Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:36 pm BST

PDB ID	:	2CKF
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 following versions of software and data (see references ①) were used in the production of this report:

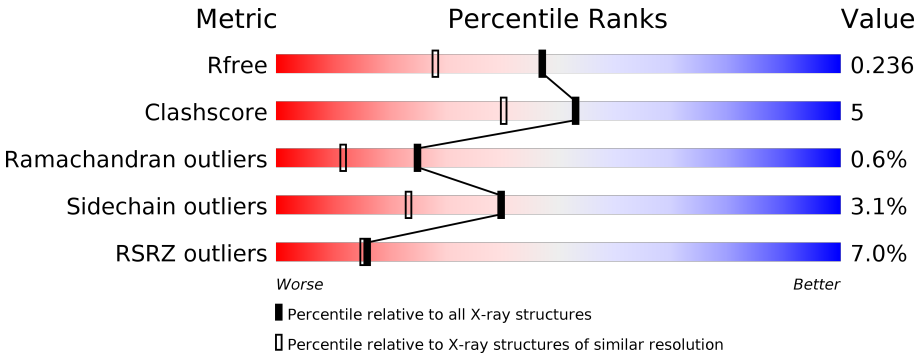
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 on 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	454	3% 86% 12%
1	C	454	10% 78% 14% 6%
1	E	454	11% 82% 11% 5%
2	B	174	3% 86% 10%
2	D	174	% 86% 10%
2	F	174	5% 85% 10%

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.

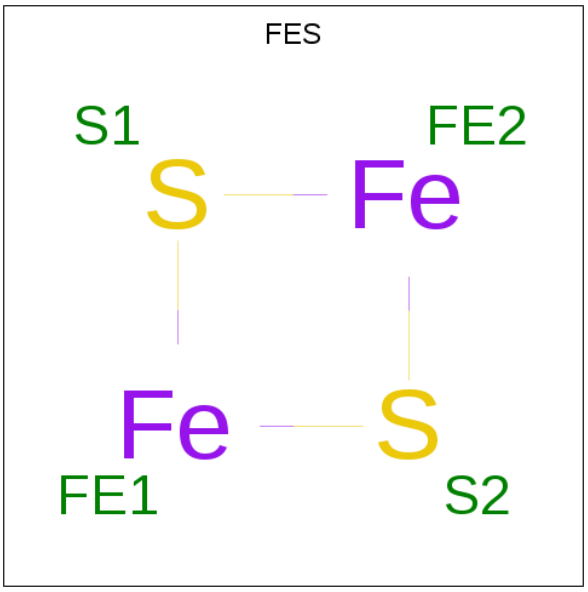
- Molecule 1 is a protein called RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT.

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 SUBUNIT.

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 (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is water.

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

Continued on next page...

Continued from previous page...

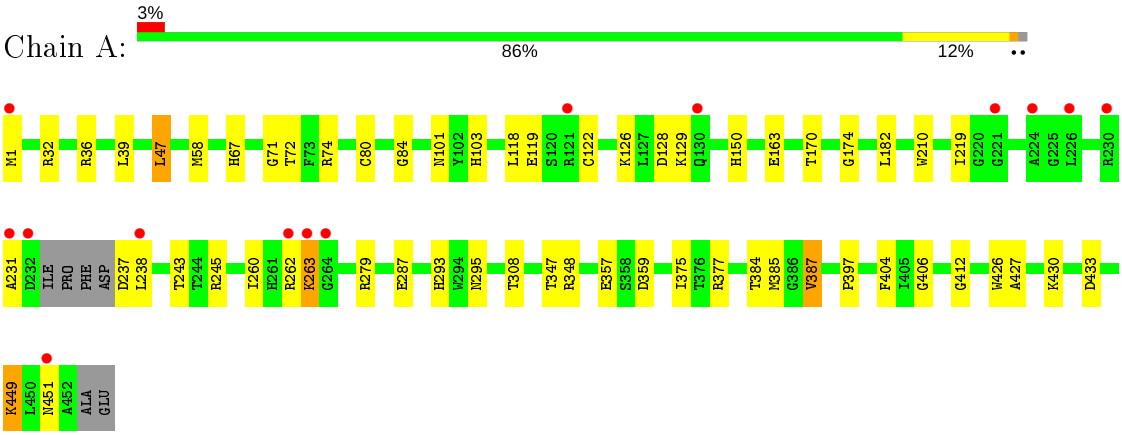
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	125	Total O 125 125	0	0
5	E	152	Total O 152 152	0	0
5	F	143	Total O 143 143	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

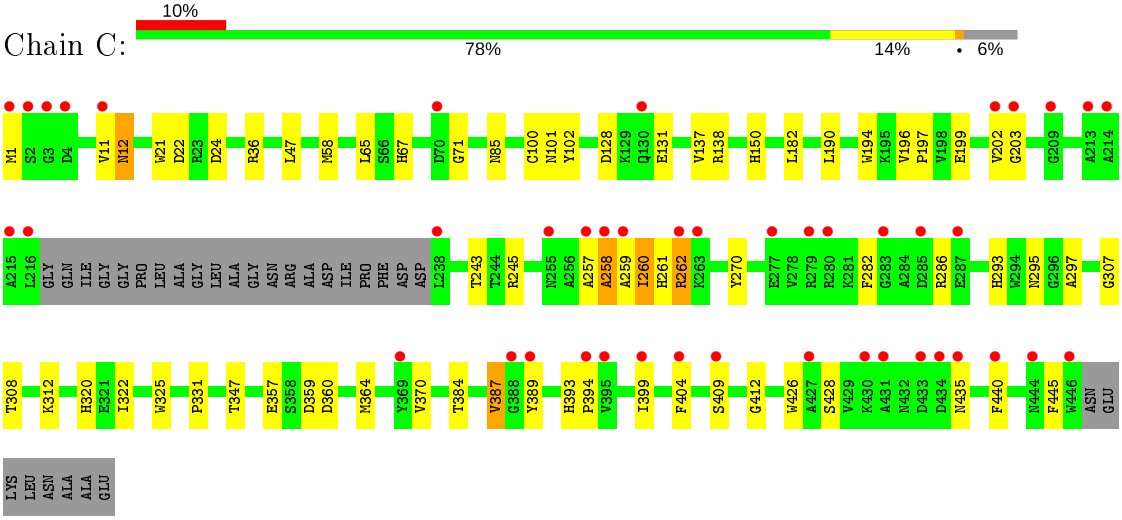
• Molecule 1: RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT

Chain A:



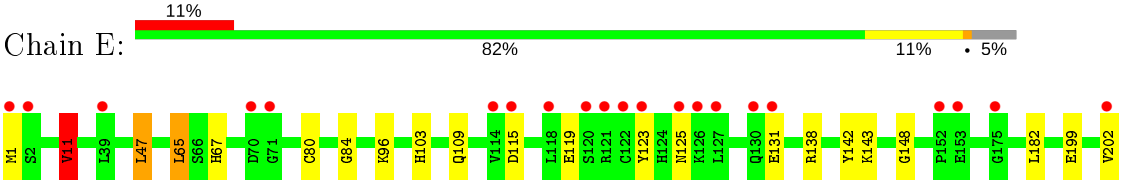
• Molecule 1: RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT

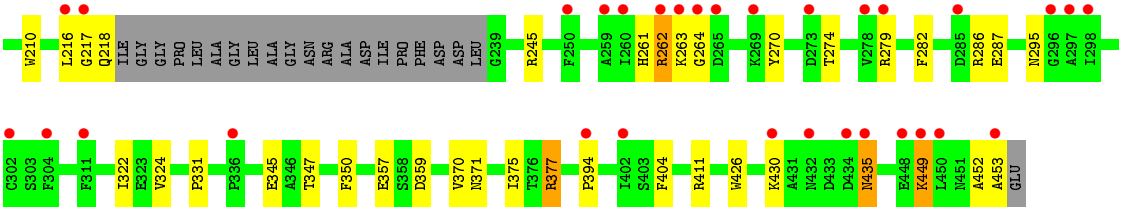
Chain C:



• Molecule 1: RING-HYDROXYLATING DIOXYGENASE ALPHA SUBUNIT

Chain E:



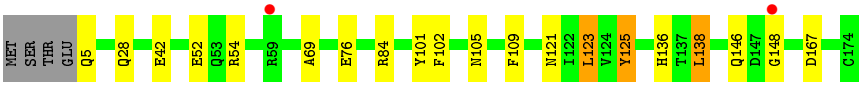


• Molecule 2: RING-HYDROXYLATING DIOXYGENASE BETA SUBUNIT

Chain B:

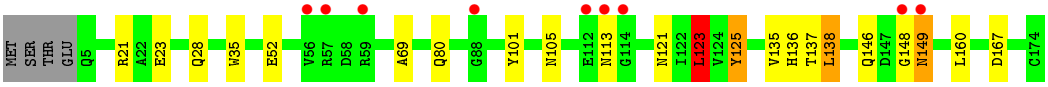
• Molecule 2: RING-HYDROXYLATING DIOXYGENASE BETA SUBUNIT

Chain D:



• Molecule 2: RING-HYDROXYLATING DIOXYGENASE BETA SUBUNIT

Chain F:



4 Data and refinement statistics (i)

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 29.89 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.00-1.85) 99.6 (29.89-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.37 , 47.9	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	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.*

[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: FE, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.90	0/3657	0.83	4/4962 (0.1%)
1	C	0.73	0/3501	0.74	1/4750 (0.0%)
1	E	0.73	0/3548	0.77	7/4814 (0.1%)
2	B	0.87	0/1498	0.91	3/2029 (0.1%)
2	D	0.84	1/1473 (0.1%)	0.80	2/1995 (0.1%)
2	F	0.75	0/1476	0.82	4/1999 (0.2%)
All	All	0.80	1/15153 (0.0%)	0.80	21/20549 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	76	GLU	CG-CD	5.04	1.59	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	84	ARG	NE-CZ-NH1	11.41	126.00	120.30
2	B	84	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	E	377	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	E	377	ARG	NE-CZ-NH1	7.45	124.03	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	123	LEU	CA-CB-CG	6.22	129.60	115.30
2	F	138	LEU	CA-CB-CG	6.17	129.49	115.30
2	B	74	ASP	CB-CG-OD1	6.14	123.83	118.30
1	E	11	VAL	C-N-CA	6.11	136.97	121.70
1	E	11	VAL	CA-C-N	5.88	130.13	117.20
1	A	263	LYS	N-CA-C	5.72	126.45	111.00
2	D	123	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	377	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	433	ASP	CB-CG-OD1	5.44	123.19	118.30
1	E	65	LEU	CA-CB-CG	5.32	127.53	115.30
2	F	160	LEU	CB-CG-CD1	-5.16	102.23	111.00
2	D	138	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	138	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	11	VAL	N-CA-C	5.09	124.74	111.00
1	E	411	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	F	21	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	377	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	43	0
1	C	3394	0	3196	45	0
1	E	3444	0	3233	38	0
2	B	1458	0	1397	18	1
2	D	1437	0	1379	14	1
2	F	1440	0	1383	19	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	155	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 5.

All (155) 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
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
1:A:427:ALA:HA	1:A:430:LYS:CE	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:449:LYS:HZ3	1:A:449:LYS:HB3	1.60	0.65
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: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:216:LEU:C	1:E:218:GLN:H	2.08	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:C:258:ALA:HB1	1:C:259:ALA:HA	1.86	0.51
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:21:TRP:O	1:C:320:HIS:HE1	1.96	0.49
1:E:47:LEU:N	1:E:47:LEU:HD23	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: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:HG2	1:A:74:ARG:HH11	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:237:ASP:O	1:A:238:LEU:HB2	2.16	0.45
1:A:39:LEU:HD12	1:A:58:MET:HB3	1.99	0.45
1:A:293:HIS:HD2	5:A:2237:HOH:O	1.98	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
2:B:147:ASP:O	2:B:149:ASN:C	2.56	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:322:ILE:C	1:C:322:ILE:HD12	2.38	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:A:126:LYS:CG	1:A:126:LYS:O	2.65	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: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: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
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:384:THR:O	1:C:387:VAL:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:ILE:HD13	1:E:324:VAL:HB	2.03	0.40
2:D:102:PHE:CE2	2:F:123:LEU:HB2	2.56	0.40
1:E:216:LEU:C	1:E:218:GLN:N	2.74	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
2:F:113:ASN:CG	2:F:113:ASN:O	2.60	0.40
1:A:293:HIS:CE1	1:A:308:THR:OG1	2.69	0.40
1:A:103:HIS:HB2	3:A:500:FES:S1	2.62	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%)	47 33
1	C	423/454 (93%)	404 (96%)	16 (4%)	3 (1%)	22 9
1	E	430/454 (95%)	403 (94%)	22 (5%)	5 (1%)	13 3
2	B	170/174 (98%)	166 (98%)	4 (2%)	0	100 100
2	D	168/174 (97%)	161 (96%)	6 (4%)	1 (1%)	25 12
2	F	168/174 (97%)	163 (97%)	5 (3%)	0	100 100
All	All	1805/1884 (96%)	1721 (95%)	74 (4%)	10 (1%)	25 12

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 (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	368/371 (99%)	358 (97%)	10 (3%)	44	29
1	C	354/371 (95%)	343 (97%)	11 (3%)	40	23
1	E	358/371 (96%)	348 (97%)	10 (3%)	43	27
2	B	156/158 (99%)	151 (97%)	5 (3%)	39	22
2	D	153/158 (97%)	148 (97%)	5 (3%)	38	21
2	F	154/158 (98%)	147 (96%)	7 (4%)	27	11
All	All	1543/1587 (97%)	1495 (97%)	48 (3%)	40	23

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	47	LEU
1	A	128	ASP
1	A	182	LEU
1	A	245	ARG
1	A	260	ILE
1	A	357	GLU
1	A	387	VAL
1	A	449	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	102	TYR
1	C	182	LEU
1	C	245	ARG
1	C	260	ILE
1	C	357	GLU
1	C	387	VAL
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	245	ARG
1	E	262	ARG
1	E	263	LYS
1	E	435	ASN
1	E	449	LYS
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	451	ASN
2	B	5	GLN
2	B	28	GLN
2	B	105	ASN
2	B	146	GLN
1	C	67	HIS
1	C	101	ASN
1	C	246	HIS
1	C	261	HIS
1	C	293	HIS
1	C	295	ASN
1	C	320	HIS
2	D	5	GLN
2	D	28	GLN
2	D	89	GLN
2	D	105	ASN
2	D	136	HIS
2	D	146	GLN
1	E	67	HIS
1	E	109	GLN
1	E	124	HIS
1	E	200	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	80	GLN
2	F	136	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 (i)

There are no carbohydrates 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	E	500	1	0,4,4	0.00	-	-		
3	FES	A	500	1	0,4,4	0.00	-	-		
3	FES	C	500	1	0,4,4	0.00	-	-		

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	E	500	1	-	-	0/1/1/1
3	FES	A	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	E	500	FES	1	0
3	A	500	FES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	448/454 (98%)	0.01	14 (3%) 49 47	12, 19, 42, 65	0
1	C	425/454 (93%)	0.58	44 (10%) 6 6	15, 31, 50, 65	0
1	E	433/454 (95%)	0.77	52 (12%) 4 4	16, 32, 53, 70	0
2	B	170/174 (97%)	-0.14	6 (3%) 44 41	13, 20, 33, 49	0
2	D	170/174 (97%)	-0.15	2 (1%) 79 79	16, 22, 35, 45	0
2	F	170/174 (97%)	0.11	9 (5%) 26 25	15, 26, 43, 50	0
All	All	1816/1884 (96%)	0.30	127 (6%) 16 15	12, 25, 49, 70	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	264	GLY	9.8
1	E	260	ILE	9.4
1	E	1	MET	6.7
1	C	214	ALA	6.6
1	C	262	ARG	6.6
1	C	1	MET	6.1
1	C	263	LYS	6.0
1	E	453	ALA	5.7
1	C	444	ASN	5.4
1	E	217	GLY	5.4
1	C	11	VAL	5.3
2	B	149	ASN	5.2
1	C	434	ASP	5.1
2	D	148	GLY	5.1
2	F	149	ASN	5.0
1	C	2	SER	4.8
2	F	59	ARG	4.7
1	A	232	ASP	4.6
1	C	213	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	216	LEU	4.5
1	E	122	CYS	4.3
1	C	446	TRP	4.3
1	E	126	LYS	4.3
1	A	224	ALA	4.2
1	E	262	ARG	4.2
1	C	238	LEU	4.1
1	E	435	ASN	4.1
1	A	230	ARG	4.1
1	E	2	SER	4.0
1	C	280	ARG	3.9
1	C	3	GLY	3.8
1	E	127	LEU	3.8
1	E	121	ARG	3.8
1	E	298	ILE	3.8
2	B	148	GLY	3.6
1	C	4	ASP	3.6
1	A	262	ARG	3.6
2	D	59	ARG	3.6
2	B	150	GLY	3.6
1	E	216	LEU	3.6
1	C	435	ASN	3.5
1	E	450	LEU	3.4
1	E	297	ALA	3.4
2	F	113	ASN	3.4
1	C	430	LYS	3.4
1	E	285	ASP	3.4
1	E	430	LYS	3.4
2	F	148	GLY	3.4
2	B	59	ARG	3.3
1	A	231	ALA	3.3
1	C	427	ALA	3.3
1	E	304	PHE	3.2
1	C	257	ALA	3.2
1	E	131	GLU	3.2
1	E	120	SER	3.2
1	C	389	TYR	3.1
1	C	258	ALA	3.1
1	E	115	ASP	3.1
2	F	112	GLU	3.0
2	F	114	GLY	3.0
1	C	202	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	130	GLN	2.9
1	C	395	VAL	2.9
1	A	121	ARG	2.8
1	E	123	TYR	2.8
1	A	1	MET	2.8
1	E	114	VAL	2.8
1	C	431	ALA	2.8
1	C	440	PHE	2.8
1	C	283	GLY	2.7
1	E	175	GLY	2.7
1	A	238	LEU	2.7
1	E	118	LEU	2.7
1	E	449	LYS	2.6
1	E	125	ASN	2.6
2	F	57	ARG	2.6
1	A	226	LEU	2.6
1	E	263	LYS	2.6
1	E	434	ASP	2.6
2	F	88	GLY	2.6
1	C	279	ARG	2.6
1	A	221	GLY	2.6
1	E	302	CYS	2.6
1	E	265	ASP	2.5
1	E	279	ARG	2.5
1	C	409	SER	2.5
1	E	70	ASP	2.5
1	C	394	PRO	2.4
1	E	152	PRO	2.4
1	E	269	LYS	2.4
1	C	287	GLU	2.4
1	E	259	ALA	2.4
1	C	255	ASN	2.4
1	E	336	PRO	2.4
1	C	70	ASP	2.4
1	C	215	ALA	2.3
1	E	278	VAL	2.3
1	A	130	GLN	2.3
2	B	111	ALA	2.3
1	E	311	PHE	2.3
1	C	277	GLU	2.3
1	E	202	VAL	2.3
1	C	285	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	264	GLY	2.2
1	C	259	ALA	2.2
1	C	209	GLY	2.2
1	E	296	GLY	2.2
1	E	448	GLU	2.2
1	E	250	PHE	2.2
1	E	394	PRO	2.1
1	C	433	ASP	2.1
1	E	71	GLY	2.1
1	E	153	GLU	2.1
1	E	39	LEU	2.1
1	A	451	ASN	2.1
1	C	130	GLN	2.1
1	A	263	LYS	2.1
1	E	273	ASP	2.1
1	C	388	GLY	2.1
1	C	404	PHE	2.1
2	F	56	VAL	2.1
1	E	402	ILE	2.1
1	C	369	TYR	2.0
1	E	432	ASN	2.0
2	B	5	GLN	2.0
1	C	399	ILE	2.0
1	C	203	GLY	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 carbohydrates 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
4	FE	C	501	1/1	0.97	0.07	29,29,29,29	0
3	FES	C	500	4/4	0.98	0.07	17,17,18,19	0
3	FES	E	500	4/4	0.98	0.06	33,33,36,36	0
3	FES	A	500	4/4	0.98	0.07	19,20,20,23	0
4	FE	E	501	1/1	0.98	0.08	23,23,23,23	0
4	FE	A	501	1/1	0.99	0.11	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.