:HD2	2.19	0.42
1:C:215:ARG:HB2	1:C:230:LEU:HD11	2.01	0.42
2:D:10:ALA:HB3	2:D:13:ASP:OD2	2.18	0.42
1:A:218:ASP:OD1	1:A:218:ASP:O	2.37	0.42
1:B:64:CYS:HB2	1:B:126:VAL:CG2	2.49	0.42
1:C:167:ILE:HB	1:C:294:HIS:CE1	2.54	0.42
1:B:263:SER:O	1:B:270:LEU:HD12	2.19	0.42
1:C:260:ASN:ND2	1:C:260:ASN:H	2.16	0.42
1:C:136:TYR:CE1	1:C:143:PRO:HD2	2.54	0.42
1:C:269:VAL:HB	1:C:285:TRP:CD1	2.54	0.42
1:A:210:ARG:HH22	2:D:21:ARG:HH12	1.65	0.42
1:C:260:ASN:C	1:C:260:ASN:ND2	2.76	0.42
1:B:151:PRO:O	1:B:152:ASN:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:CYS:HB2	2:F:13:ASP:OD2	2.20	0.42
1:A:287:VAL:HA	1:A:288:PRO:HD3	1.91	0.41
1:A:333:ASP:O	1:A:337:ARG:HG3	2.20	0.41
1:B:12:VAL:HG21	1:B:19:VAL:HG21	2.02	0.41
1:B:48:LEU:HD23	1:B:137:LEU:HD23	2.02	0.41
1:A:194:LYS:HE3	5:A:901:HOH:O	2.19	0.41
1:C:280:MET:HE3	1:C:313:TYR:HE1	1.86	0.41
2:F:53:LEU:HD11	2:F:88:LEU:HD11	2.01	0.41
1:A:65:LEU:CD2	1:A:123:THR:HG22	2.46	0.41
1:B:191:ILE:O	1:B:195:ASP:HB2	2.21	0.41
1:C:15:TRP:CZ3	1:C:363:VAL:HG13	2.55	0.41
2:E:68:HIS:HB2	4:E:201:FES:S2	2.60	0.41
1:A:290:ASP:CG	1:A:293:THR:HG22	2.44	0.41
1:B:291:GLU:HG2	5:B:698:HOH:O	2.20	0.41
1:B:206:PRO:HG2	1:B:357:GLU:HB3	2.03	0.41
1:C:293:THR:HG21	5:C:846:HOH:O	2.21	0.41
1:A:108:LEU:HD12	1:A:108:LEU:N	2.36	0.41
1:A:222:VAL:HG23	1:A:224:ARG:HG3	2.02	0.41
1:A:280:MET:HE3	1:A:313:TYR:CE1	2.54	0.41
1:C:104:LEU:HD21	1:C:107:ILE:HD11	2.02	0.41
1:C:184:ILE:HD11	1:C:200:LEU:HD11	2.02	0.41
1:B:192:LEU:HD12	1:B:324:MET:SD	2.60	0.41
2:F:96:LYS:HE2	2:F:101:TYR:CZ	2.56	0.41
2:D:90:VAL:HG23	2:D:107:LYS:HE3	2.03	0.40
1:A:275:PHE:CG	1:A:276:PRO:HA	2.57	0.40
1:B:269:VAL:HB	1:B:285:TRP:CD1	2.56	0.40
1:A:176:GLU:O	1:A:180:ASP:HB2	2.21	0.40
1:A:211:LYS:H	1:A:211:LYS:HG3	1.63	0.40
1:B:143:PRO:HG3	1:B:147:ARG:CZ	2.52	0.40
1:C:275:PHE:CG	1:C:276:PRO:HA	2.57	0.40
1:C:389:HIS:CE1	2:E:62:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	368 (95%)	16 (4%)	2 (0%)	24	21
1	B	386/392 (98%)	364 (94%)	21 (5%)	1 (0%)	36	35
1	C	386/392 (98%)	366 (95%)	18 (5%)	2 (0%)	24	21
2	D	103/115 (90%)	97 (94%)	6 (6%)	0	100	100
2	E	108/115 (94%)	102 (94%)	5 (5%)	1 (1%)	14	9
2	F	102/115 (89%)	99 (97%)	3 (3%)	0	100	100
All	All	1471/1521 (97%)	1396 (95%)	69 (5%)	6 (0%)	30	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	C	268	GLY
1	A	71	HIS
1	A	268	GLY
1	C	71	HIS
2	E	109	GLU

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	335/339 (99%)	328 (98%)	7 (2%)	47	52
1	B	335/339 (99%)	328 (98%)	7 (2%)	47	52
1	C	335/339 (99%)	328 (98%)	7 (2%)	47	52
2	D	83/93 (89%)	83 (100%)	0	100	100
2	E	88/93 (95%)	87 (99%)	1 (1%)	65	73
2	F	82/93 (88%)	81 (99%)	1 (1%)	63	70
All	All	1258/1296 (97%)	1235 (98%)	23 (2%)	51	58

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	47	LYS
1	A	137	LEU
1	A	262	LEU
1	A	293	THR
1	A	356	PHE
1	A	368	LEU
1	B	10	LYS
1	B	46	LEU
1	B	137	LEU
1	B	246	GLU
1	B	260	ASN
1	B	356	PHE
1	B	368	LEU
1	C	137	LEU
1	C	257	ILE
1	C	260	ASN
1	C	307	ASP
1	C	356	PHE
1	C	368	LEU
1	C	371	GLU
2	E	2	ASN
2	F	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	213	GLN
1	A	282	GLN
1	A	315	GLN
1	A	330	ASN
1	A	379	GLN
1	B	127	GLN
1	B	165	GLN
1	B	260	ASN
1	B	282	GLN
1	B	298	GLN
1	B	330	ASN
1	B	388	HIS
1	C	75	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	GLN
1	C	260	ASN
1	C	273	ASN
1	C	282	GLN
1	C	315	GLN
1	C	330	ASN
1	C	389	HIS
2	E	2	ASN
2	E	110	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 oligosaccharides 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	E	201	2	0,4,4	-	-	-		
4	FES	C	502	1	0,4,4	-	-	-		
4	FES	A	502	1	0,4,4	-	-	-		
4	FES	D	201	2	0,4,4	-	-	-		
4	FES	B	502	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FES	F	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
4	FES	E	201	2	-	-	0/1/1/1
4	FES	C	502	1	-	-	0/1/1/1
4	FES	A	502	1	-	-	0/1/1/1
4	FES	D	201	2	-	-	0/1/1/1
4	FES	B	502	1	-	-	0/1/1/1
4	FES	F	201	2	-	-	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	201	FES	1	0
4	C	502	FES	1	0
4	A	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, 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	388/392 (98%)	-0.09	9 (2%) 61 60	18, 26, 41, 48	0
1	B	388/392 (98%)	0.00	6 (1%) 72 71	19, 29, 45, 51	0
1	C	388/392 (98%)	-0.01	4 (1%) 79 79	21, 29, 42, 48	0
2	D	105/115 (91%)	0.61	7 (6%) 24 22	23, 39, 49, 51	0
2	E	110/115 (95%)	0.37	4 (3%) 46 45	25, 34, 45, 51	0
2	F	104/115 (90%)	0.86	10 (9%) 13 12	26, 38, 47, 52	0
All	All	1483/1521 (97%)	0.10	40 (2%) 56 55	18, 30, 45, 52	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	HIS	3.8
2	D	4	ILE	3.7
2	E	111	HIS	3.7
1	A	387	HIS	3.7
2	F	4	ILE	3.6
1	B	389	HIS	3.5
2	D	108	LEU	3.5
2	F	6	LEU	3.5
2	F	101	TYR	3.5
1	A	221	VAL	3.3
1	C	389	HIS	3.3
1	A	2	ALA	3.1
1	A	220	ASP	3.1
1	B	221	VAL	3.1
2	D	6	LEU	3.1
2	E	110	HIS	3.0
2	F	107	LYS	2.9
2	F	100	VAL	2.8
2	E	2	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	25	VAL	2.5
1	A	308	GLU	2.5
1	B	308	GLU	2.5
2	F	95	VAL	2.4
2	D	104	GLY	2.4
2	D	38	GLN	2.4
1	B	235	GLY	2.4
1	A	218	ASP	2.4
1	B	305	ALA	2.4
2	F	102	VAL	2.4
1	C	388	HIS	2.3
1	B	2	ALA	2.3
1	A	388	HIS	2.2
2	F	93	VAL	2.2
1	A	210	ARG	2.2
1	C	307	ASP	2.2
1	C	235	GLY	2.1
2	F	92	GLU	2.1
2	E	4	ILE	2.1
2	D	102	VAL	2.1
2	D	89	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	FE2	A	501	1/1	0.99	0.02	24,24,24,24	0
3	FE2	B	501	1/1	0.99	0.02	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FES	A	502	4/4	0.99	0.04	22,22,22,22	0
4	FES	B	502	4/4	0.99	0.03	18,20,21,21	0
4	FES	C	502	4/4	0.99	0.03	23,23,24,25	0
4	FES	E	201	4/4	0.99	0.04	24,25,25,30	0
4	FES	F	201	4/4	0.99	0.04	25,27,28,28	0
3	FE2	C	501	1/1	1.00	0.02	28,28,28,28	0
4	FES	D	201	4/4	1.00	0.02	24,24,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.