



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:01 PM UTC

PDB ID : 2CKF / pdb_00002ckf
Title : Crystal Structure of the Terminal Component of the PAH-hydroxylating Dioxygenase from Sphingomonas sp CHY-1
Authors : Jakoncic, J.; Meyer, C.; Jouanneau, Y.; Stojanoff, V.
Deposited on : 2006-04-18
Resolution : 1.85 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

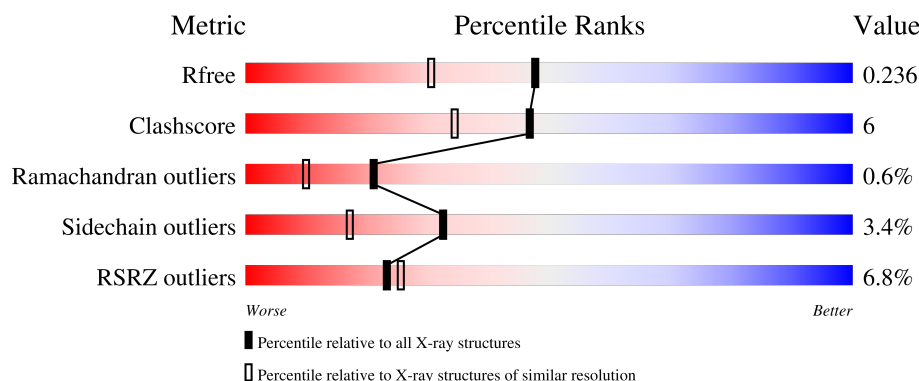
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	454	5% 85% 13% ..
1	C	454	8% 78% 14% 6%
1	E	454	11% 82% 12% 5%
2	B	174	3% 86% 11% ..
2	D	174	2% 87% 10% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	174	3% 84% 11% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15833 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.

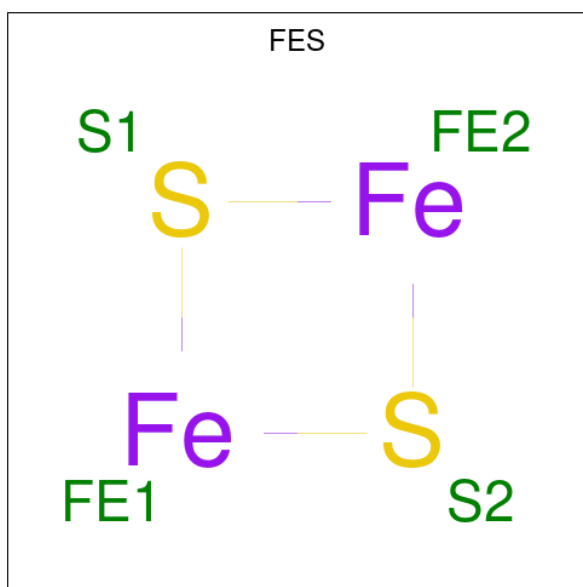
- Molecule 1 is a protein called RING-HYDROXYLATING DIOXYGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	2	0
			3549	2245	621	666	17			
1	C	425	Total	C	N	O	S	0	2	0
			3394	2155	591	631	17			
1	E	433	Total	C	N	O	S	0	1	0
			3444	2181	602	644	17			

- Molecule 2 is a protein called RING-HYDROXYLATING DIOXYGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	2	0
			1458	924	260	270	4			
2	D	170	Total	C	N	O	S	0	0	0
			1437	910	258	265	4			
2	F	170	Total	C	N	O	S	0	0	0
			1440	911	259	266	4			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		
4	E	1	Total	Fe	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	357	Total	O	0	0
			357	357		
5	B	172	Total	O	0	0
			172	172		
5	C	147	Total	O	0	0
			147	147		

Continued on next page...

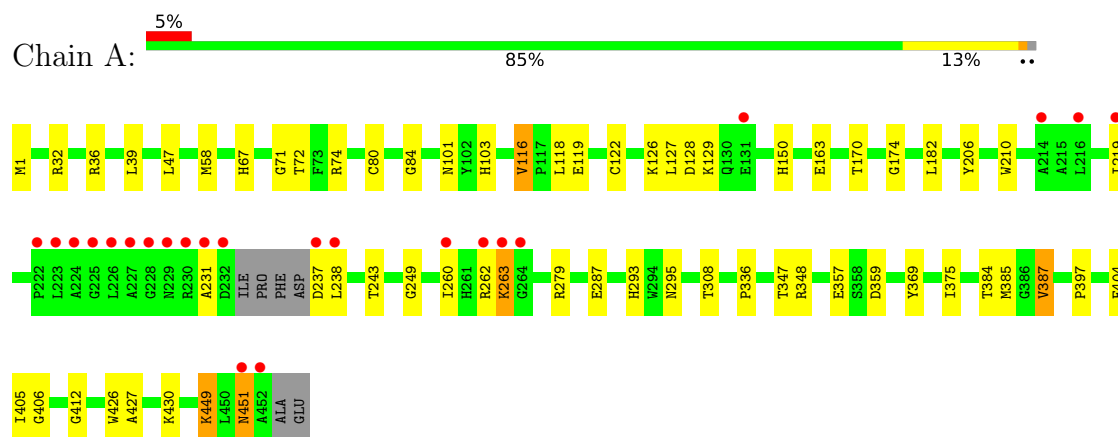
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	125	Total 125	O 125	0	0
5	E	152	Total 152	O 152	0	0
5	F	143	Total 143	O 143	0	0

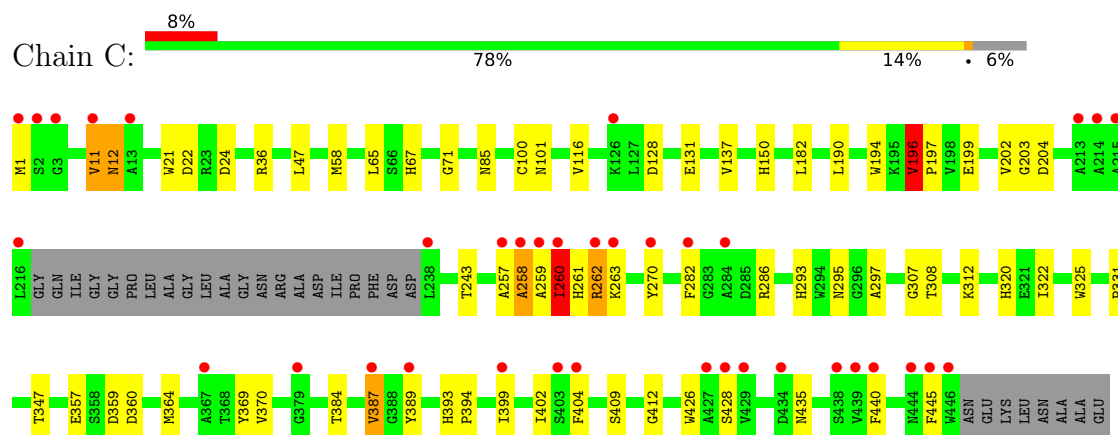
3 Residue-property plots [i](#)

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.

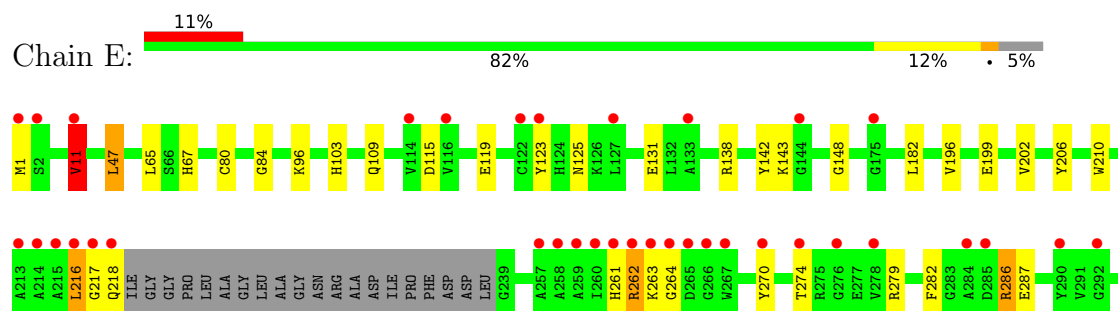
• Molecule 1: RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT



• Molecule 1: RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT

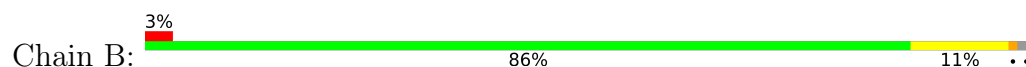


• Molecule 1: RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT

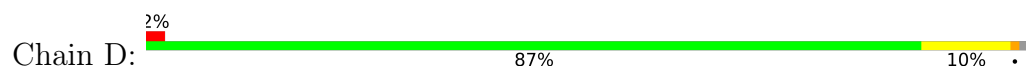




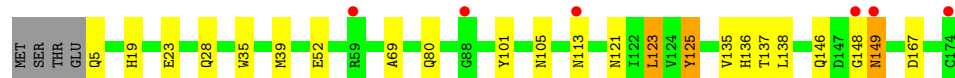
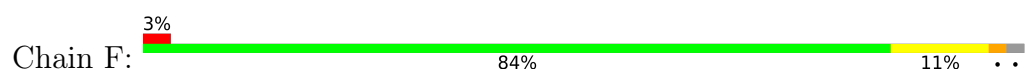
• Molecule 2: RING-HYDROXYLATING DIOXYGENASE BETA SUBUNIT



• Molecule 2: RING-HYDROXYLATING DIOXYGENASE BETA SUBUNIT



• Molecule 2: RING-HYDROXYLATING DIOXYGENASE BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.64Å 112.73Å 190.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.85 35.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.00-1.85) 99.6 (35.00-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.236 0.197 , 0.236	Depositor DCC
R_{free} test set	8495 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	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	0.95	EDS
Total number of atoms	15833	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, FE

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	1.02	3/3657 (0.1%)	1.02	4/4962 (0.1%)
1	C	0.86	1/3501 (0.0%)	0.94	6/4750 (0.1%)
1	E	0.86	0/3548	0.99	8/4814 (0.2%)
2	B	0.98	1/1498 (0.1%)	0.93	0/2029
2	D	0.96	0/1473	0.92	0/1995
2	F	0.86	0/1476	0.92	0/1999
All	All	0.92	5/15153 (0.0%)	0.97	18/20549 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	GLY	N-CA	5.96	1.51	1.45
1	A	405	ILE	CA-CB	5.80	1.60	1.53
1	C	260	ILE	CA-CB	5.58	1.60	1.54
2	B	153	VAL	CA-CB	5.21	1.60	1.54
1	A	116	VAL	CA-CB	5.00	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	VAL	N-CA-C	10.37	120.18	110.74
1	A	263	LYS	N-CA-C	9.29	126.45	114.75
1	E	452	ALA	N-CA-C	9.12	121.30	111.36
1	E	11	VAL	CA-C-N	8.08	136.97	121.54
1	E	11	VAL	C-N-CA	8.08	136.97	121.54
1	E	11	VAL	N-CA-C	7.40	124.74	109.34
1	C	11	VAL	CA-C-N	6.50	133.39	121.70
1	C	11	VAL	C-N-CA	6.50	133.39	121.70
1	A	127	LEU	CA-C-N	-6.31	114.64	122.84
1	A	127	LEU	C-N-CA	-6.31	114.64	122.84
1	E	452	ALA	CA-C-N	6.14	132.75	121.70
1	E	452	ALA	C-N-CA	6.14	132.75	121.70
1	E	11	VAL	O-C-N	-6.13	114.90	122.57
1	C	263	LYS	N-CA-C	6.03	121.31	111.37
1	C	196	VAL	N-CA-CB	5.81	114.98	110.45
1	C	369	TYR	N-CA-C	5.38	119.10	112.54
1	A	369	TYR	N-CA-C	5.18	118.86	112.54
1	E	309	ASN	N-CA-C	5.03	118.72	112.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	LYS	Peptide
1	E	11	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3549	0	3337	45	0
1	C	3394	0	3196	46	0
1	E	3444	0	3233	41	0
2	B	1458	0	1397	19	1
2	D	1437	0	1379	14	1
2	F	1440	0	1383	20	0
3	A	4	0	0	1	0
3	C	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	4	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	357	0	0	2	0
5	B	172	0	0	0	0
5	C	147	0	0	0	0
5	D	125	0	0	1	0
5	E	152	0	0	2	0
5	F	143	0	0	1	0
All	All	15833	0	13925	162	1

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 6.

All (162) 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:258:ALA:HB3	1:C:259:ALA:HA	1.21	1.14
2:B:84:ARG:HD3	2:B:171:TYR:OH	1.52	1.09
1:C:258:ALA:CB	1:C:259:ALA:HA	1.82	1.09
2:B:121:ASN:HD21	2:F:28:GLN:HE22	1.19	0.89
1:A:262:ARG:HH22	1:A:348:ARG:HH11	1.19	0.89
1:A:430:LYS:HD3	5:A:2332:HOH:O	1.77	0.85
2:B:84:ARG:HD3	2:B:171:TYR:CZ	2.11	0.85
2:D:28:GLN:HE22	2:F:121:ASN:HD21	1.24	0.83
1:A:262:ARG:HH22	1:A:348:ARG:NH1	1.78	0.82
2:B:84:ARG:CD	2:B:171:TYR:OH	2.27	0.82
1:C:258:ALA:HB3	1:C:259:ALA:CA	2.09	0.80
1:C:258:ALA:CB	1:C:259:ALA:CA	2.61	0.79
1:A:210:TRP:HE1	1:C:101:ASN:HD22	1.27	0.78
1:C:295:ASN:HD21	1:C:404:PHE:HE2	1.32	0.78
1:A:101:ASN:HD22	1:E:210:TRP:HE1	1.34	0.74
1:A:119:GLU:OE2	1:A:129:LYS:HE2	1.89	0.73
2:F:19:HIS:CE1	2:F:39:MET:HE2	2.25	0.72
1:A:427:ALA:HA	1:A:430:LYS:HE2	1.74	0.70
2:B:28:GLN:HE22	2:D:121:ASN:HD21	1.38	0.70
2:D:28:GLN:HE21	2:D:101:TYR:H	1.37	0.70
1:A:449:LYS:NZ	1:A:449:LYS:HB3	2.07	0.69
1:A:126:LYS:O	1:A:126:LYS:HG3	1.93	0.68
1:C:347:THR:HG21	2:D:69:ALA:O	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:HA	1:A:430:LYS:CE	2.23	0.68
1:A:449:LYS:HB3	1:A:449:LYS:HZ3	1.58	0.68
2:B:28:GLN:HE21	2:B:101:TYR:H	1.43	0.66
1:E:452:ALA:HB3	1:E:453:ALA:HB3	1.76	0.66
1:E:426:TRP:O	1:E:430:LYS:HG3	1.96	0.66
1:A:293:HIS:HE1	1:A:308:THR:OG1	1.80	0.64
1:A:36:ARG:HG3	1:A:426:TRP:NE1	2.13	0.64
2:D:136:HIS:HE1	2:D:167:ASP:OD2	1.82	0.62
1:A:219:ILE:HD13	1:A:262:ARG:HD3	1.80	0.62
2:D:28:GLN:HE22	2:F:121:ASN:ND2	1.96	0.62
1:E:282:PHE:HB3	1:E:286:ARG:HD3	1.80	0.62
2:B:121:ASN:ND2	2:F:28:GLN:HE22	1.93	0.61
2:F:136:HIS:HD2	5:F:2043:HOH:O	1.83	0.60
1:A:295:ASN:HD21	1:A:404:PHE:HE2	1.49	0.60
2:B:123:LEU:HD13	2:B:125[A]:TYR:HE2	1.67	0.60
1:E:216:LEU:C	1:E:218:GLN:H	2.08	0.60
1:A:384:THR:O	1:A:387:VAL:HG22	2.02	0.60
2:F:28:GLN:HE21	2:F:101:TYR:H	1.48	0.60
1:C:22:ASP:HB3	1:C:24:ASP:OD1	2.01	0.59
1:E:449:LYS:O	1:E:453:ALA:HB3	2.01	0.59
1:A:359:ASP:OD1	2:B:84:ARG:NH2	2.36	0.59
1:E:270:TYR:O	1:E:274:THR:OG1	2.16	0.59
1:E:371:ASN:O	1:E:377:ARG:HD3	2.02	0.59
1:A:347:THR:HG21	2:B:69:ALA:O	2.03	0.58
2:D:136:HIS:HD2	5:D:2044:HOH:O	1.86	0.57
1:C:67:HIS:HE1	1:C:71:GLY:HA2	1.69	0.57
1:C:243:THR:OG1	1:C:412:GLY:HA3	2.05	0.56
1:C:36:ARG:HG2	1:C:426:TRP:NE1	2.21	0.56
2:F:136:HIS:HE1	2:F:167:ASP:OD2	1.89	0.56
1:E:1:MET:HB3	5:E:2003:HOH:O	2.06	0.55
1:E:96:LYS:HA	1:E:109:GLN:HE21	1.71	0.55
1:C:257:ALA:O	1:C:307:GLY:HA2	2.06	0.55
1:C:359:ASP:OD1	2:D:84:ARG:NH2	2.28	0.55
1:C:11:VAL:CA	1:C:12:ASN:HB2	2.36	0.54
1:E:216:LEU:O	1:E:218:GLN:N	2.41	0.54
2:D:28:GLN:NE2	2:D:101:TYR:H	2.06	0.53
1:A:118:LEU:HD13	1:A:122:CYS:SG	2.49	0.52
1:A:262:ARG:NH2	1:A:348:ARG:NH1	2.54	0.52
1:E:47:LEU:O	1:E:67:HIS:HD2	1.92	0.52
1:E:206:TYR:CG	1:E:385:MET:HE1	2.46	0.51
1:C:258:ALA:HB1	1:C:259:ALA:HA	1.86	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:HIS:HE1	1:C:308:THR:OG1	1.95	0.50
1:C:11:VAL:HB	1:C:12:ASN:HB2	1.93	0.50
1:E:261:HIS:HD2	1:E:345:GLU:CB	2.25	0.50
2:B:28:GLN:HE22	2:D:121:ASN:ND2	2.06	0.49
1:A:36:ARG:HG3	1:A:426:TRP:CD1	2.47	0.49
2:B:147:ASP:O	2:B:149:ASN:C	2.56	0.49
1:E:270:TYR:CZ	1:E:331:PRO:HB3	2.47	0.49
1:E:347:THR:HG21	2:F:69:ALA:O	2.12	0.49
1:E:262:ARG:HG2	2:F:80:GLN:HE22	1.77	0.49
2:B:92:MET:HE1	2:B:168:LYS:HD3	1.93	0.49
1:C:21:TRP:O	1:C:320:HIS:HE1	1.96	0.49
1:E:47:LEU:HD23	1:E:47:LEU:N	2.28	0.49
1:A:32:ARG:O	1:A:36:ARG:HD2	2.12	0.48
1:C:196:VAL:HB	1:C:197:PRO:HD3	1.95	0.48
1:E:80:CYS:O	1:E:84:GLY:HA2	2.13	0.48
1:C:322:ILE:C	1:C:322:ILE:HD12	2.38	0.48
1:C:199:GLU:HA	1:C:202:VAL:HG12	1.96	0.48
1:C:128:ASP:OD1	1:C:131[A]:GLU:OE1	2.31	0.48
1:C:282:PHE:O	1:C:286:ARG:HD3	2.13	0.48
2:B:147:ASP:O	2:B:150:GLY:N	2.47	0.47
1:E:359:ASP:O	5:E:2120:HOH:O	2.20	0.47
1:C:67:HIS:CE1	1:C:71:GLY:HA2	2.49	0.47
2:B:121:ASN:HD21	2:F:28:GLN:NE2	2.00	0.47
1:C:370:VAL:HG21	1:E:84:GLY:O	2.15	0.46
2:F:28:GLN:NE2	2:F:101:TYR:H	2.14	0.46
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.81	0.46
2:B:135:VAL:HG11	2:F:125:TYR:OH	2.15	0.46
1:E:295:ASN:HD21	1:E:404:PHE:HE2	1.64	0.46
1:C:202:VAL:HG23	1:C:297:ALA:HB3	1.98	0.46
1:E:279:ARG:HB2	1:E:287:GLU:OE1	2.15	0.45
1:E:119:GLU:O	1:E:123:TYR:HB2	2.17	0.45
1:A:84:GLY:O	1:E:370:VAL:HG21	2.17	0.45
1:A:39:LEU:HD12	1:A:58:MET:HB3	1.99	0.45
1:A:237:ASP:O	1:A:238:LEU:HB2	2.16	0.45
1:A:293:HIS:HD2	5:A:2237:HOH:O	1.98	0.45
1:E:216:LEU:C	1:E:218:GLN:N	2.74	0.45
1:A:243:THR:OG1	1:A:412:GLY:HA3	2.16	0.45
2:F:123:LEU:HD23	2:F:137:THR:HG22	1.99	0.45
1:A:72:THR:OG1	1:A:74:ARG:NH1	2.48	0.44
1:A:170:THR:O	1:A:174:GLY:HA2	2.18	0.44
1:E:199:GLU:HA	1:E:202:VAL:HG12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:GLN:HG2	2:D:109:PHE:HB3	1.98	0.44
1:E:142:TYR:CD1	1:E:143:LYS:HG2	2.52	0.44
2:B:81:ARG:O	2:B:84:ARG:HG2	2.16	0.44
1:A:279:ARG:HD3	1:A:287:GLU:OE1	2.18	0.44
1:A:427:ALA:HA	1:A:430:LYS:HE3	1.97	0.44
1:C:11:VAL:N	1:C:12:ASN:HB2	2.33	0.44
1:C:194:TRP:HA	1:C:322:ILE:HG21	1.99	0.44
1:C:261:HIS:O	1:C:262:ARG:HB2	2.17	0.44
1:E:449:LYS:O	1:E:453:ALA:CB	2.65	0.44
1:C:257:ALA:O	1:C:307:GLY:CA	2.66	0.44
1:C:190:LEU:HB3	1:C:322:ILE:HD11	1.99	0.44
1:A:47:LEU:O	1:A:67:HIS:HD2	2.00	0.43
1:A:80:CYS:O	1:A:84:GLY:HA2	2.18	0.43
2:F:113:ASN:O	2:F:113:ASN:CG	2.60	0.43
1:A:385:MET:SD	1:A:406:GLY:HA2	2.58	0.43
1:A:375:ILE:HG13	1:C:150:HIS:CD2	2.54	0.43
1:E:138:ARG:O	1:E:148:GLY:HA2	2.17	0.43
2:F:148:GLY:HA2	2:F:149:ASN:HA	1.63	0.43
1:E:261:HIS:HD2	1:E:345:GLU:HB2	1.84	0.43
1:C:389:TYR:HA	1:C:445:PHE:CE2	2.54	0.43
2:F:123:LEU:HD23	2:F:137:THR:CG2	2.49	0.43
1:E:350:PHE:HA	1:E:357:GLU:HB2	2.01	0.43
1:A:262:ARG:HH22	1:A:348:ARG:HD2	1.84	0.42
1:C:360:ASP:O	1:C:364:MET:HG2	2.19	0.42
1:E:282:PHE:O	1:E:286:ARG:HD3	2.19	0.42
1:A:126:LYS:O	1:A:126:LYS:CG	2.65	0.42
1:E:103:HIS:HB2	3:E:500:FES:S1	2.59	0.42
1:A:150:HIS:CD2	1:E:375:ILE:HG13	2.54	0.42
2:B:28:GLN:NE2	2:B:101:TYR:H	2.12	0.42
1:A:67:HIS:CE1	1:A:71:GLY:HA2	2.54	0.42
2:F:23:GLU:HG3	2:F:35:TRP:CD1	2.54	0.42
2:D:52:GLU:HG3	2:D:54:ARG:HG3	2.02	0.42
1:E:279:ARG:HD3	1:E:287:GLU:OE1	2.19	0.42
2:B:148:GLY:HA2	2:B:149:ASN:HA	1.70	0.42
1:C:58:MET:SD	1:C:137:VAL:HG11	2.60	0.42
1:C:203:GLY:CA	1:C:409:SER:HB2	2.49	0.42
1:C:203:GLY:HA3	1:C:409:SER:HB2	2.02	0.41
1:A:206:TYR:CG	1:A:385:MET:HE1	2.55	0.41
1:E:142:TYR:CE1	1:E:143:LYS:HG2	2.56	0.41
1:C:260:ILE:HD13	1:C:261:HIS:CD2	2.55	0.41
1:C:399:ILE:HG13	1:C:440:PHE:CD1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:TYR:CD1	1:E:385:MET:HE1	2.56	0.41
1:A:163:GLU:HB3	1:A:397:PRO:HB2	2.03	0.41
1:C:85:ASN:HB3	1:C:100:CYS:SG	2.61	0.41
1:C:11:VAL:H	1:C:12:ASN:HB2	1.85	0.41
1:C:312:LYS:HA	1:C:325:TRP:O	2.21	0.41
1:C:270:TYR:CZ	1:C:331:PRO:HB3	2.56	0.40
1:C:204:ASP:CG	1:E:103:HIS:HE2	2.27	0.40
1:C:384:THR:O	1:C:387:VAL:HG22	2.21	0.40
2:D:102:PHE:CE2	2:F:123:LEU:HB2	2.56	0.40
1:E:322:ILE:HD13	1:E:324:VAL:HB	2.03	0.40
1:C:393:HIS:CG	1:C:394:PRO:HD2	2.56	0.40
2:D:125:TYR:OH	2:F:135:VAL:HG11	2.21	0.40
1:A:103:HIS:HB2	3:A:500:FES:S1	2.62	0.40
1:A:293:HIS:CE1	1:A:308:THR:OG1	2.69	0.40
1:A:451:ASN:CG	1:A:451:ASN:O	2.64	0.40
1:E:435:ASN:HD22	1:E:435:ASN:HA	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76[A]:GLU:CG	2:D:42:GLU:OE1[3_655]	2.13	0.07

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	446/454 (98%)	424 (95%)	21 (5%)	1 (0%)	43	31
1	C	423/454 (93%)	404 (96%)	16 (4%)	3 (1%)	18	8
1	E	430/454 (95%)	403 (94%)	22 (5%)	5 (1%)	10	2
2	B	170/174 (98%)	166 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	168/174 (97%)	161 (96%)	6 (4%)	1 (1%)	21	10
2	F	168/174 (97%)	163 (97%)	5 (3%)	0	100	100
All	All	1805/1884 (96%)	1721 (95%)	74 (4%)	10 (1%)	21	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	12	ASN
1	C	258	ALA
1	E	125	ASN
1	A	231	ALA
2	D	148	GLY
1	E	11	VAL
1	E	217	GLY
1	E	264	GLY
1	E	394	PRO
1	C	262	ARG

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	368/371 (99%)	358 (97%)	10 (3%)	39	24
1	C	354/371 (95%)	342 (97%)	12 (3%)	32	17
1	E	358/371 (96%)	346 (97%)	12 (3%)	32	17
2	B	156/158 (99%)	151 (97%)	5 (3%)	34	19
2	D	153/158 (97%)	148 (97%)	5 (3%)	33	18
2	F	154/158 (98%)	146 (95%)	8 (5%)	21	7
All	All	1543/1587 (97%)	1491 (97%)	52 (3%)	32	17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	116	VAL
1	A	128	ASP
1	A	182	LEU
1	A	260	ILE
1	A	336	PRO
1	A	357	GLU
1	A	387	VAL
1	A	449	LYS
1	A	451	ASN
2	B	98	LYS
2	B	105	ASN
2	B	123	LEU
2	B	146	GLN
2	B	168	LYS
1	C	1	MET
1	C	47	LEU
1	C	65	LEU
1	C	116	VAL
1	C	182	LEU
1	C	196	VAL
1	C	260	ILE
1	C	357	GLU
1	C	387	VAL
1	C	402	ILE
1	C	428	SER
1	C	435	ASN
2	D	105	ASN
2	D	123	LEU
2	D	125	TYR
2	D	138	LEU
2	D	146	GLN
1	E	47	LEU
1	E	65	LEU
1	E	115	ASP
1	E	131	GLU
1	E	182	LEU
1	E	196	VAL
1	E	216	LEU
1	E	262	ARG
1	E	263	LYS
1	E	286	ARG
1	E	435	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	449	LYS
2	F	5	GLN
2	F	52	GLU
2	F	105	ASN
2	F	123	LEU
2	F	125	TYR
2	F	138	LEU
2	F	146	GLN
2	F	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	101	ASN
1	A	261	HIS
1	A	293	HIS
1	A	444	ASN
1	A	447	ASN
1	A	451	ASN
2	B	28	GLN
2	B	105	ASN
2	B	146	GLN
1	C	67	HIS
1	C	85	ASN
1	C	101	ASN
1	C	109	GLN
1	C	191	HIS
1	C	246	HIS
1	C	261	HIS
1	C	293	HIS
1	C	295	ASN
1	C	320	HIS
1	C	432	ASN
2	D	5	GLN
2	D	28	GLN
2	D	31	GLN
2	D	89	GLN
2	D	136	HIS
2	D	146	GLN
1	E	67	HIS
1	E	85	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	101	ASN
1	E	109	GLN
1	E	124	HIS
1	E	125	ASN
1	E	261	HIS
1	E	295	ASN
1	E	320	HIS
1	E	435	ASN
2	F	5	GLN
2	F	28	GLN
2	F	37	HIS
2	F	80	GLN
2	F	136	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
3	FES	A	500	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FES	E	500	1	0,4,4	-	-	-		
3	FES	C	500	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
3	FES	A	500	1	-	-	0/1/1/1
3	FES	E	500	1	-	-	0/1/1/1
3	FES	C	500	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
3	A	500	FES	1	0
3	E	500	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	448/454 (98%)	-0.13	23 (5%)	33	36	12, 19, 42, 65	2 (0%)
1	C	425/454 (93%)	0.62	37 (8%)	16	16	15, 31, 50, 65	2 (0%)
1	E	433/454 (95%)	0.85	49 (11%)	10	9	16, 32, 53, 70	1 (0%)
2	B	170/174 (97%)	-0.16	5 (2%)	53	57	9, 20, 33, 49	2 (1%)
2	D	170/174 (97%)	-0.11	4 (2%)	59	63	16, 22, 35, 45	0
2	F	170/174 (97%)	0.16	6 (3%)	47	51	15, 26, 43, 50	0
All	All	1816/1884 (96%)	0.30	124 (6%)	23	25	9, 25, 49, 70	7 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	260	ILE	6.1
1	C	216	LEU	5.4
1	C	214	ALA	5.2
1	E	264	GLY	5.1
1	E	1	MET	5.1
1	C	213	ALA	4.6
1	A	262	ARG	4.4
1	A	231	ALA	4.3
1	E	257	ALA	4.2
1	C	258	ALA	4.1
1	A	264	GLY	4.1
1	C	2	SER	3.9
1	A	229	ASN	3.7
1	E	450	LEU	3.7
1	C	257	ALA	3.7
1	C	262	ARG	3.7
1	C	404	PHE	3.7
1	A	226	LEU	3.7
1	C	11	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	444	ASN	3.5
1	C	215	ALA	3.5
1	C	1	MET	3.5
2	B	150	GLY	3.5
1	A	238	LEU	3.5
1	E	2	SER	3.4
1	A	228	GLY	3.4
1	C	440	PHE	3.4
2	F	148	GLY	3.3
1	E	453	ALA	3.3
1	A	232	ASP	3.3
2	D	148	GLY	3.3
2	B	148	GLY	3.2
1	E	214	ALA	3.2
1	C	238	LEU	3.2
1	E	259	ALA	3.1
2	F	149	ASN	3.1
1	C	446	TRP	3.0
1	E	266	GLY	3.0
1	E	267	TRP	3.0
1	C	263	LYS	2.9
1	E	285	ASP	2.9
1	E	217	GLY	2.9
1	E	122	CYS	2.9
1	E	216	LEU	2.9
1	E	114	VAL	2.9
1	A	260	ILE	2.9
1	A	230	ARG	2.9
1	A	219	ILE	2.9
2	B	149	ASN	2.8
1	E	263	LYS	2.8
1	E	265	ASP	2.8
1	C	259	ALA	2.8
1	E	452	ALA	2.8
1	A	227	ALA	2.7
1	E	261	HIS	2.7
1	C	429	VAL	2.7
1	E	213	ALA	2.7
2	D	59	ARG	2.7
1	C	439	VAL	2.7
1	C	389	TYR	2.7
1	E	11	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	13	ALA	2.6
1	A	237	ASP	2.6
2	F	174	CYS	2.6
1	E	175	GLY	2.6
1	A	452	ALA	2.6
1	E	270	TYR	2.6
1	A	225	GLY	2.6
1	A	223	LEU	2.5
1	E	133	ALA	2.5
1	E	278	VAL	2.5
1	E	127	LEU	2.5
1	A	451	ASN	2.5
1	E	284	ALA	2.5
1	C	282	PHE	2.5
1	C	399	ILE	2.5
1	E	258	ALA	2.5
1	E	123	TYR	2.4
1	E	333	ASP	2.4
2	F	59	ARG	2.4
2	B	88	GLY	2.4
2	F	113	ASN	2.4
1	A	131	GLU	2.4
1	A	263	LYS	2.3
1	E	218	GLN	2.3
1	C	445	PHE	2.3
1	E	435	ASN	2.3
1	C	367	ALA	2.3
1	C	260	ILE	2.3
1	E	432	ASN	2.3
1	E	290	TYR	2.3
1	A	214	ALA	2.3
1	E	262	ARG	2.3
1	E	292	GLY	2.3
2	F	88	GLY	2.3
1	A	222	PRO	2.2
1	E	274	THR	2.2
1	A	224	ALA	2.2
1	E	306	TYR	2.2
1	C	284	ALA	2.2
1	E	215	ALA	2.2
2	B	59	ARG	2.2
1	C	438	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	276	GLY	2.1
1	E	404	PHE	2.1
1	E	144	GLY	2.1
1	A	216	LEU	2.1
1	E	451	ASN	2.1
2	D	149	ASN	2.1
1	C	270	TYR	2.1
1	C	428	SER	2.1
1	E	394	PRO	2.1
1	E	334	ALA	2.1
1	C	434	ASP	2.1
1	C	403	SER	2.0
1	C	427	ALA	2.0
2	D	76	GLU	2.0
1	C	126[A]	LYS	2.0
1	E	445	PHE	2.0
1	C	3	GLY	2.0
1	C	379	GLY	2.0
1	E	336	PRO	2.0
1	C	387	VAL	2.0
1	E	116	VAL	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($\text{\AA}^2$)	Q<0.9
3	FES	E	500	4/4	0.97	0.06	33,33,36,36	0
4	FE	E	501	1/1	0.97	0.04	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FES	A	500	4/4	0.98	0.04	19,20,20,23	0
4	FE	C	501	1/1	0.98	0.04	29,29,29,29	0
3	FES	C	500	4/4	0.98	0.04	17,17,18,19	0
4	FE	A	501	1/1	0.99	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.