



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:35 AM UTC

PDB ID : 3MPS / pdb\_00003mps  
Title : Peroxide Bound Oxidized Rubrerythrin from *Pyrococcus furiosus*  
Authors : Dillard, B.D.; Adams, M.W.W.; Lanzilotta, W.N.  
Deposited on : 2010-04-27  
Resolution : 2.00 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](mailto: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>.

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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

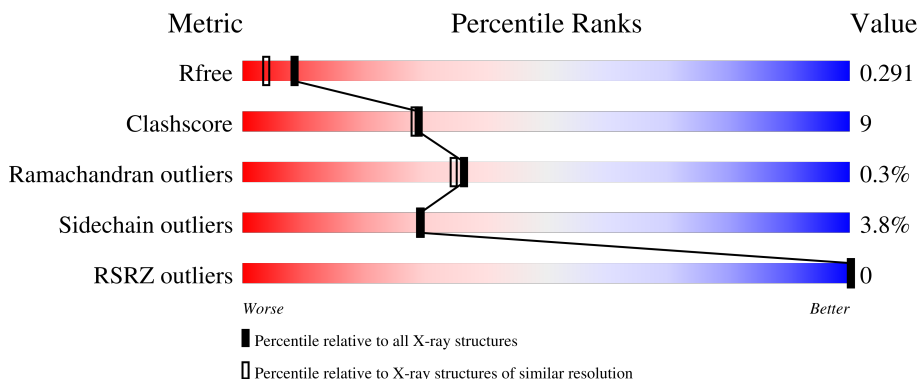
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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  $\geq 3$ , 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	170	85% 14% .
1	B	170	85% 14% .
1	D	170	80% 18% .
1	F	170	85% 15% .
1	G	170	84% 15% .

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Mol	Chain	Length	Quality of chain
1	H	170	 73% 24%
1	I	170	 79% 19%
1	K	170	 77% 22%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11289 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 Rubrerythrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	170	1357	875	220	253	9	0	0	0
1	B	170	1354	874	218	253	9	0	0	0
1	D	170	1353	873	220	251	9	0	0	0
1	F	170	1336	858	218	251	9	0	0	0
1	G	170	1363	880	221	253	9	0	0	0
1	H	170	1363	880	221	253	9	0	0	0
1	I	170	1358	877	221	251	9	0	0	0
1	K	170	1360	879	219	253	9	0	0	0

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

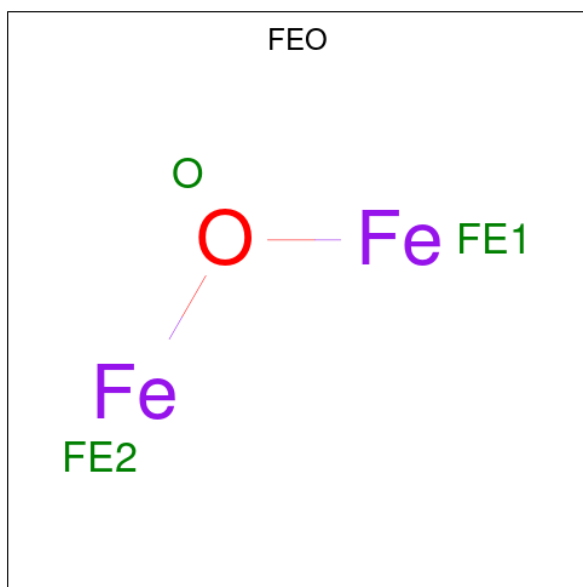
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	D	3	Total	Fe	0	0
			3	3		
2	F	3	Total	Fe	0	0
			3	3		
2	G	4	Total	Fe	0	0
			4	4		
2	H	2	Total	Fe	0	0
			2	2		

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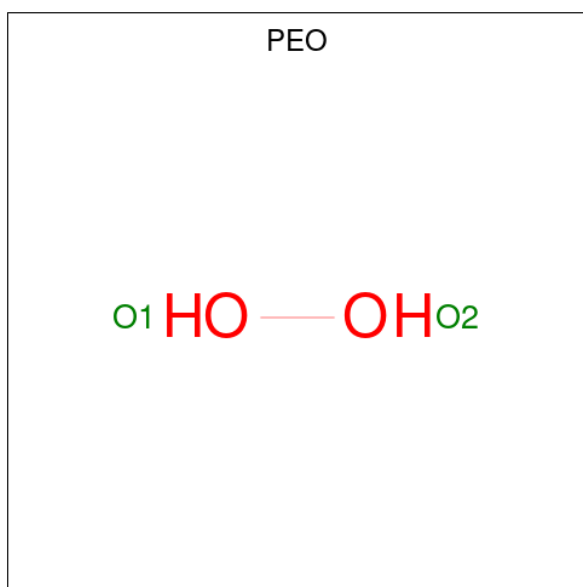
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0

- Molecule 3 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe<sub>2</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe O 3 2 1	0	0
3	B	1	Total Fe O 3 2 1	0	0
3	I	1	Total Fe O 3 2 1	0	0
3	K	1	Total Fe O 3 2 1	0	0

- Molecule 4 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O 2 2	0	0


- Molecule 5 is water.

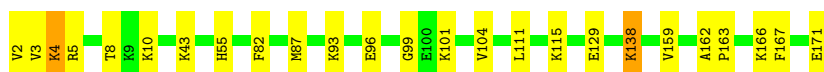
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	B	64	Total O 64 64	0	0
5	D	35	Total O 35 35	0	0
5	F	51	Total O 51 51	0	0
5	G	52	Total O 52 52	0	0
5	H	74	Total O 74 74	0	0
5	I	24	Total O 24 24	0	0
5	K	57	Total O 57 57	0	0

### 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: Rubrerythrin

Chain A:  85% 14%




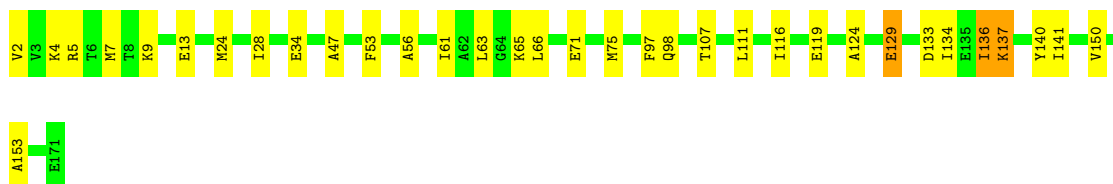
- Molecule 1: Rubrerythrin

Chain B:  85% 14%




- Molecule 1: Rubrerythrin

Chain D:  80% 18%




- Molecule 1: Rubrerythrin

Chain F:  85% 15%



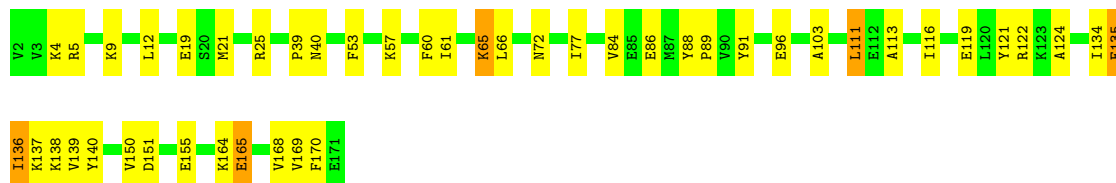
- Molecule 1: Rubrerythrin

Chain G:  84% 15%




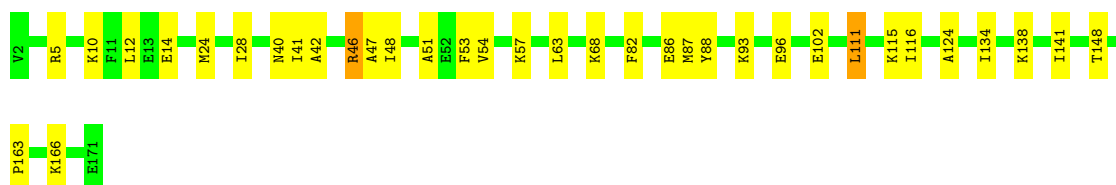
- Molecule 1: Rubrerythrin

Chain H:  73% 24%




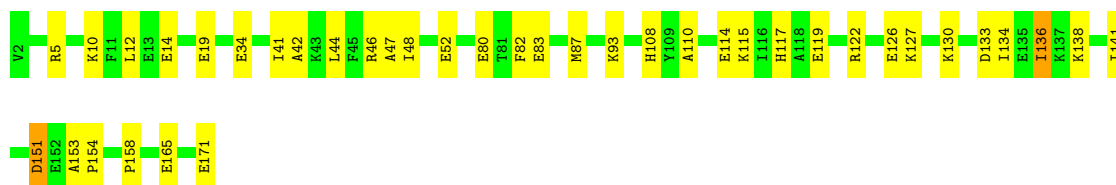
- Molecule 1: Rubrerythrin

Chain I:  79% 19%



- Molecule 1: Rubrerythrin

Chain K:  77% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.40Å 105.16Å 105.22Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	105.41 – 2.00 105.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (105.41-2.00) 99.1 (105.22-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.00Å)	Xtrriage
Refinement program	REFMAC, CNS	Depositor
R, $R_{free}$	0.242 , 0.291 0.242 , 0.291	Depositor DCC
$R_{free}$ test set	5896 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 23.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.319 for -h,l,k 0.347 for -h,-l,-k 0.319 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, PEO, FEO

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	0.66	0/1388	0.94	0/1864
1	B	0.69	0/1384	0.96	1/1860 (0.1%)
1	D	0.68	0/1384	0.95	0/1858
1	F	0.66	1/1363 (0.1%)	0.90	0/1827
1	G	0.72	0/1394	0.96	0/1871
1	H	0.69	0/1394	0.90	0/1871
1	I	0.67	0/1389	0.94	0/1865
1	K	0.68	0/1391	0.99	3/1867 (0.2%)
All	All	0.68	1/11087 (0.0%)	0.94	4/14883 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	144	ILE	CA-CB	5.70	1.61	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	VAL	CB-CA-C	-7.18	102.78	111.97
1	K	117	HIS	N-CA-C	5.42	117.19	111.28
1	K	115	LYS	CA-C-N	5.08	127.16	120.60
1	K	115	LYS	C-N-CA	5.08	127.16	120.60

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	1357	0	1328	18	1
1	B	1354	0	1311	23	0
1	D	1353	0	1324	32	0
1	F	1336	0	1266	18	0
1	G	1363	0	1345	32	0
1	H	1363	0	1345	42	0
1	I	1358	0	1336	29	1
1	K	1360	0	1340	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	3	0	0	0	0
2	F	3	0	0	0	0
2	G	4	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	K	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	I	3	0	0	0	0
3	K	3	0	0	0	0
4	F	2	0	0	0	0
5	A	58	0	0	7	0
5	B	64	0	0	5	0
5	D	35	0	0	2	0
5	F	51	0	0	4	0
5	G	52	0	0	7	0
5	H	74	0	0	12	0
5	I	24	0	0	6	0
5	K	57	0	0	6	0
All	All	11289	0	10595	186	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 9.

All (186) 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:D:4:LYS:HD2	1:G:71:GLU:HG2	1.33	1.05
1:G:116:ILE:HD11	5:G:183:HOH:O	1.60	1.01
1:G:111:LEU:O	1:G:115:LYS:HE3	1.66	0.94
1:H:88:TYR:HB3	1:H:111:LEU:HD22	1.51	0.93
1:G:24:MET:O	1:G:28:ILE:HD13	1.69	0.92
1:B:169:VAL:HG12	5:B:209:HOH:O	1.74	0.87
1:H:103:ALA:HA	5:H:175:HOH:O	1.74	0.87
1:B:114:GLU:HG3	5:B:198:HOH:O	1.74	0.87
1:K:126:GLU:O	1:K:130:LYS:HD3	1.73	0.86
1:H:119:GLU:HG2	1:H:122:ARG:HH11	1.41	0.83
1:H:116:ILE:HG22	5:H:219:HOH:O	1.78	0.82
1:D:71:GLU:HG2	1:G:4:LYS:HD3	1.61	0.79
1:B:86:GLU:OE1	1:H:5:ARG:CZ	2.30	0.78
1:H:9:LYS:HE2	5:H:197:HOH:O	1.81	0.78
1:H:168:VAL:O	5:H:202:HOH:O	2.03	0.77
1:K:119:GLU:OE1	1:K:122:ARG:NH2	2.17	0.76
1:G:116:ILE:HD13	5:G:198:HOH:O	1.87	0.74
1:I:82:PHE:HE1	1:I:87:MET:HE2	1.53	0.73
1:D:141:ILE:HD11	1:I:47:ALA:HB1	1.70	0.73
1:D:129:GLU:HG2	1:G:5:ARG:NH2	2.05	0.70
1:H:113:ALA:O	5:H:219:HOH:O	2.08	0.70
1:K:82:PHE:HE1	1:K:87:MET:CE	2.03	0.70
1:K:83:GLU:HB2	5:K:194:HOH:O	1.90	0.70
1:D:53:PHE:CE1	1:I:28:ILE:HD13	2.27	0.70
5:A:180:HOH:O	1:B:5:ARG:HD3	1.92	0.70
1:H:170:PHE:HD1	5:H:202:HOH:O	1.76	0.69
1:F:10:LYS:O	1:F:14:GLU:HG3	1.94	0.68
1:A:162:ALA:HB1	1:A:166:LYS:HD2	1.75	0.68
1:G:116:ILE:HG12	5:G:221:HOH:O	1.96	0.66
1:K:10:LYS:HE2	1:K:14:GLU:OE2	1.96	0.65
1:K:82:PHE:CE1	1:K:87:MET:HE3	2.32	0.65
1:A:2:VAL:O	1:A:4:LYS:HD2	1.97	0.64
1:G:87:MET:HE3	5:G:185:HOH:O	1.97	0.64
1:I:51:ALA:HA	5:I:192:HOH:O	1.96	0.64
1:H:135:GLU:HG2	5:H:193:HOH:O	1.97	0.63
1:K:138:LYS:HG3	5:K:253:HOH:O	1.97	0.63
1:D:56:ALA:HB1	5:D:225:HOH:O	1.98	0.62
1:D:4:LYS:CD	1:G:71:GLU:HG2	2.19	0.62
1:K:34:GLU:HG2	1:K:42:ALA:CB	2.31	0.61
1:D:28:ILE:HD13	1:I:53:PHE:CE1	2.35	0.61
1:K:82:PHE:HE1	1:K:87:MET:HE3	1.63	0.61
1:G:14:GLU:OE1	1:H:91:TYR:OH	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ILE:HD12	1:H:53:PHE:CE1	2.36	0.61
1:K:119:GLU:CD	1:K:122:ARG:NH2	2.59	0.61
1:K:48:ILE:O	1:K:52:GLU:HG2	2.01	0.60
1:G:43:LYS:HD2	5:H:184:HOH:O	2.02	0.60
1:I:10:LYS:HE2	1:I:14:GLU:OE2	2.01	0.59
1:K:127:LYS:HG3	1:K:134:ILE:HG22	1.85	0.59
1:H:139:VAL:O	5:H:202:HOH:O	2.17	0.59
1:K:110:ALA:O	1:K:114:GLU:HB2	2.02	0.59
1:B:129:GLU:HA	1:B:129:GLU:OE1	2.02	0.58
1:D:136:ILE:O	1:D:137:LYS:HB2	2.03	0.58
1:D:56:ALA:CB	5:D:225:HOH:O	2.53	0.57
1:K:151:ASP:HA	5:K:253:HOH:O	2.03	0.57
1:A:163:PRO:HD2	1:A:166:LYS:HE3	1.86	0.57
1:H:138:LYS:O	1:H:151:ASP:N	2.31	0.57
1:G:125:LYS:O	1:G:129:GLU:HG2	2.06	0.56
1:G:133:ASP:OD1	1:H:39:PRO:HD2	2.05	0.56
1:K:108:HIS:HE1	5:K:190:HOH:O	1.87	0.56
1:B:80:GLU:O	1:B:84:VAL:HG23	2.05	0.56
1:I:42:ALA:O	1:I:46:ARG:HG2	2.05	0.56
1:D:63:LEU:HD13	1:D:65:LYS:HE3	1.88	0.56
1:K:82:PHE:HE1	1:K:87:MET:HE2	1.72	0.55
1:I:54:VAL:CG2	5:I:192:HOH:O	2.54	0.55
1:D:47:ALA:HB1	1:I:141:ILE:HD11	1.89	0.54
1:D:141:ILE:HG21	5:I:192:HOH:O	2.08	0.54
1:B:147:TYR:CE1	1:B:158:PRO:HG2	2.44	0.53
1:H:165:GLU:H	1:H:165:GLU:CD	2.16	0.53
1:I:82:PHE:HE1	1:I:87:MET:CE	2.20	0.53
1:A:82:PHE:CE1	1:A:87:MET:HE3	2.44	0.53
1:G:28:ILE:HD12	1:H:53:PHE:HE1	1.72	0.53
1:A:93:LYS:HD2	5:A:179:HOH:O	2.09	0.53
1:B:5:ARG:CZ	1:H:86:GLU:OE1	2.57	0.53
1:D:129:GLU:HG2	1:G:5:ARG:CZ	2.39	0.52
1:H:61:ILE:HD11	1:H:66:LEU:HD22	1.90	0.52
1:H:150:VAL:HG13	5:H:224:HOH:O	2.10	0.52
1:H:57:LYS:O	1:H:61:ILE:HD13	2.10	0.52
1:H:60:PHE:CZ	1:H:65:LYS:HB3	2.45	0.52
1:F:65:LYS:HE3	5:F:183:HOH:O	2.10	0.52
1:A:138:LYS:HB2	5:A:202:HOH:O	2.09	0.52
1:B:100:GLU:O	1:B:104:VAL:HG23	2.10	0.52
1:D:9:LYS:HE2	1:D:13:GLU:OE1	2.10	0.51
1:F:144:ILE:HD11	5:F:214:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:TYR:CE2	1:H:169:VAL:HG22	2.45	0.51
1:B:86:GLU:OE1	1:H:5:ARG:NH1	2.43	0.51
1:B:93:LYS:HE3	1:G:93:LYS:HE3	1.92	0.51
1:H:77:ILE:HD12	1:H:122:ARG:HG3	1.91	0.51
1:D:7:MET:HG2	1:F:86:GLU:OE2	2.11	0.51
1:B:86:GLU:OE1	1:H:5:ARG:NE	2.43	0.51
1:A:55:HIS:HD2	5:B:184:HOH:O	1.94	0.51
1:A:82:PHE:HE1	1:A:87:MET:HE3	1.75	0.51
1:F:60:PHE:CZ	1:F:65:LYS:HB3	2.46	0.51
1:H:124:ALA:HA	1:H:134:ILE:CG2	2.41	0.51
1:H:89:PRO:HG3	1:H:111:LEU:HD11	1.93	0.50
1:D:134:ILE:HG12	1:I:41:ILE:HD13	1.93	0.50
1:K:82:PHE:CE1	1:K:87:MET:CE	2.89	0.50
1:K:138:LYS:HB3	1:K:171:GLU:HB3	1.94	0.50
1:F:47:ALA:HB1	1:K:141:ILE:HD11	1.94	0.50
1:I:116:ILE:HG21	1:I:148:THR:HB	1.94	0.49
1:K:80:GLU:O	5:K:194:HOH:O	2.20	0.49
1:B:5:ARG:NE	1:H:86:GLU:OE1	2.46	0.49
1:G:43:LYS:NZ	1:H:137:LYS:O	2.42	0.49
1:D:24:MET:O	1:D:28:ILE:HG12	2.12	0.49
1:B:110:ALA:O	1:B:114:GLU:HB2	2.12	0.48
1:F:97:PHE:CD2	1:I:93:LYS:HE3	2.49	0.48
1:G:10:LYS:HE3	1:G:14:GLU:OE2	2.13	0.48
1:G:127:LYS:HD3	1:G:134:ILE:HA	1.95	0.48
1:H:88:TYR:HB3	1:H:111:LEU:CD2	2.32	0.48
1:H:96:GLU:HB2	5:H:195:HOH:O	2.14	0.48
1:F:141:ILE:HD11	1:K:47:ALA:HB1	1.96	0.48
1:I:24:MET:O	1:I:28:ILE:HG12	2.13	0.47
1:D:140:TYR:CD2	1:D:153:ALA:HB2	2.49	0.47
1:G:87:MET:CE	5:G:185:HOH:O	2.59	0.47
1:G:55:HIS:HD2	5:H:177:HOH:O	1.96	0.47
1:D:141:ILE:CG2	5:I:192:HOH:O	2.63	0.47
1:G:34:GLU:OE2	1:G:39:PRO:HA	2.15	0.47
1:G:43:LYS:HE3	1:H:136:ILE:HD12	1.97	0.47
1:K:34:GLU:HG2	1:K:42:ALA:HB1	1.96	0.47
1:H:134:ILE:HD12	1:H:136:ILE:HG12	1.96	0.47
1:K:119:GLU:CD	1:K:122:ARG:HH22	2.12	0.46
1:D:133:ASP:OD2	1:I:41:ILE:HG12	2.15	0.46
1:H:77:ILE:HD13	1:H:121:TYR:HB2	1.96	0.46
1:G:117:HIS:CD2	5:G:221:HOH:O	2.68	0.46
1:B:154:PRO:O	1:B:164:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:LEU:O	1:K:48:ILE:HG12	2.16	0.46
5:A:198:HOH:O	1:B:55:HIS:HE1	1.99	0.46
1:B:116:ILE:HG21	1:B:148:THR:HB	1.98	0.45
1:I:124:ALA:HA	1:I:134:ILE:CG2	2.46	0.45
1:D:97:PHE:CD2	1:K:93:LYS:HE3	2.51	0.45
1:F:23:HIS:HE1	5:F:194:HOH:O	1.98	0.45
1:A:111:LEU:O	1:A:115:LYS:NZ	2.36	0.45
1:K:154:PRO:HG2	1:K:158:PRO:HD3	1.99	0.45
1:A:43:LYS:HB3	1:A:43:LYS:HE2	1.78	0.45
1:D:71:GLU:CG	1:G:4:LYS:HD3	2.40	0.45
1:I:12:LEU:HB2	1:I:63:LEU:HD21	1.97	0.45
1:I:54:VAL:HG23	5:I:192:HOH:O	2.17	0.45
1:K:19:GLU:OE2	1:K:19:GLU:HA	2.18	0.44
1:K:41:ILE:O	1:K:44:LEU:HB3	2.17	0.44
1:D:134:ILE:HG13	1:I:40:ASN:HB3	1.98	0.44
1:D:98:GLN:HB3	1:I:5:ARG:HD3	1.99	0.44
1:A:96:GLU:HB2	5:A:194:HOH:O	2.17	0.44
1:F:46:ARG:HD3	5:F:192:HOH:O	2.16	0.44
1:A:101:LYS:HA	1:A:101:LYS:HD3	1.71	0.44
1:F:41:ILE:HG13	1:K:133:ASP:OD2	2.17	0.44
1:G:126:GLU:O	1:G:130:LYS:HG3	2.17	0.44
1:A:159:VAL:O	5:A:203:HOH:O	2.21	0.44
1:I:86:GLU:OE1	1:K:5:ARG:NE	2.50	0.44
1:K:10:LYS:CE	1:K:14:GLU:OE2	2.64	0.44
1:I:54:VAL:HG21	5:I:192:HOH:O	2.15	0.43
1:I:82:PHE:CE1	1:I:87:MET:CE	3.02	0.43
1:A:138:LYS:HG2	1:A:171:GLU:HB3	2.01	0.43
1:D:124:ALA:HB1	1:I:41:ILE:HD12	2.00	0.43
1:D:28:ILE:HD12	1:I:57:LYS:HB2	2.01	0.43
1:B:5:ARG:HA	1:B:5:ARG:HE	1.84	0.42
1:G:10:LYS:O	1:G:14:GLU:HG3	2.18	0.42
1:G:134:ILE:HG13	1:H:40:ASN:HB3	2.00	0.42
1:F:74:GLN:NE2	1:F:78:GLU:OE2	2.41	0.42
1:D:28:ILE:CD1	1:I:57:LYS:HB2	2.49	0.42
1:F:40:ASN:HB3	1:K:136:ILE:HD13	2.01	0.42
1:H:155:GLU:HA	1:H:164:LYS:HD2	2.02	0.42
1:F:141:ILE:HD12	1:F:170:PHE:CD1	2.55	0.42
1:A:3:VAL:HG11	1:A:8:THR:HG22	2.00	0.42
1:F:55:HIS:HE1	5:K:180:HOH:O	2.02	0.42
1:H:19:GLU:HA	1:H:19:GLU:OE1	2.20	0.42
1:G:13:GLU:OE2	5:G:187:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:ILE:CD1	1:H:136:ILE:HG12	2.49	0.41
1:A:104:VAL:HG13	5:A:194:HOH:O	2.20	0.41
1:B:138:LYS:HB3	5:B:209:HOH:O	2.19	0.41
1:I:163:PRO:HG2	1:I:166:LYS:HG2	2.02	0.41
1:A:5:ARG:HD2	1:B:98:GLN:HB3	2.02	0.41
1:G:29:PHE:CG	1:H:72:ASN:HB3	2.56	0.41
1:F:84:VAL:HG21	1:F:115:LYS:HG2	2.02	0.41
1:F:102:GLU:HA	1:F:105:ARG:NH1	2.35	0.41
1:A:167:PHE:N	1:A:167:PHE:CD1	2.88	0.41
1:B:169:VAL:CG1	5:B:209:HOH:O	2.52	0.41
1:H:21:MET:O	1:H:25:ARG:HG3	2.20	0.41
1:I:88:TYR:HB3	1:I:111:LEU:HD13	2.03	0.41
1:B:32:LYS:HA	1:B:32:LYS:HD3	1.96	0.41
1:B:143:PRO:HG2	1:B:144:ILE:HD12	2.02	0.41
1:D:61:ILE:HD12	1:D:66:LEU:HB3	2.02	0.41
1:D:75:MET:HE3	1:D:75:MET:HB2	1.97	0.41
1:F:19:GLU:OE1	1:F:19:GLU:HA	2.21	0.40
1:H:119:GLU:HG2	1:H:122:ARG:NH1	2.23	0.40
1:D:2:VAL:N	1:I:102:GLU:OE1	2.55	0.40
1:D:107:THR:O	1:D:111:LEU:HB2	2.22	0.40
1:K:42:ALA:O	1:K:46:ARG:HG3	2.22	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)
1:A:99:GLY:O	1:I:68:LYS:NZ[1_455]	2.18	0.02

## 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	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
1	B	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
1	D	168/170 (99%)	160 (95%)	6 (4%)	2 (1%)	10	6
1	F	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
1	G	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
1	H	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
1	I	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
1	K	168/170 (99%)	163 (97%)	3 (2%)	2 (1%)	10	6
All	All	1344/1360 (99%)	1309 (97%)	31 (2%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	153	ALA
1	D	136	ILE
1	D	137	LYS
1	K	151	ASP

### 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	136/138 (99%)	132 (97%)	4 (3%)	37	40
1	B	134/138 (97%)	129 (96%)	5 (4%)	30	30
1	D	135/138 (98%)	129 (96%)	6 (4%)	25	24
1	F	128/138 (93%)	124 (97%)	4 (3%)	35	37
1	G	138/138 (100%)	133 (96%)	5 (4%)	31	31
1	H	138/138 (100%)	130 (94%)	8 (6%)	18	15
1	I	136/138 (99%)	130 (96%)	6 (4%)	25	24
1	K	137/138 (99%)	134 (98%)	3 (2%)	45	50
All	All	1082/1104 (98%)	1041 (96%)	41 (4%)	29	29

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	10	LYS
1	A	129	GLU
1	A	138	LYS
1	B	12	LEU
1	B	32	LYS
1	B	68	LYS
1	B	166	LYS
1	B	169	VAL
1	D	5	ARG
1	D	34	GLU
1	D	116	ILE
1	D	119	GLU
1	D	129	GLU
1	D	150	VAL
1	F	31	GLU
1	F	32	LYS
1	F	166	LYS
1	F	169	VAL
1	G	28	ILE
1	G	111	LEU
1	G	116	ILE
1	G	136	ILE
1	G	165	GLU
1	H	4	LYS
1	H	12	LEU
1	H	65	LYS
1	H	84	VAL
1	H	111	LEU
1	H	135	GLU
1	H	136	ILE
1	H	165	GLU
1	I	46	ARG
1	I	48	ILE
1	I	96	GLU
1	I	111	LEU
1	I	115	LYS
1	I	138	LYS
1	K	12	LEU
1	K	136	ILE
1	K	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	108	HIS
1	B	55	HIS
1	B	108	HIS
1	D	108	HIS
1	F	55	HIS
1	F	108	HIS
1	G	55	HIS
1	H	55	HIS
1	H	108	HIS
1	I	55	HIS
1	K	108	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 21 ligands modelled in this entry, 16 are monoatomic - leaving 5 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	FEO	I	1	1	0,2,2	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FEO	A	173	1	0,2,2	-	-	-		
3	FEO	B	173	1	0,2,2	-	-	-		
4	PEO	F	6079	2	1,1,1	0.35	0	-		
3	FEO	K	173	1	0,2,2	-	-	-		

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.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	170/170 (100%)	-1.14	0 100 100	14, 23, 35, 38	0
1	B	170/170 (100%)	-1.14	0 100 100	15, 21, 32, 35	0
1	D	170/170 (100%)	-1.10	0 100 100	14, 24, 35, 39	0
1	F	170/170 (100%)	-1.02	0 100 100	16, 25, 38, 46	0
1	G	170/170 (100%)	-1.15	0 100 100	15, 22, 32, 36	0
1	H	170/170 (100%)	-1.14	0 100 100	14, 21, 31, 36	0
1	I	170/170 (100%)	-1.12	0 100 100	16, 23, 32, 36	0
1	K	170/170 (100%)	-1.13	0 100 100	16, 23, 32, 34	0
All	All	1360/1360 (100%)	-1.12	0 100 100	14, 23, 33, 46	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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
2	FE	A	172	1/1	1.00	0.02	22,22,22,22	0
2	FE	B	172	1/1	1.00	0.01	20,20,20,20	0
2	FE	D	1	1/1	1.00	0.01	23,23,23,23	0
2	FE	D	172	1/1	1.00	0.01	22,22,22,22	0
2	FE	D	173	1/1	1.00	0.01	22,22,22,22	0
2	FE	F	172	1/1	1.00	0.01	24,24,24,24	0
2	FE	F	173	1/1	1.00	0.01	22,22,22,22	0
2	FE	F	174	1/1	1.00	0.02	22,22,22,22	0
2	FE	G	172	1/1	1.00	0.02	19,19,19,19	0
2	FE	G	173	1/1	1.00	0.02	21,21,21,21	0
2	FE	G	174	1/1	1.00	0.03	18,18,18,18	0
2	FE	G	175	1/1	1.00	0.01	22,22,22,22	0
2	FE	H	172	1/1	1.00	0.02	18,18,18,18	0
2	FE	H	173	1/1	1.00	0.01	20,20,20,20	0
2	FE	I	172	1/1	1.00	0.01	22,22,22,22	0
2	FE	K	172	1/1	1.00	0.01	22,22,22,22	0
3	FEO	A	173	3/3	1.00	0.02	17,17,21,22	0
3	FEO	B	173	3/3	1.00	0.01	16,16,19,22	0
3	FEO	I	1	3/3	1.00	0.01	16,16,19,22	0
3	FEO	K	173	3/3	1.00	0.02	19,19,20,20	0
4	PEO	F	6079	2/2	1.00	0.03	23,23,23,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.