



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:36 am BST

PDB ID : 4X6G  
Title : Full-length OxyR C199D from pseudomonas aeruginosa  
Authors : Jo, I.; Ha, N.C.  
Deposited on : 2014-12-08  
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.

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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 : 1.8.5 (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

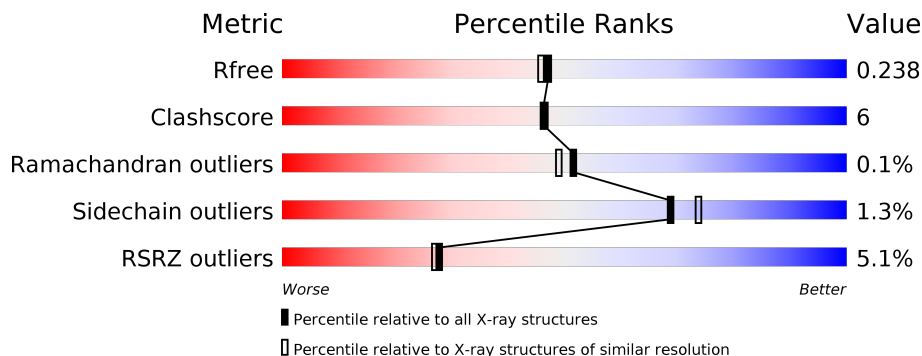
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



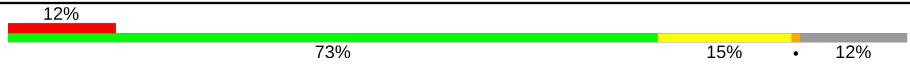

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	316	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
1	B	316	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
1	C	316	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
1	D	316	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div>
1	E	316	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div>
1	F	316	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	316	
1	H	316	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19805 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 OxyR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	Total 2338	C 1495	N 411	O 425	S 7	0	1	0
1	B	296	Total 2326	C 1490	N 412	O 417	S 7	0	1	0
1	C	295	Total 2307	C 1477	N 404	O 420	S 6	0	0	0
1	D	302	Total 2362	C 1511	N 415	O 429	S 7	0	0	0
1	E	307	Total 2414	C 1542	N 425	O 440	S 7	0	1	0
1	F	300	Total 2356	C 1507	N 415	O 427	S 7	0	1	0
1	G	279	Total 2176	C 1398	N 376	O 396	S 6	0	0	0
1	H	292	Total 2278	C 1461	N 398	O 412	S 7	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9HTL4
A	-4	HIS	-	expression tag	UNP Q9HTL4
A	-3	HIS	-	expression tag	UNP Q9HTL4
A	-2	HIS	-	expression tag	UNP Q9HTL4
A	-1	HIS	-	expression tag	UNP Q9HTL4
A	0	HIS	-	expression tag	UNP Q9HTL4
A	199	ASP	CYS	engineered mutation	UNP Q9HTL4
B	-5	HIS	-	expression tag	UNP Q9HTL4
B	-4	HIS	-	expression tag	UNP Q9HTL4
B	-3	HIS	-	expression tag	UNP Q9HTL4
B	-2	HIS	-	expression tag	UNP Q9HTL4
B	-1	HIS	-	expression tag	UNP Q9HTL4
B	0	HIS	-	expression tag	UNP Q9HTL4

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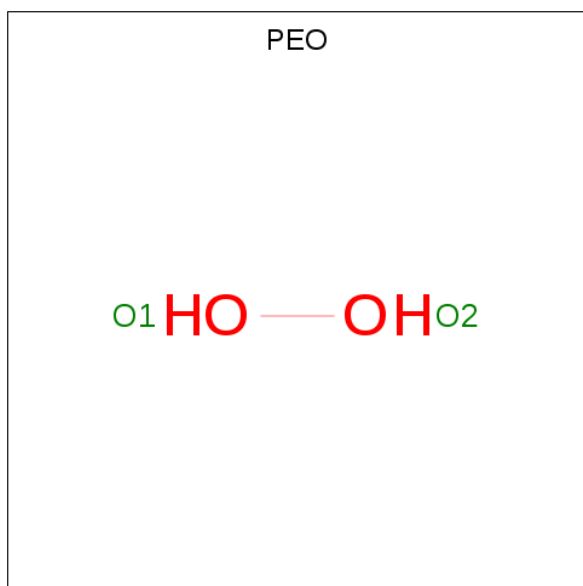
Chain	Residue	Modelled	Actual	Comment	Reference
B	199	ASP	CYS	engineered mutation	UNP Q9HTL4
C	-5	HIS	-	expression tag	UNP Q9HTL4
C	-4	HIS	-	expression tag	UNP Q9HTL4
C	-3	HIS	-	expression tag	UNP Q9HTL4
C	-2	HIS	-	expression tag	UNP Q9HTL4
C	-1	HIS	-	expression tag	UNP Q9HTL4
C	0	HIS	-	expression tag	UNP Q9HTL4
C	199	ASP	CYS	engineered mutation	UNP Q9HTL4
D	-5	HIS	-	expression tag	UNP Q9HTL4
D	-4	HIS	-	expression tag	UNP Q9HTL4
D	-3	HIS	-	expression tag	UNP Q9HTL4
D	-2	HIS	-	expression tag	UNP Q9HTL4
D	-1	HIS	-	expression tag	UNP Q9HTL4
D	0	HIS	-	expression tag	UNP Q9HTL4
D	199	ASP	CYS	engineered mutation	UNP Q9HTL4
E	-5	HIS	-	expression tag	UNP Q9HTL4
E	-4	HIS	-	expression tag	UNP Q9HTL4
E	-3	HIS	-	expression tag	UNP Q9HTL4
E	-2	HIS	-	expression tag	UNP Q9HTL4
E	-1	HIS	-	expression tag	UNP Q9HTL4
E	0	HIS	-	expression tag	UNP Q9HTL4
E	199	ASP	CYS	engineered mutation	UNP Q9HTL4
F	-5	HIS	-	expression tag	UNP Q9HTL4
F	-4	HIS	-	expression tag	UNP Q9HTL4
F	-3	HIS	-	expression tag	UNP Q9HTL4
F	-2	HIS	-	expression tag	UNP Q9HTL4
F	-1	HIS	-	expression tag	UNP Q9HTL4
F	0	HIS	-	expression tag	UNP Q9HTL4
F	199	ASP	CYS	engineered mutation	UNP Q9HTL4
G	-5	HIS	-	expression tag	UNP Q9HTL4
G	-4	HIS	-	expression tag	UNP Q9HTL4
G	-3	HIS	-	expression tag	UNP Q9HTL4
G	-2	HIS	-	expression tag	UNP Q9HTL4
G	-1	HIS	-	expression tag	UNP Q9HTL4
G	0	HIS	-	expression tag	UNP Q9HTL4
G	199	ASP	CYS	engineered mutation	UNP Q9HTL4
H	-5	HIS	-	expression tag	UNP Q9HTL4
H	-4	HIS	-	expression tag	UNP Q9HTL4
H	-3	HIS	-	expression tag	UNP Q9HTL4
H	-2	HIS	-	expression tag	UNP Q9HTL4
H	-1	HIS	-	expression tag	UNP Q9HTL4
H	0	HIS	-	expression tag	UNP Q9HTL4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	199	ASP	CYS	engineered mutation	UNP Q9HTL4

- Molecule 2 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 2 2	0	0
2	B	1	Total O 2 2	0	0
2	C	1	Total O 2 2	0	0
2	D	1	Total O 2 2	0	0
2	E	1	Total O 2 2	0	0
2	F	1	Total O 2 2	0	0
2	G	1	Total O 2 2	0	0
2	H	1	Total O 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

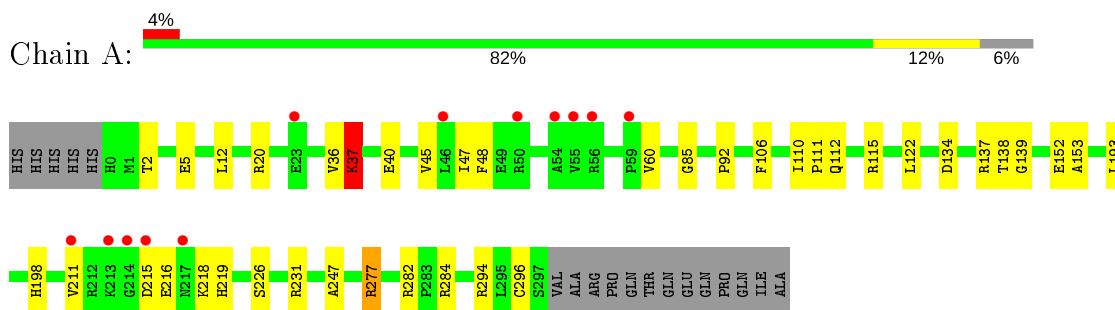
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	123	Total	O	0	0
			123	123		
4	C	149	Total	O	0	0
			149	149		
4	D	166	Total	O	0	0
			166	166		
4	E	164	Total	O	0	0
			164	164		
4	F	111	Total	O	0	0
			111	111		
4	G	138	Total	O	0	0
			138	138		
4	H	129	Total	O	0	0
			129	129		



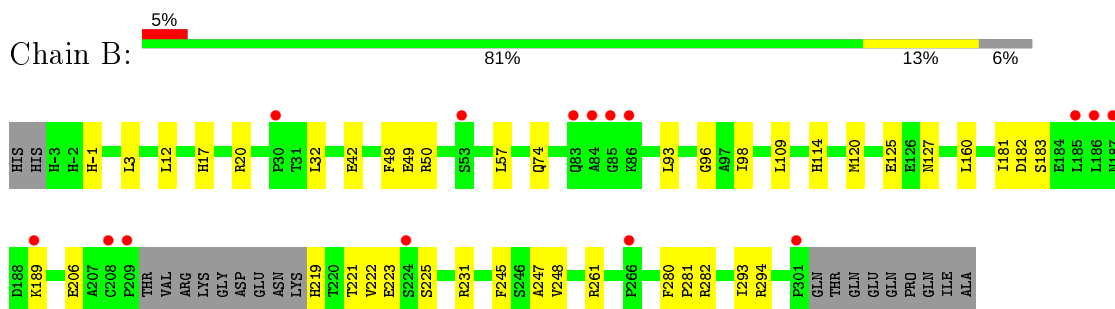
### 3 Residue-property plots [i](#)

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.

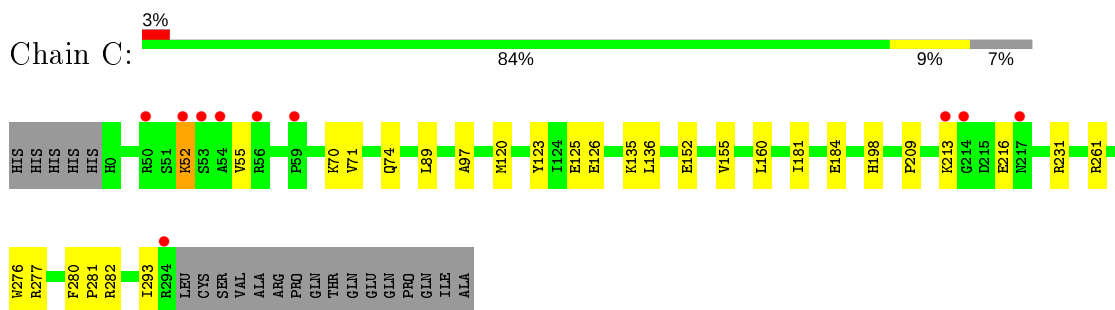
- Molecule 1: OxyR



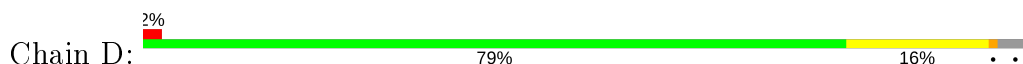
- Molecule 1: OxyR

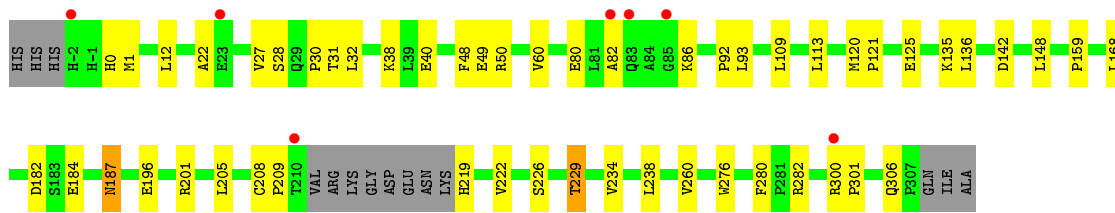


- Molecule 1: OxyR

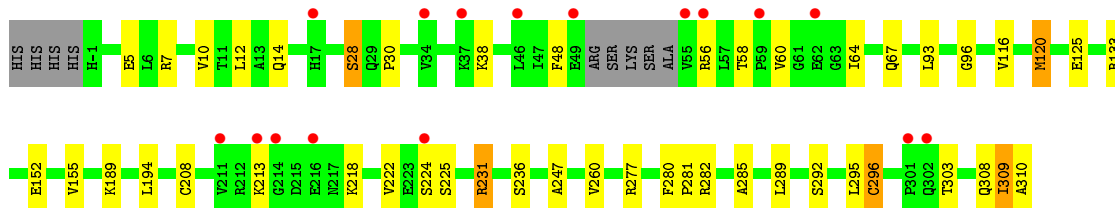
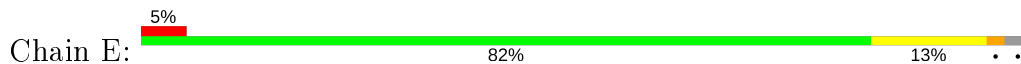


- Molecule 1: OxyR

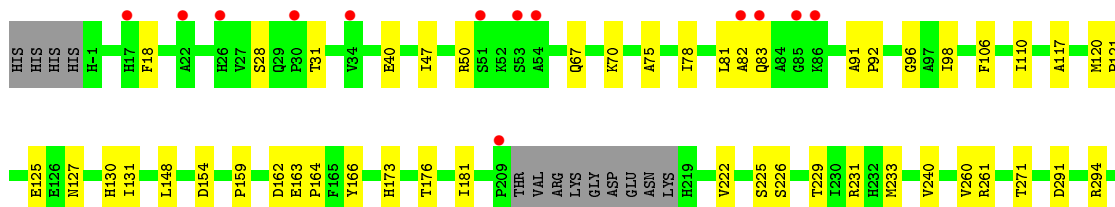
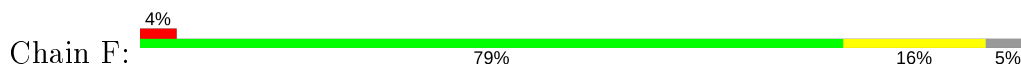




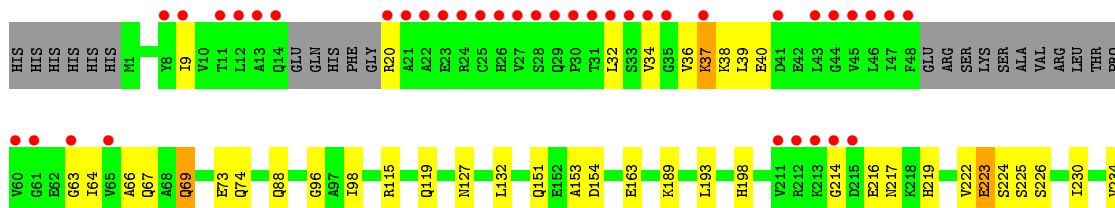
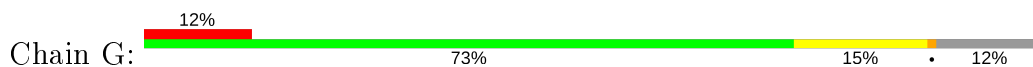
• Molecule 1: OxyR



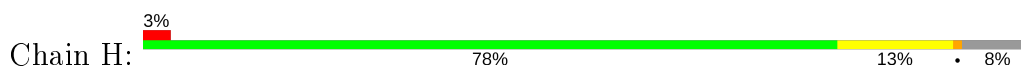
• Molecule 1: OxyR

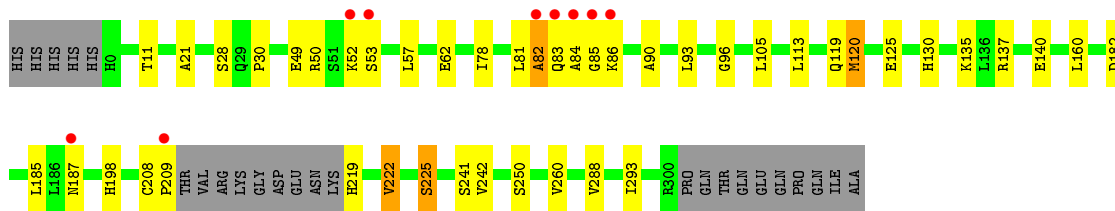


• Molecule 1: OxyR



• Molecule 1: OxyR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.64Å 151.13Å 141.58Å 90.00° 97.28° 90.00°	Depositor
Resolution (Å)	19.96 – 2.00 30.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.3 (19.96-2.00) 75.4 (30.20-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.186 , 0.237 0.189 , 0.238	Depositor DCC
$R_{free}$ test set	8656 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2852e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

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

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	0.61	1/2392 (0.0%)	0.72	4/3254 (0.1%)
1	B	0.59	0/2383	0.72	4/3245 (0.1%)
1	C	0.59	0/2361	0.71	1/3213 (0.0%)
1	D	0.61	0/2419	0.71	1/3295 (0.0%)
1	E	0.62	0/2470	0.71	2/3361 (0.1%)
1	F	0.61	0/2412	0.70	1/3284 (0.0%)
1	G	0.61	0/2224	0.74	0/3026
1	H	0.58	0/2331	0.70	0/3173
All	All	0.60	1/18992 (0.0%)	0.71	13/25851 (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)
1	A	296	CYS	CB-SG	-5.42	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	LEU	CA-CB-CG	8.38	134.58	115.30
1	A	277	ARG	NE-CZ-NH2	-7.50	116.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	VAL	C-N-CA	-7.11	103.94	121.70
1	C	231	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	E	120	MET	CB-CG-SD	-6.52	92.84	112.40
1	B	109	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	37	LYS	CA-CB-CG	5.89	126.35	113.40
1	B	294	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	F	231	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	277	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	231	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	282	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	57	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	LYS	Peptide
1	E	309	ILE	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	2338	0	2376	30	1
1	B	2326	0	2357	25	0
1	C	2307	0	2343	17	0
1	D	2362	0	2388	36	0
1	E	2414	0	2443	38	1
1	F	2356	0	2386	37	0
1	G	2176	0	2218	40	0
1	H	2278	0	2316	31	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	18	0	24	3	0
3	B	18	0	24	4	0
3	C	12	0	16	0	0
3	D	12	0	16	1	0
3	E	6	0	8	2	0
3	F	6	0	8	2	0
3	G	6	0	8	3	0
3	H	12	0	16	2	0
4	A	162	0	0	5	0
4	B	123	0	0	2	0
4	C	149	0	0	4	0
4	D	166	0	0	3	0
4	E	164	0	0	5	0
4	F	111	0	0	2	0
4	G	138	0	0	2	0
4	H	129	0	0	1	0
All	All	19805	0	18947	237	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 (237) 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:A:37:LYS:HB2	1:A:40:GLU:HB2	1.39	1.04
1:H:187:ASN:HB3	1:H:209:PRO:HG2	1.49	0.94
1:A:137:ARG:NH2	1:A:152:GLU:OE1	2.06	0.88
1:D:187:ASN:ND2	1:D:209:PRO:O	2.10	0.85
1:G:66:ALA:O	1:G:69:GLN:HG3	1.76	0.83
1:E:225:SER:O	3:E:402:GOL:O3	1.97	0.82
1:F:78:ILE:HG12	1:G:67:GLN:HB3	1.62	0.81
1:G:214:GLY:HA2	1:G:216:GLU:HG3	1.63	0.78
1:B:231:ARG:NH2	1:B:247:ALA:O	2.17	0.78
1:A:40:GLU:OE2	1:A:47:ILE:N	2.18	0.75
1:D:113:LEU:HD21	1:D:120:MET:HE2	1.70	0.70
1:F:294[A]:ARG:HD2	1:F:302:GLN:HE22	1.56	0.70
1:D:142:ASP:OD1	4:D:527:HOH:O	2.10	0.70
1:E:7[B]:ARG:NH2	4:E:610:HOH:O	2.25	0.69
1:E:93:LEU:HD22	1:E:120:MET:CE	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASP:HB2	1:A:218:LYS:HE3	1.75	0.68
1:E:133:ARG:NH1	1:E:152:GLU:OE1	2.26	0.67
1:H:182:ASP:HB2	1:H:185:LEU:HD13	1.77	0.67
1:H:52:LYS:C	1:H:52:LYS:HD2	2.15	0.67
1:F:154:ASP:OD2	4:F:586:HOH:O	2.12	0.66
1:C:160:LEU:HD13	1:C:293:ILE:HG21	1.78	0.66
1:H:82:ALA:O	1:H:83:GLN:HG3	1.96	0.66
1:G:88:GLN:HE22	1:G:284:ARG:H	1.44	0.65
1:G:36:VAL:O	1:G:40:GLU:HG3	1.97	0.65
1:A:231:ARG:NH2	1:A:247:ALA:O	2.26	0.65
1:F:117:ALA:O	1:F:120:MET:HB2	1.99	0.63
1:F:91:ALA:H	1:F:120:MET:HE1	1.64	0.63
1:E:309:ILE:HA	1:E:310:ALA:HB3	1.83	0.61
1:B:17:HIS:CD2	1:B:20:ARG:HH21	2.18	0.61
1:E:5:GLU:OE2	1:E:38:LYS:NZ	2.34	0.60
1:F:294[A]:ARG:HD2	1:F:302:GLN:NE2	2.15	0.60
1:B:93:LEU:HB2	1:B:120:MET:HE1	1.84	0.59
1:G:69:GLN:O	1:G:73:GLU:HG3	2.03	0.59
1:D:184:GLU:HA	1:D:209:PRO:HG2	1.83	0.58
1:E:281:PRO:HG3	1:H:49:GLU:HG2	1.85	0.58
1:D:92:PRO:O	1:D:282:ARG:NH2	2.36	0.58
1:F:91:ALA:H	1:F:120:MET:CE	2.16	0.58
1:D:27:VAL:HG13	1:D:31:THR:HB	1.85	0.58
1:A:211:VAL:HG21	1:A:216:GLU:HB3	1.85	0.58
1:E:64:ILE:HD11	1:H:82:ALA:HA	1.86	0.58
1:F:92:PRO:HB3	1:F:121:PRO:HG2	1.86	0.58
1:A:277:ARG:NH2	1:D:49:GLU:OE1	2.35	0.57
1:F:67:GLN:HE22	1:G:74:GLN:NE2	2.01	0.57
1:D:125:GLU:OE1	1:D:135:LYS:HE2	2.04	0.57
1:H:62:GLU:OE1	1:H:137:ARG:NH2	2.38	0.57
1:H:113:LEU:HD12	1:H:288:VAL:HG12	1.86	0.57
1:G:88:GLN:NE2	1:G:284:ARG:H	2.02	0.57
1:C:280:PHE:CE2	1:C:282:ARG:HB2	2.40	0.56
1:E:93:LEU:HD22	1:E:120:MET:HE2	1.86	0.56
1:E:292:SER:O	1:E:296:CYS:HB3	2.05	0.56
1:H:93:LEU:HB2	1:H:120:MET:CE	2.36	0.56
1:A:45:VAL:HG11	1:A:60:VAL:HG11	1.86	0.56
1:B:96:GLY:HA2	1:B:125:GLU:O	2.07	0.55
1:B:225:SER:O	3:B:402:GOL:H12	2.07	0.55
1:E:236:SER:HB3	1:F:110:ILE:HD12	1.86	0.55
1:E:295:LEU:HB3	1:E:303:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLU:HB3	1:E:155:VAL:HB	1.89	0.55
1:E:309:ILE:HA	1:E:310:ALA:CB	2.37	0.54
1:G:222:VAL:HG13	1:G:225:SER:OG	2.08	0.54
1:B:189:LYS:HG3	1:B:219:HIS:N	2.23	0.54
1:G:283:PRO:O	1:G:287:GLU:HG2	2.06	0.54
1:A:37:LYS:HA	1:A:40:GLU:H	1.73	0.54
1:B:181:ILE:HD13	1:B:261:ARG:HB2	1.90	0.54
1:C:136:LEU:HD11	1:C:276:TRP:HA	1.90	0.54
1:D:280:PHE:CE2	1:D:282:ARG:HB2	2.43	0.53
1:D:92:PRO:HB3	1:D:121:PRO:HG2	1.90	0.53
1:H:84:ALA:HB1	1:H:85:GLY:HA2	1.90	0.53
1:F:96:GLY:HA2	1:F:125:GLU:O	2.08	0.53
1:F:173:HIS:O	1:F:176:THR:OG1	2.20	0.53
1:H:11:THR:HG22	1:H:21:ALA:HA	1.91	0.53
1:F:181:ILE:HD13	1:F:261:ARG:HB2	1.90	0.53
1:E:189:LYS:HA	1:E:218:LYS:O	2.09	0.53
1:F:28:SER:HB3	1:F:31:THR:OG1	2.09	0.52
1:B:206:GLU:HG3	4:B:619:HOH:O	2.08	0.52
1:B:12:LEU:HD23	1:B:48:PHE:CE2	2.45	0.52
1:G:96:GLY:HA3	1:G:132:LEU:HD22	1.92	0.52
1:H:187:ASN:HA	1:H:219:HIS:HE1	1.74	0.52
1:F:222:VAL:O	1:F:225:SER:OG	2.24	0.52
1:B:50:ARG:HD3	3:B:404:GOL:H31	1.90	0.51
1:D:306:GLN:NE2	4:D:501:HOH:O	2.37	0.51
1:H:222:VAL:O	1:H:225:SER:OG	2.27	0.51
4:A:659:HOH:O	1:B:114:HIS:HD2	1.93	0.51
1:G:119:GLN:HG2	4:G:590:HOH:O	2.10	0.51
1:G:37:LYS:HG3	1:G:38:LYS:N	2.25	0.51
1:G:66:ALA:HA	1:G:69:GLN:CG	2.41	0.51
1:A:198:HIS:HE1	3:A:402:GOL:H11	1.76	0.50
1:H:57:LEU:HD13	1:H:62:GLU:HG2	1.93	0.50
1:B:160:LEU:HD13	1:B:293:ILE:HG21	1.92	0.50
1:D:219:HIS:N	4:D:662:HOH:O	2.43	0.50
4:C:595:HOH:O	1:D:229:THR:HG21	2.11	0.50
1:F:70:LYS:HE2	1:G:74:GLN:HG3	1.93	0.50
1:H:52:LYS:HE3	1:H:53:SER:HB2	1.92	0.50
1:D:300:ARG:HG2	1:D:301:PRO:HD3	1.94	0.50
1:E:280:PHE:CE2	1:E:282:ARG:HB2	2.47	0.50
1:H:28:SER:HB2	1:H:30:PRO:HD2	1.94	0.50
1:F:78:ILE:CG1	1:G:67:GLN:HB3	2.40	0.49
1:C:70:LYS:O	1:C:74:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:NH2	4:A:501:HOH:O	2.39	0.48
1:A:106:PHE:O	1:A:110:ILE:HG12	2.12	0.48
1:F:226:SER:HB3	3:F:402:GOL:H11	1.95	0.48
1:D:182:ASP:HB3	1:D:184:GLU:OE2	2.13	0.48
1:G:198:HIS:CE1	3:G:402:GOL:H12	2.48	0.48
1:A:137:ARG:NH2	1:A:152:GLU:HB3	2.29	0.48
1:G:189:LYS:NZ	4:G:632:HOH:O	2.47	0.48
1:A:2:THR:OG1	1:A:5:GLU:HG2	2.14	0.48
1:C:213:LYS:HA	1:C:216:GLU:OE2	2.14	0.48
1:E:222:VAL:HG13	1:E:225:SER:OG	2.14	0.48
1:F:78:ILE:N	1:G:67:GLN:HG2	2.29	0.48
1:B:280:PHE:CD1	1:B:281:PRO:HD2	2.48	0.48
1:C:181:ILE:HD13	1:C:261:ARG:HB2	1.96	0.48
1:E:208:CYS:HB3	4:E:608:HOH:O	2.14	0.48
1:F:291:ASP:OD2	1:F:294[B]:ARG:NH2	2.48	0.47
1:A:277:ARG:HH22	1:D:49:GLU:CD	2.17	0.47
1:G:115:ARG:HH11	1:G:115:ARG:HG3	1.80	0.47
1:G:98:ILE:HA	1:G:127:ASN:O	2.14	0.47
1:G:88:GLN:O	1:G:282:ARG:HD2	2.13	0.47
3:A:404:GOL:H31	1:D:1:MET:HE1	1.96	0.47
1:D:136:LEU:HD11	1:D:276:TRP:HA	1.96	0.47
1:F:222:VAL:HG12	1:F:225:SER:HB3	1.97	0.47
1:A:110:ILE:HB	1:A:111:PRO:HD3	1.97	0.47
1:D:168:LEU:HG	1:D:234:VAL:HG11	1.97	0.47
1:C:52:LYS:HG3	1:C:52:LYS:H	1.44	0.47
1:F:229:THR:HG22	1:F:233:MET:CE	2.44	0.47
1:E:225:SER:O	3:E:402:GOL:H12	2.15	0.46
1:A:92:PRO:O	1:A:282:ARG:NH2	2.48	0.46
1:A:40:GLU:HG2	1:A:47:ILE:HG13	1.97	0.46
1:G:280:PHE:CE2	1:G:282:ARG:HB2	2.50	0.46
1:B:74:GLN:HB2	1:C:71:VAL:HG22	1.96	0.46
1:G:193:LEU:HD12	1:G:219:HIS:CD2	2.50	0.46
1:F:130:HIS:CE1	1:F:131:ILE:HG13	2.50	0.46
1:G:9:ILE:HG21	1:G:39:LEU:HD23	1.96	0.46
1:B:50:ARG:CD	3:B:404:GOL:H31	2.46	0.46
1:G:115:ARG:NH1	1:G:115:ARG:HG3	2.30	0.46
1:A:193:LEU:HD12	1:A:219:HIS:CD2	2.51	0.46
1:H:130:HIS:HD2	4:H:583:HOH:O	1.98	0.46
1:G:66:ALA:HA	1:G:69:GLN:HG2	1.98	0.46
1:A:85:GLY:HA3	1:D:60:VAL:HG21	1.98	0.45
1:E:231:ARG:NH2	1:E:247:ALA:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:LYS:NZ	4:E:503:HOH:O	2.48	0.45
1:D:148:LEU:HD11	1:D:159:PRO:HG3	1.98	0.45
1:F:98:ILE:HA	1:F:127:ASN:O	2.16	0.45
1:H:96:GLY:HA2	1:H:125:GLU:O	2.17	0.45
1:A:12:LEU:HD23	1:A:48:PHE:CE1	2.52	0.45
1:B:93:LEU:HB2	1:B:120:MET:CE	2.45	0.45
1:G:223:GLU:HA	1:G:224:SER:HA	1.30	0.45
1:C:280:PHE:HA	1:C:281:PRO:HD3	1.70	0.45
1:E:116:VAL:HG22	1:E:308:GLN:HB3	1.97	0.45
1:H:222:VAL:HG13	1:H:225:SER:OG	2.16	0.45
1:A:115[A]:ARG:HG3	4:A:603:HOH:O	2.17	0.44
1:D:226:SER:HB3	3:D:402:GOL:H31	1.98	0.44
1:C:89:LEU:HA	1:C:120:MET:CE	2.47	0.44
1:H:90:ALA:HA	1:H:119:GLN:HB3	1.99	0.44
1:A:226:SER:HA	3:A:402:GOL:O1	2.16	0.44
1:D:208:CYS:HA	1:D:209:PRO:HD2	1.79	0.44
1:G:63:GLY:O	1:G:66:ALA:HB3	2.16	0.44
1:D:0:HIS:N	1:D:0:HIS:CD2	2.83	0.44
1:E:224:SER:O	1:E:224:SER:OG	2.35	0.44
1:G:34:VAL:HG23	1:G:37:LYS:HE3	1.99	0.44
1:H:241:SER:OG	1:H:242:VAL:N	2.50	0.44
1:C:97:ALA:O	1:C:126:GLU:HA	2.17	0.44
1:G:214:GLY:HA2	1:G:216:GLU:N	2.33	0.44
1:F:83:GLN:NE2	4:F:602:HOH:O	2.51	0.43
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.85	0.43
1:D:38:LYS:HE3	1:D:38:LYS:HB2	1.77	0.43
1:D:80:GLU:OE2	1:D:86:LYS:NZ	2.51	0.43
1:F:78:ILE:HG23	1:G:64:ILE:HG23	2.00	0.43
1:B:222:VAL:O	1:B:225:SER:OG	2.20	0.43
1:B:261:ARG:NH2	4:B:616:HOH:O	2.50	0.43
1:F:81:LEU:HD23	1:F:81:LEU:HA	1.85	0.43
1:C:125:GLU:OE2	1:C:135:LYS:NZ	2.41	0.43
1:E:12:LEU:HD23	1:E:48:PHE:CE2	2.54	0.43
1:F:40:GLU:OE2	1:F:47:ILE:N	2.44	0.43
1:D:196:GLU:HA	1:D:201:ARG:HD3	2.01	0.43
1:E:28:SER:HB3	1:E:30:PRO:HD2	2.01	0.43
1:E:58:THR:CG2	1:E:60:VAL:HG12	2.49	0.43
1:C:152:GLU:HB3	1:C:155:VAL:HB	2.01	0.43
1:C:184:GLU:HB2	1:C:209:PRO:HG2	2.00	0.43
1:D:93:LEU:HD22	1:D:120:MET:HE1	2.00	0.43
1:B:3:LEU:HD23	4:C:582:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:LEU:HD13	1:H:293:ILE:HG21	1.99	0.42
1:G:274:ILE:CD1	1:G:289:LEU:HD23	2.49	0.42
1:H:135:LYS:HB3	1:H:140:GLU:HB3	2.01	0.42
1:H:250:SER:O	1:H:250:SER:OG	2.27	0.42
1:E:67:GLN:HB3	1:H:78:ILE:HD13	2.01	0.42
1:B:-1:HIS:HB3	1:B:42:GLU:OE1	2.19	0.42
1:C:198:HIS:HD2	4:C:513:HOH:O	2.03	0.42
1:F:75:ALA:O	1:F:78:ILE:HB	2.20	0.42
1:G:225:SER:O	3:G:402:GOL:H11	2.19	0.42
1:H:187:ASN:HA	1:H:219:HIS:CE1	2.53	0.42
1:H:198:HIS:NE2	3:H:403:GOL:H12	2.34	0.42
1:B:245:PHE:O	1:B:248:VAL:HG22	2.19	0.42
1:D:125:GLU:CD	1:D:135:LYS:HE2	2.40	0.42
1:C:123:TYR:OH	1:D:222:VAL:HG13	2.20	0.42
1:E:67:GLN:HG3	1:H:81:LEU:HD22	2.01	0.42
1:G:226:SER:HA	3:G:402:GOL:H11	2.01	0.42
1:H:105:LEU:HA	1:H:105:LEU:HD12	1.85	0.42
1:B:182:ASP:OD1	1:B:183:SER:N	2.53	0.42
1:A:139:GLY:HA2	4:A:543:HOH:O	2.19	0.42
1:D:12:LEU:HD23	1:D:48:PHE:CE2	2.55	0.42
1:F:106:PHE:O	1:F:110:ILE:HG12	2.20	0.42
1:E:280:PHE:HA	1:E:281:PRO:HD3	1.72	0.41
1:G:230:ILE:O	1:G:234:VAL:HG23	2.19	0.41
1:A:137:ARG:NH1	1:A:153:ALA:O	2.52	0.41
1:F:225:SER:O	3:F:402:GOL:H12	2.19	0.41
1:B:98:ILE:HA	1:B:127:ASN:O	2.21	0.41
1:E:116:VAL:HG21	4:E:548:HOH:O	2.20	0.41
1:E:10:VAL:O	1:E:14:GLN:HG3	2.20	0.41
1:E:93:LEU:HD23	1:E:289:LEU:HD22	2.03	0.41
1:E:96:GLY:HA2	1:E:125:GLU:O	2.21	0.41
1:F:163:GLU:HA	1:F:164:PRO:HD2	1.97	0.41
1:G:217:ASN:HB2	1:G:219:HIS:CE1	2.55	0.41
1:A:134:ASP:O	1:A:138:THR:HG23	2.21	0.41
1:D:40:GLU:OE1	1:D:50:ARG:NH1	2.49	0.41
1:E:7[B]:ARG:HA	1:E:7[B]:ARG:HD3	1.85	0.41
1:A:137:ARG:HH22	1:A:152:GLU:HB3	1.84	0.41
1:E:277:ARG:HD3	4:E:533:HOH:O	2.19	0.41
1:F:148:LEU:HD11	1:F:159:PRO:HG3	2.01	0.41
1:H:50:ARG:NH2	3:H:402:GOL:O1	2.53	0.41
1:B:49:GLU:O	3:B:404:GOL:H32	2.21	0.41
1:G:153:ALA:HA	1:G:154:ASP:HA	1.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:CYS:HB3	1:H:209:PRO:HD2	2.02	0.41
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.85	0.41
1:F:82:ALA:HB2	1:G:64:ILE:HD11	2.02	0.41
1:A:211:VAL:HG21	1:A:216:GLU:CA	2.51	0.41
1:B:221:THR:HG22	1:B:223:GLU:HG2	2.03	0.41
1:E:194:LEU:HA	1:E:194:LEU:HD23	1.91	0.41
1:E:58:THR:HG22	1:E:60:VAL:HG12	2.03	0.41
1:F:91:ALA:N	1:F:120:MET:HE1	2.32	0.41
1:D:22:ALA:HA	1:D:32:LEU:HD13	2.03	0.40
1:F:166:TYR:HB3	1:F:260:VAL:HG13	2.02	0.40
1:A:110:ILE:CD1	1:A:122:LEU:HD12	2.52	0.40
1:E:120:MET:CE	1:E:285:ALA:HB1	2.52	0.40
1:A:112:GLN:HG3	4:A:546:HOH:O	2.21	0.40
1:F:162:ASP:OD1	1:F:271:THR:OG1	2.21	0.40
1:G:163:GLU:OE2	1:G:246:SER:OG	2.29	0.40
1:C:277:ARG:HD3	4:C:521:HOH:O	2.22	0.40
1:D:28:SER:OG	1:D:30:PRO:HD2	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:294:ARG:NH1	1:E:310:ALA:OXT[1_554]	2.11	0.09

## 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	297/316 (94%)	291 (98%)	6 (2%)	0	100	100
1	B	293/316 (93%)	284 (97%)	9 (3%)	0	100	100
1	C	293/316 (93%)	285 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	298/316 (94%)	289 (97%)	8 (3%)	1 (0%)	41	37
1	E	304/316 (96%)	296 (97%)	8 (3%)	0	100	100
1	F	297/316 (94%)	287 (97%)	10 (3%)	0	100	100
1	G	273/316 (86%)	266 (97%)	7 (3%)	0	100	100
1	H	288/316 (91%)	273 (95%)	13 (4%)	2 (1%)	22	16
All	All	2343/2528 (93%)	2271 (97%)	69 (3%)	3 (0%)	51	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	82	ALA
1	H	82	ALA
1	H	86	LYS

### 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	254/269 (94%)	252 (99%)	2 (1%)	81	86
1	B	252/269 (94%)	251 (100%)	1 (0%)	91	93
1	C	250/269 (93%)	248 (99%)	2 (1%)	81	86
1	D	257/269 (96%)	254 (99%)	3 (1%)	71	76
1	E	262/269 (97%)	257 (98%)	5 (2%)	57	61
1	F	256/269 (95%)	253 (99%)	3 (1%)	71	76
1	G	236/269 (88%)	230 (98%)	6 (2%)	47	49
1	H	247/269 (92%)	243 (98%)	4 (2%)	62	67
All	All	2014/2152 (94%)	1988 (99%)	26 (1%)	69	74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	37	LYS
1	B	32	LEU
1	C	52	LYS
1	C	55	VAL
1	D	187	ASN
1	D	229	THR
1	D	260	VAL
1	E	28	SER
1	E	56	ARG
1	E	213	LYS
1	E	260	VAL
1	E	296	CYS
1	F	18	PHE
1	F	50	ARG
1	F	240	VAL
1	G	20	ARG
1	G	32	LEU
1	G	37	LYS
1	G	69	GLN
1	G	151	GLN
1	G	223	GLU
1	H	120	MET
1	H	222	VAL
1	H	225	SER
1	H	260	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	B	114	HIS
1	C	198	HIS
1	C	252	HIS
1	D	0	HIS
1	D	114	HIS
1	E	304	GLN
1	F	114	HIS
1	F	130	HIS
1	F	302	GLN
1	G	74	GLN
1	G	76	GLN
1	G	83	GLN

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Mol	Chain	Res	Type
1	G	88	GLN
1	H	0	HIS
1	H	130	HIS
1	H	219	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

23 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	PEO	G	401	-	1,1,1	0.25	0	-		
2	PEO	A	401	-	1,1,1	0.29	0	-		
2	PEO	D	401	-	1,1,1	0.01	0	-		
3	GOL	F	402	-	5,5,5	0.43	0	5,5,5	1.15	1 (20%)
3	GOL	H	403	-	5,5,5	0.36	0	5,5,5	0.46	0
3	GOL	B	404	-	5,5,5	0.42	0	5,5,5	0.52	0
3	GOL	A	402	-	5,5,5	0.34	0	5,5,5	0.89	0
2	PEO	F	401	-	1,1,1	0.22	0	-		
3	GOL	A	404	-	5,5,5	0.46	0	5,5,5	0.41	0
3	GOL	B	402	-	5,5,5	0.39	0	5,5,5	0.77	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	403	-	5,5,5	0.40	0	5,5,5	0.48	0
2	PEO	E	401	-	1,1,1	0.16	0	-		
3	GOL	C	402	-	5,5,5	0.66	0	5,5,5	0.82	0
2	PEO	H	401	-	1,1,1	0.26	0	-		
3	GOL	H	402	-	5,5,5	0.38	0	5,5,5	0.50	0
2	PEO	B	401	-	1,1,1	0.25	0	-		
3	GOL	A	403	-	5,5,5	0.29	0	5,5,5	0.95	0
3	GOL	C	403	-	5,5,5	0.31	0	5,5,5	0.47	0
3	GOL	G	402	-	5,5,5	0.34	0	5,5,5	0.71	0
2	PEO	C	401	-	1,1,1	0.31	0	-		
3	GOL	D	402	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	B	403	-	5,5,5	0.43	0	5,5,5	0.68	0
3	GOL	E	402	-	5,5,5	0.29	0	5,5,5	0.72	0

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	GOL	H	402	-	-	1/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	F	402	-	-	4/4/4/4	-
3	GOL	A	404	-	-	4/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	H	403	-	-	2/4/4/4	-
3	GOL	D	403	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	C	403	-	-	4/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	E	402	-	-	4/4/4/4	-
3	GOL	G	402	-	-	0/4/4/4	-
3	GOL	A	402	-	-	4/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	F	402	GOL	O1-C1-C2	2.12	120.36	110.20

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	402	GOL	O1-C1-C2-C3
3	H	403	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-C3
3	A	402	GOL	O1-C1-C2-C3
3	A	402	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	D	403	GOL	O1-C1-C2-C3
3	C	402	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	D	402	GOL	O1-C1-C2-O2
3	D	402	GOL	O1-C1-C2-C3
3	E	402	GOL	O1-C1-C2-O2
3	E	402	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-O2
3	A	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O1-C1-C2-O2
3	C	403	GOL	O1-C1-C2-O2
3	C	403	GOL	O1-C1-C2-C3
3	B	403	GOL	O1-C1-C2-C3
3	E	402	GOL	C1-C2-C3-O3
3	F	402	GOL	O1-C1-C2-O2
3	H	403	GOL	O2-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	D	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-O2
3	E	402	GOL	O2-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
3	C	403	GOL	O2-C2-C3-O3
3	F	402	GOL	O2-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	C	403	GOL	C1-C2-C3-O3
3	F	402	GOL	C1-C2-C3-O3
3	H	402	GOL	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	GOL	2	0
3	H	403	GOL	1	0
3	B	404	GOL	3	0
3	A	402	GOL	2	0
3	A	404	GOL	1	0
3	B	402	GOL	1	0
3	H	402	GOL	1	0
3	G	402	GOL	3	0
3	D	402	GOL	1	0
3	E	402	GOL	2	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, 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	298/316 (94%)	-0.09	12 (4%) 38 37	11, 29, 75, 102	0
1	B	296/316 (93%)	-0.10	15 (5%) 28 27	13, 31, 66, 85	0
1	C	295/316 (93%)	-0.31	10 (3%) 45 44	11, 28, 66, 103	0
1	D	302/316 (95%)	-0.19	7 (2%) 60 59	12, 27, 63, 87	0
1	E	307/316 (97%)	-0.04	16 (5%) 27 26	13, 30, 76, 92	0
1	F	300/316 (94%)	-0.05	14 (4%) 31 30	12, 34, 74, 96	0
1	G	279/316 (88%)	0.27	39 (13%) 2 2	10, 30, 100, 110	0
1	H	292/316 (92%)	-0.19	9 (3%) 49 48	14, 30, 70, 88	0
All	All	2369/2528 (93%)	-0.09	122 (5%) 28 27	10, 30, 75, 110	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	6.7
1	G	215	ASP	6.4
1	G	28	SER	5.8
1	A	211	VAL	5.8
1	G	25	CYS	5.6
1	G	27	VAL	5.6
1	G	47	ILE	5.1
1	G	45	VAL	5.1
1	G	34	VAL	5.0
1	G	44	GLY	5.0
1	G	214	GLY	5.0
1	G	26	HIS	5.0
1	G	31	THR	4.9
1	G	60	VAL	4.9
1	G	213	LYS	4.9
1	H	86	LYS	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	213	LYS	4.8
1	H	53	SER	4.8
1	G	21	ALA	4.7
1	G	61	GLY	4.5
1	G	24	ARG	4.4
1	G	33	SER	4.4
1	E	213	LYS	4.4
1	C	54	ALA	4.2
1	C	53	SER	4.2
1	E	216	GLU	4.2
1	G	29	GLN	4.2
1	H	52	LYS	4.1
1	G	11	THR	4.1
1	C	52	LYS	4.1
1	G	9	ILE	4.1
1	D	300	ARG	3.9
1	A	54	ALA	3.8
1	D	83	GLN	3.8
1	E	59	PRO	3.8
1	G	48	PHE	3.8
1	B	208	CYS	3.7
1	D	210	THR	3.7
1	H	85	GLY	3.7
1	G	35	GLY	3.6
1	D	23	GLU	3.6
1	H	209	PRO	3.6
1	G	12	LEU	3.6
1	F	53	SER	3.6
1	F	30	PRO	3.6
1	G	30	PRO	3.5
1	E	214	GLY	3.5
1	A	50	ARG	3.4
1	G	63	GLY	3.4
1	G	43	LEU	3.3
1	A	215	ASP	3.3
1	E	56	ARG	3.3
1	G	13	ALA	3.3
1	H	82	ALA	3.2
1	H	83	GLN	3.2
1	F	83	GLN	3.2
1	G	41	ASP	3.1
1	C	50	ARG	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	56	ARG	3.1
1	E	55	VAL	3.1
1	B	187	ASN	3.0
1	B	185	LEU	2.9
1	E	211	VAL	2.8
1	G	20	ARG	2.8
1	G	46	LEU	2.8
1	E	37	LYS	2.8
1	E	301	PRO	2.8
1	C	214	GLY	2.8
1	B	186	LEU	2.8
1	B	224	SER	2.8
1	H	187	ASN	2.8
1	G	8	TYR	2.7
1	B	53	SER	2.7
1	G	22	ALA	2.7
1	F	54	ALA	2.6
1	G	23	GLU	2.6
1	A	55	VAL	2.6
1	B	85	GLY	2.6
1	E	46	LEU	2.6
1	E	34	VAL	2.6
1	A	46	LEU	2.5
1	B	84	ALA	2.5
1	E	49	GLU	2.5
1	A	59	PRO	2.4
1	B	209	PRO	2.4
1	E	224	SER	2.4
1	B	30	PRO	2.4
1	F	26	HIS	2.4
1	D	-2	HIS	2.3
1	F	209	PRO	2.3
1	C	213	LYS	2.3
1	F	306	GLN	2.3
1	C	217	ASN	2.3
1	F	34	VAL	2.3
1	B	301	PRO	2.3
1	A	217	ASN	2.3
1	B	86	LYS	2.2
1	F	51	SER	2.2
1	F	85	GLY	2.2
1	F	86	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	84	ALA	2.2
1	G	37	LYS	2.2
1	F	82	ALA	2.2
1	A	23	GLU	2.2
1	C	59	PRO	2.2
1	E	302	GLN	2.2
1	F	22	ALA	2.2
1	B	189	LYS	2.2
1	G	14	GLN	2.1
1	G	65	VAL	2.1
1	G	211	VAL	2.1
1	E	62	GLU	2.1
1	B	83	GLN	2.1
1	B	266	PRO	2.1
1	D	82	ALA	2.1
1	G	32	LEU	2.1
1	G	212	ARG	2.1
1	D	85	GLY	2.1
1	C	294	ARG	2.0
1	F	17	HIS	2.0
1	C	56	ARG	2.0
1	E	17	HIS	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<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(Å <sup>2</sup> )	Q<0.9
3	GOL	E	402	6/6	0.83	0.19	40,51,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	402	6/6	0.84	0.23	39,42,45,48	0
3	GOL	A	404	6/6	0.84	0.13	51,60,64,65	0
3	GOL	G	402	6/6	0.85	0.16	39,41,46,55	0
3	GOL	B	402	6/6	0.85	0.17	39,44,60,64	0
3	GOL	A	403	6/6	0.89	0.22	44,49,51,59	0
3	GOL	C	403	6/6	0.89	0.35	54,58,65,68	0
3	GOL	F	402	6/6	0.90	0.11	30,45,47,49	0
3	GOL	A	402	6/6	0.91	0.14	32,45,46,47	0
3	GOL	B	404	6/6	0.91	0.22	30,59,60,64	0
3	GOL	D	402	6/6	0.92	0.10	28,38,41,43	0
3	GOL	H	403	6/6	0.93	0.12	29,49,55,57	0
3	GOL	D	403	6/6	0.93	0.19	41,51,53,54	0
3	GOL	B	403	6/6	0.94	0.13	37,39,41,44	0
3	GOL	H	402	6/6	0.94	0.15	33,37,50,52	0
2	PEO	C	401	2/2	0.97	0.11	11,11,11,33	0
2	PEO	D	401	2/2	0.98	0.12	15,15,15,22	0
2	PEO	B	401	2/2	0.98	0.10	14,14,14,26	0
2	PEO	H	401	2/2	0.98	0.10	16,16,16,24	0
2	PEO	E	401	2/2	0.99	0.09	8,8,8,26	0
2	PEO	A	401	2/2	0.99	0.09	15,15,15,24	0
2	PEO	G	401	2/2	0.99	0.10	13,13,13,24	0
2	PEO	F	401	2/2	0.99	0.08	20,20,20,20	0

## 6.5 Other polymers

There are no such residues in this entry.