



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:49 AM GMT

PDB ID : 1E5D  
Title : RUBREDOXIN OXYGEN:OXIDOREDUCTASE(ROO) FROM ANAEROBIC DESULFOVIBRIO GIGAS  
Authors : Frazao, C.; Silva, G.; Gomes, C.M.; Matias, P.; Coelho, R.; Sieker, L.; Macedo, S.; Liu, M.Y.; Oliveira, S.; Teixeira, M.; Xavier, A.V.; Rodrigues-Pousada, C.; Carrondo, M.A.; Le Gall, J.  
Deposited on : 2000-07-24  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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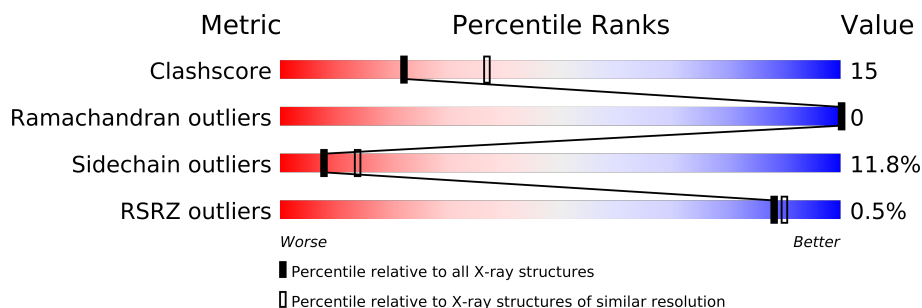
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	402	
1	B	402	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	OXY	A	405	-	X
4	OXY	B	405	-	X

## 2 Entry composition i

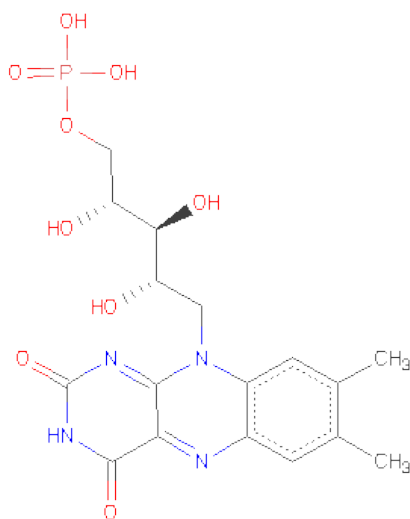
There are 5 unique types of molecules in this entry. The entry contains 6568 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RUBREDOXIN\;OXYGENOXIDOREDUCTASE.

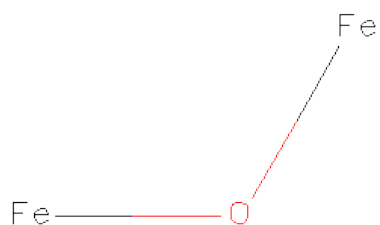
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	3	0
			3160	2026	527	588	19			
1	B	401	Total	C	N	O	S	0	4	0
			3166	2028	528	591	19			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



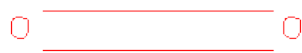
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



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

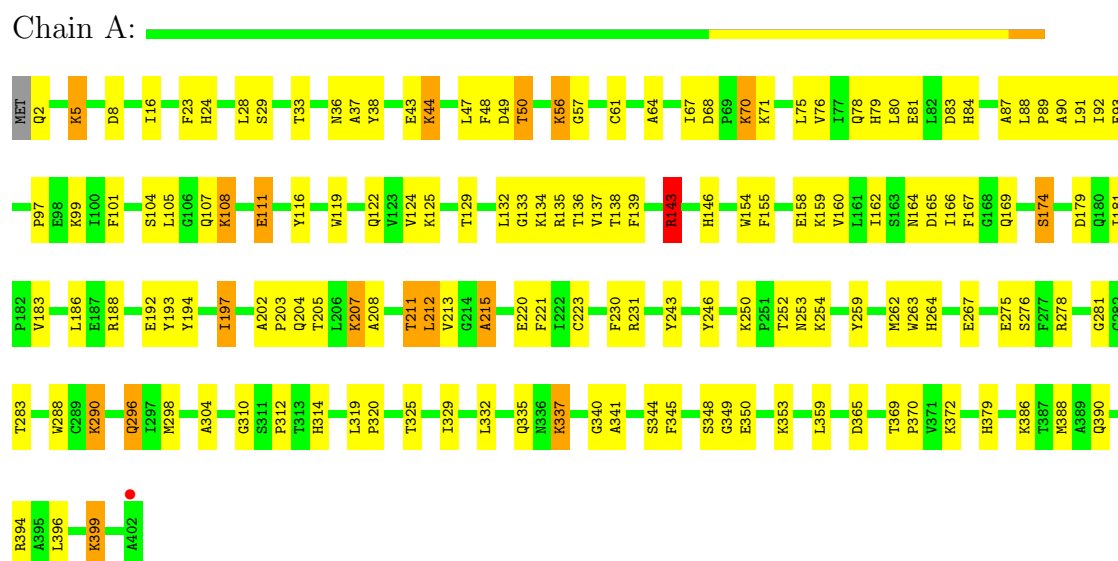
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total 84	O 84	0	0
5	B	86	Total 86	O 86	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RUBREDOXIN\ : OXYGENOXIDOREDUCTASE



#### • Molecule 1: RUBREDOXIN\ : OXYGENOXIDOREDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.24Å 101.25Å 90.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 14.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.50) 95.8 (14.97-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.22 (at 2.51Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.179 , 0.248 0.157 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.0	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31671 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.31	0/3253	0.87	6/4415 (0.1%)
1	B	0.31	0/3263	0.88	4/4428 (0.1%)
All	All	0.31	0/6516	0.88	10/8843 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	ARG	CD-NE-CZ	7.30	133.82	123.60
1	B	21	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	243	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	B	243	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	79	HIS	CA-CB-CG	5.23	122.49	113.60
1	A	215	ALA	C-N-CA	-5.12	111.56	122.30
1	A	143	ARG	CD-NE-CZ	5.07	130.69	123.60
1	A	143	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	215	ALA	C-N-CA	-5.03	111.73	122.30
1	A	164	ASN	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the



chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3160	0	3103	98	0
1	B	3166	0	3102	97	0
2	A	31	0	19	3	0
2	B	31	0	19	0	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	84	0	0	4	0
5	B	86	0	0	5	0
All	All	6568	0	6243	190	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (190) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:GLU:HG2	1:A:133:GLY:HA3	1.54	0.89
1:B:370:PRO:HA	1:B:388:MET:HE1	1.61	0.83
1:A:28:LEU:HD12	1:A:296:GLN:HE22	1.43	0.82
1:A:5:LYS:HE2	1:A:8:ASP:HA	1.62	0.79
1:B:209:ILE:O	1:B:213:VAL:HG23	1.84	0.75
1:B:207:LYS:O	1:B:210:GLU:HG3	1.87	0.73
1:A:2:GLN:HG2	5:A:2001:HOH:O	1.88	0.73
1:B:59:LEU:HD21	1:B:91:LEU:HD11	1.71	0.73
1:B:125:LYS:NZ	1:B:128:GLU:HB2	2.06	0.70
1:B:179:ASP:OD2	1:B:231:ARG:HD2	1.92	0.70
1:B:394:ARG:HH11	1:B:394:ARG:HG2	1.55	0.70
1:A:28:LEU:HD12	1:A:296:GLN:NE2	2.07	0.69
1:A:174:SER:HB2	5:A:2033:HOH:O	1.93	0.69
1:B:43:GLU:HB2	1:B:133:GLY:HA3	1.76	0.68
1:B:353:LYS:HE2	1:B:357[B]:GLU:OE2	1.94	0.67
1:A:335:GLN:O	1:A:337:LYS:HE3	1.94	0.67
1:B:394:ARG:HD2	1:B:397:LYS:NZ	2.10	0.66
1:B:207:LYS:O	1:B:211:THR:HG23	1.96	0.66
1:B:235:GLN:O	1:B:238:PHE:HB3	1.95	0.66
1:B:159:LYS:NZ	1:B:220:GLU:HG3	2.11	0.66
1:B:210:GLU:OE1	1:B:211:THR:HG22	1.97	0.64
1:B:130:LEU:HB3	1:B:137:VAL:HG13	1.79	0.64
1:B:78:GLN:HE22	1:B:162:ILE:HG22	1.61	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:146:HIS:CE1	1:B:197:ILE:HD11	2.34	0.63
1:B:276:SER:HB3	1:B:386:LYS:HE3	1.79	0.63
1:A:262:MET:HB3	1:B:24:HIS:O	1.99	0.63
1:B:207:LYS:HB2	1:B:207:LYS:NZ	2.13	0.63
1:B:38:TYR:CZ	1:B:223:CYS:HB3	2.33	0.63
1:A:38:TYR:CZ	1:A:223:CYS:HB3	2.34	0.63
1:A:105:LEU:HD12	1:A:143:ARG:HD2	1.81	0.63
1:B:255:VAL:HG22	1:B:306:ALA:HB3	1.80	0.62
1:B:304:ALA:O	1:B:337:LYS:HE2	1.99	0.62
1:A:179:ASP:OD2	1:A:231:ARG:HD2	1.99	0.62
1:B:188:ARG:O	1:B:192:GLU:HG3	2.00	0.61
1:A:181:ILE:HD11	1:A:186:LEU:HB2	1.82	0.60
1:B:44:LYS:N	1:B:44:LYS:HD2	2.18	0.59
1:A:129:THR:HG22	1:A:138:THR:OG1	2.02	0.58
1:A:158:GLU:HB3	1:A:160:VAL:HG23	1.86	0.58
1:A:23:PHE:HE1	1:A:33:THR:HG21	1.69	0.57
1:A:64:ALA:HA	1:A:67:ILE:O	2.04	0.57
1:A:24:HIS:O	1:B:262:MET:HB3	2.03	0.57
1:B:341:ALA:O	1:B:388:MET:HE1	2.05	0.57
1:A:202:ALA:O	1:A:205:THR:HB	2.05	0.57
1:A:252:THR:HB	5:A:2056:HOH:O	2.05	0.57
1:B:125:LYS:HZ2	1:B:128:GLU:HB2	1.70	0.56
1:A:335:GLN:HA	5:A:2076:HOH:O	2.04	0.56
1:B:59:LEU:CD2	1:B:91:LEU:HD11	2.34	0.56
1:B:394:ARG:HD2	1:B:397:LYS:HZ3	1.67	0.56
1:A:370:PRO:HA	1:A:388:MET:HE1	1.87	0.56
1:A:37:ALA:HA	1:A:49[B]:ASP:HB2	1.86	0.56
1:A:50:THR:OG1	1:A:91:LEU:HD12	2.06	0.56
1:A:207:LYS:O	1:A:211:THR:HG23	2.05	0.56
1:B:50:THR:OG1	1:B:91:LEU:HD12	2.07	0.55
1:A:314:HIS:CD2	2:A:403:FMN:HM73	2.40	0.55
1:A:76:VAL:HG22	1:A:101:PHE:HB2	1.87	0.55
1:A:56:LYS:NZ	1:A:90:ALA:HB2	2.22	0.55
1:A:259:TYR:OH	1:A:267:GLU:HG3	2.06	0.55
1:B:50:THR:HG23	1:B:87:ALA:HB3	1.88	0.55
2:A:403:FMN:H9	1:B:147:TRP:HZ2	1.70	0.54
1:A:75:LEU:HD12	1:A:97:PRO:HG3	1.87	0.54
1:A:263:TRP:CH2	1:B:83:ASP:HB3	2.42	0.54
1:B:130:LEU:HB3	1:B:137:VAL:CG1	2.37	0.54
1:B:78:GLN:NE2	1:B:162:ILE:HG22	2.23	0.54
1:A:221:PHE:HA	1:A:230:PHE:O	2.08	0.54
1:B:259:TYR:OH	1:B:267:GLU:HG3	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:403:FMN:H9	1:B:147:TRP:CZ2	2.43	0.53
1:B:193:TYR:O	1:B:197:ILE:HG22	2.08	0.53
1:B:50:THR:HG22	1:B:84:HIS:O	2.09	0.53
1:A:263:TRP:HH2	1:B:83:ASP:HB3	1.73	0.52
1:A:208:ALA:O	1:A:212:LEU:HD23	2.10	0.52
1:B:102:THR:O	1:B:123:VAL:HA	2.10	0.52
1:A:37:ALA:HA	1:A:49[B]:ASP:CB	2.40	0.51
1:B:390:GLN:O	1:B:394:ARG:HD3	2.10	0.51
1:B:48[B]:PHE:O	1:B:76:VAL:O	2.29	0.51
1:A:48[B]:PHE:O	1:A:76:VAL:O	2.29	0.51
1:A:188:ARG:HE	1:A:192:GLU:CG	2.24	0.51
1:B:77:ILE:HD11	1:B:88:LEU:HD13	1.92	0.51
1:B:60:LEU:HD21	1:B:91:LEU:HD23	1.93	0.50
1:B:202:ALA:O	1:B:205:THR:HB	2.10	0.50
1:B:278:ARG:HG2	1:B:278:ARG:HH11	1.77	0.50
1:B:213:VAL:O	1:B:215:ALA:O	2.30	0.50
1:A:83:ASP:OD1	3:A:404:FEO:O	2.30	0.50
1:A:36:ASN:O	1:A:49[B]:ASP:OD2	2.30	0.50
1:A:213:VAL:O	1:A:215:ALA:O	2.29	0.50
1:A:132:LEU:HD11	1:A:137:VAL:HG12	1.95	0.48
1:B:125:LYS:HZ3	1:B:128:GLU:HB2	1.78	0.48
1:B:197:ILE:HG22	5:B:2009:HOH:O	2.13	0.48
1:A:288:TRP:CE2	1:A:290:LYS:HB2	2.47	0.48
1:A:312:PRO:HA	1:A:344:SER:O	2.14	0.48
1:A:188:ARG:O	1:A:192:GLU:HG3	2.13	0.48
1:B:105:LEU:HB2	5:B:2023:HOH:O	2.13	0.48
1:B:186:LEU:O	1:B:190:MET:HG3	2.14	0.48
1:B:338:ILE:HG23	1:B:365:ASP:O	2.14	0.47
1:B:394:ARG:NH1	1:B:394:ARG:HG2	2.26	0.47
1:A:50:THR:HG22	1:A:84:HIS:O	2.14	0.47
1:A:92:ILE:HD13	1:A:119:TRP:CE2	2.48	0.47
1:A:221:PHE:CE1	1:A:231:ARG:HG3	2.49	0.47
1:B:88:LEU:HB3	1:B:89:PRO:HD3	1.96	0.47
1:A:68:ASP:OD1	1:A:70:LYS:HD3	2.15	0.47
1:B:86:GLY:HA3	5:B:2015:HOH:O	2.14	0.47
1:A:345:PHE:CB	1:A:349:GLY:HA2	2.45	0.47
1:B:154:TRP:CH2	1:B:159:LYS:HA	2.49	0.47
1:A:83:ASP:HB3	1:B:263:TRP:CH2	2.50	0.47
1:B:166:ILE:O	1:B:167:PHE:HB2	2.14	0.47
1:A:154:TRP:CH2	1:A:159:LYS:HA	2.49	0.47
1:A:348:SER:HB2	1:A:350:GLU:OE1	2.15	0.47
1:B:159:LYS:CE	1:B:220:GLU:HG3	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:ALA:O	1:A:388:MET:HE1	2.14	0.47
1:A:132:LEU:CD1	1:A:137:VAL:HG12	2.44	0.46
1:A:116:TYR:CD2	1:A:119:TRP:HB2	2.49	0.46
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.97	0.46
1:A:135:ARG:HD3	1:A:158:GLU:OE2	2.15	0.46
1:A:275:GLU:HG3	1:A:278:ARG:HH21	1.81	0.45
1:B:401:ALA:O	1:B:402:ALA:HB2	2.16	0.45
1:A:124:VAL:HG11	1:A:139:PHE:CE2	2.51	0.45
1:A:325:THR:O	1:A:329:ILE:HG13	2.15	0.45
1:B:253[A]:ASN:ND2	1:B:281:GLY:O	2.50	0.45
1:B:234:ASP:OD1	1:B:234:ASP:N	2.50	0.45
1:A:319:LEU:HA	1:A:320:PRO:HD3	1.83	0.45
1:A:340:GLY:O	1:A:359:LEU:HD11	2.17	0.45
1:B:378:THR:O	1:B:381:ASP:N	2.50	0.45
1:A:37:ALA:HA	1:A:49[B]:ASP:CG	2.36	0.45
1:A:56:LYS:HG3	1:A:57:GLY:N	2.31	0.45
1:B:298:MET:HG2	1:B:332:LEU:HD13	1.99	0.45
1:B:179:ASP:OD1	1:B:231:ARG:NH1	2.50	0.44
1:A:75:LEU:CD1	1:A:97:PRO:HG3	2.47	0.44
1:B:352:THR:OG1	1:B:372:LYS:NZ	2.50	0.44
1:A:259:TYR:CZ	1:A:267:GLU:HG3	2.52	0.44
1:A:44:LYS:HD2	1:A:44:LYS:HA	1.73	0.44
1:A:253:ASN:ND2	1:A:281:GLY:O	2.50	0.44
1:A:50:THR:HG23	1:A:87:ALA:HB3	1.99	0.44
1:B:127:GLY:N	1:B:139:PHE:O	2.50	0.44
1:A:365:ASP:OD2	1:A:399:LYS:NZ	2.50	0.44
1:A:254:LYS:HB3	1:A:304:ALA:HA	2.00	0.44
1:A:386:LYS:HE2	1:A:390:GLN:HE22	1.82	0.44
1:B:252:THR:OG1	1:B:303:ASP:O	2.30	0.44
1:B:210:GLU:OE1	1:B:211:THR:N	2.50	0.44
1:A:68:ASP:O	1:A:71:LYS:HG3	2.18	0.44
1:A:105:LEU:HD12	1:A:143:ARG:CD	2.46	0.43
1:A:155:PHE:O	1:A:159:LYS:N	2.50	0.43
1:B:380:ALA:O	1:B:383:GLU:HB2	2.17	0.43
1:B:50:THR:CG2	1:B:87:ALA:H	2.31	0.43
1:A:44:LYS:HB2	1:A:132:LEU:O	2.18	0.43
1:B:250:LYS:HA	1:B:251:PRO:HD3	1.73	0.43
1:B:254:LYS:HD3	1:B:304:ALA:HB2	2.00	0.43
1:A:166:ILE:O	1:A:167:PHE:HB2	2.19	0.43
1:A:49[B]:ASP:OD1	1:A:49[B]:ASP:N	2.50	0.43
1:B:208:ALA:O	1:B:212:LEU:HG	2.18	0.43
1:B:335:GLN:O	1:B:337:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:LEU:HD21	1:B:230:PHE:HE1	1.84	0.43
1:B:146:HIS:ND1	1:B:197:ILE:HD11	2.33	0.43
1:A:23:PHE:HB2	1:A:29:SER:HB3	2.01	0.43
1:B:257:ILE:HA	1:B:308:ILE:O	2.19	0.43
1:A:81:GLU:HG2	1:A:83:ASP:OD1	2.19	0.43
1:B:370:PRO:HA	1:B:388:MET:CE	2.40	0.42
1:A:78:GLN:HE22	1:A:162:ILE:HG22	1.83	0.42
1:A:259:TYR:HA	1:A:310:GLY:O	2.19	0.42
1:B:254:LYS:HB3	1:B:304:ALA:HA	2.00	0.42
1:A:202:ALA:HB3	1:A:203:PRO:HD3	2.01	0.42
1:A:193:TYR:O	1:A:197:ILE:HG22	2.19	0.42
1:B:108:LYS:HA	1:B:108:LYS:HD3	1.84	0.42
1:A:204:GLN:N	1:A:204:GLN:OE1	2.49	0.42
1:B:75:LEU:HA	1:B:75:LEU:HD12	1.74	0.42
1:B:153:SER:O	1:B:161:LEU:HD12	2.19	0.42
1:B:263:TRP:O	1:B:264:HIS:HB2	2.20	0.42
1:A:188:ARG:NE	1:A:192:GLU:OE2	2.50	0.42
1:A:143:ARG:H	1:A:143:ARG:HG2	1.67	0.42
1:A:146:HIS:CE1	1:A:197:ILE:HD11	2.55	0.42
1:B:19:ASN:ND2	5:B:2004:HOH:O	2.53	0.42
1:B:75:LEU:HD22	1:B:97:PRO:HG3	2.02	0.42
1:B:288:TRP:CE2	1:B:290:LYS:HB2	2.55	0.42
1:B:176:ARG:HA	1:B:176:ARG:HD2	1.76	0.41
1:A:50:THR:CG2	1:A:87:ALA:H	2.33	0.41
1:B:321:TYR:HB2	5:B:2072:HOH:O	2.19	0.41
1:A:68:ASP:HB3	1:A:71:LYS:HG3	2.01	0.41
1:B:378:THR:OG1	1:B:379:HIS:N	2.52	0.41
1:A:108:LYS:O	1:A:111:GLU:HG3	2.20	0.41
1:A:165:ASP:HB3	1:A:193:TYR:OH	2.20	0.41
1:B:83:ASP:OD2	1:B:226:HIS:HE1	2.04	0.41
1:A:263:TRP:O	1:A:264:HIS:HB2	2.20	0.41
1:B:186:LEU:HD21	1:B:230:PHE:CE1	2.55	0.41
1:A:80:LEU:HD13	1:A:80:LEU:HA	1.93	0.41
1:B:106:GLY:HA2	1:B:149:ASP:HB3	2.01	0.41
1:B:38:TYR:CE2	1:B:223:CYS:HB3	2.56	0.40
1:A:181:ILE:HD11	1:A:186:LEU:CB	2.48	0.40
1:A:298:MET:HG2	1:A:332:LEU:HD13	2.02	0.40
1:A:37:ALA:HA	1:A:49[B]:ASP:OD2	2.22	0.40
1:A:56:LYS:HZ2	1:A:90:ALA:HB2	1.84	0.40
1:B:259:TYR:HA	1:B:310:GLY:O	2.22	0.40
1:A:194:TYR:CD2	1:A:246:TYR:HB3	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	402/402 (100%)	381 (95%)	21 (5%)	0	100	100
1	B	403/402 (100%)	379 (94%)	24 (6%)	0	100	100
All	All	805/804 (100%)	760 (94%)	45 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	338/336 (101%)	298 (88%)	40 (12%)	8	14
1	B	339/336 (101%)	300 (88%)	39 (12%)	8	15
All	All	677/672 (101%)	598 (88%)	79 (12%)	8	14

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	ILE
1	A	44	LYS
1	A	47	LEU
1	A	50	THR
1	A	56	LYS
1	A	61	CYS
1	A	70	LYS
1	A	93	GLU
1	A	99	LYS
1	A	104	SER

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Mol	Chain	Res	Type
1	A	107	GLN
1	A	108	LYS
1	A	111	GLU
1	A	122	GLN
1	A	125	LYS
1	A	134	LYS
1	A	136	THR
1	A	143	ARG
1	A	169	GLN
1	A	174	SER
1	A	183	VAL
1	A	197	ILE
1	A	207	LYS
1	A	211	THR
1	A	212	LEU
1	A	220	GLU
1	A	250	LYS
1	A	276	SER
1	A	283	THR
1	A	290	LYS
1	A	296	GLN
1	A	337	LYS
1	A	353	LYS
1	A	369	THR
1	A	372	LYS
1	A	379	HIS
1	A	394	ARG
1	A	396	LEU
1	A	399	LYS
1	B	2	GLN
1	B	5	LYS
1	B	16	ILE
1	B	43	GLU
1	B	44	LYS
1	B	47	LEU
1	B	50	THR
1	B	52	LYS
1	B	56	LYS
1	B	61	CYS
1	B	70	LYS
1	B	71	LYS
1	B	75	LEU

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Mol	Chain	Res	Type
1	B	96	GLN
1	B	104	SER
1	B	107	GLN
1	B	125	LYS
1	B	136	THR
1	B	149	ASP
1	B	159	LYS
1	B	169	GLN
1	B	174	SER
1	B	181	ILE
1	B	183	VAL
1	B	197	ILE
1	B	207	LYS
1	B	210	GLU
1	B	211	THR
1	B	250	LYS
1	B	276	SER
1	B	369	THR
1	B	372	LYS
1	B	374	LYS
1	B	378	THR
1	B	386	LYS
1	B	394	ARG
1	B	396	LEU
1	B	397	LYS
1	B	399	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	170	ASN
1	A	235	GLN
1	A	296	GLN
1	A	335	GLN
1	A	390	GLN
1	B	19	ASN
1	B	78	GLN
1	B	96	GLN
1	B	170	ASN
1	B	315	ASN
1	B	335	GLN

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Mol	Chain	Res	Type
1	B	375	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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	$\# Z  > 2$
2	FMN	A	403	-	33,33,33	1.79	10 (30%)	46,50,50	1.38	7 (15%)
3	FEO	A	404	1,5,4	0,2,2	0.00	-	0,1,1	0.00	-
4	OXY	A	405	3	1,1,1	0.39	0	0,0,0	0.00	-
2	FMN	B	403	-	33,33,33	1.75	10 (30%)	46,50,50	1.24	7 (15%)
3	FEO	B	404	1,5,4	0,2,2	0.00	-	0,1,1	0.00	-
4	OXY	B	405	3	1,1,1	0.60	0	0,0,0	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
2	FMN	A	403	-	-	0/18/18/18	0/0/3/3
3	FEO	A	404	1,5,4	-	0/0/0/0	0/0/0/0
4	OXY	A	405	3	-	0/0/0/0	0/0/0/0
2	FMN	B	403	-	-	0/18/18/18	0/0/3/3
3	FEO	B	404	1,5,4	-	0/0/0/0	0/0/0/0
4	OXY	B	405	3	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	FMN	P-O2P	-4.19	1.39	1.54
2	A	403	FMN	P-O2P	-4.08	1.39	1.54
2	A	403	FMN	C1'-C2'	4.06	1.55	1.51
2	B	403	FMN	C1'-C2'	3.64	1.55	1.51
2	B	403	FMN	C4A-C10	3.32	1.46	1.40
2	A	403	FMN	C9A-N10	3.06	1.43	1.38
2	A	403	FMN	O5'-C5'	3.06	1.57	1.44
2	B	403	FMN	C4-C4A	2.98	1.46	1.41
2	B	403	FMN	C9A-N10	2.93	1.43	1.38
2	A	403	FMN	C4-C4A	2.93	1.46	1.41
2	B	403	FMN	O5'-C5'	2.92	1.56	1.44
2	A	403	FMN	C4A-C10	2.90	1.45	1.40
2	A	403	FMN	C2-N3	2.66	1.42	1.37
2	A	403	FMN	C10-N10	-2.56	1.33	1.38
2	B	403	FMN	C2-N3	2.49	1.42	1.37
2	B	403	FMN	P-O5'	-2.40	1.51	1.60
2	A	403	FMN	P-O3P	-2.27	1.46	1.54
2	B	403	FMN	P-O3P	-2.26	1.46	1.54
2	B	403	FMN	C10-N10	-2.19	1.34	1.38
2	A	403	FMN	P-O5'	-2.10	1.52	1.60

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	403	FMN	C2-N1-C10	5.17	120.19	114.98
2	B	403	FMN	C4A-C10-N1	-3.62	119.11	122.73
2	B	403	FMN	C2-N1-C10	3.01	118.01	114.98
2	A	403	FMN	C4A-C10-N10	-2.72	119.15	120.51
2	B	403	FMN	C5'-C4'-C3'	-2.69	106.99	112.06
2	A	403	FMN	C5'-C4'-C3'	-2.56	107.24	112.06
2	A	403	FMN	C4-N3-C2	-2.54	120.18	125.39
2	A	403	FMN	C4A-C10-N1	-2.40	120.33	122.73
2	B	403	FMN	O2P-P-O1P	2.39	118.26	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	FMN	O2P-P-O5'	2.18	112.68	106.65
2	B	403	FMN	C4A-C10-N10	-2.14	119.44	120.51
2	A	403	FMN	O2P-P-O5'	2.08	112.39	106.65
2	B	403	FMN	C4-N3-C2	-2.07	121.14	125.39
2	A	403	FMN	C1'-N10-C9A	-2.01	116.92	118.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	401/402 (99%)	-0.63	1 (0%) 93 94	8, 23, 49, 115	0
1	B	401/402 (99%)	-0.60	3 (0%) 84 86	8, 23, 49, 123	0
All	All	802/804 (99%)	-0.61	4 (0%) 88 90	8, 23, 49, 123	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	ALA	7.0
1	A	402	ALA	4.9
1	B	401	ALA	4.0
1	B	117	LYS	2.5

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OXY	B	405	2/2	0.32	17.94	14,14,14,15	0
4	OXY	A	405	2/2	0.27	10.17	13,13,13,15	0
2	FMN	B	403	31/31	0.09	-0.07	6,10,18,23	0
2	FMN	A	403	31/31	0.08	-0.75	6,10,18,23	0
3	FEO	A	404	3/3	0.04	-3.89	11,11,15,24	0
3	FEO	B	404	3/3	0.04	-4.06	12,12,16,24	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.