



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2017 – 09:20 PM EST

PDB ID : 5B8A  
Title : Crystal structure of oxidized chimeric EcAhpC1-186-YFSKHN  
Authors : Kamariah, N.; Sek, M.F.; Eisenhaber, B.; Eisenhaber, F.; Gruber, G.  
Deposited on : 2016-06-14  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

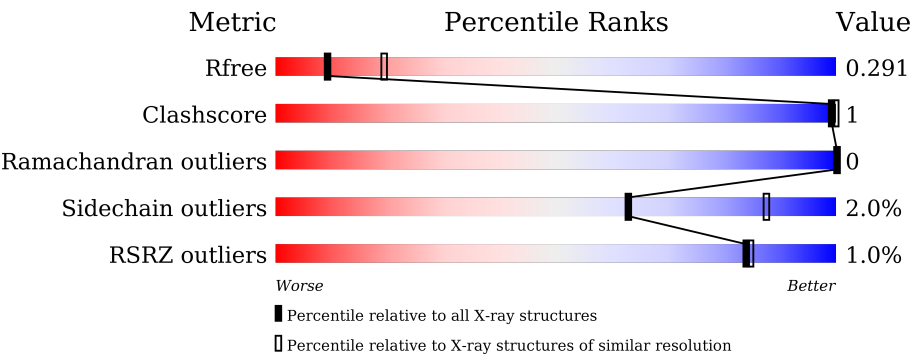
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	192	<div><div></div><div>85%13%</div></div>
1	B	192	<div><div>3%</div><div>85%14%</div></div>
1	C	192	<div><div>%</div><div>82%15%</div></div>
1	D	192	<div><div>%</div><div>80%16%</div></div>
1	E	192	<div><div>%</div><div>83%15%</div></div>
1	F	192	<div><div>%</div><div>84%14%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	192	
1	H	192	
1	I	192	
1	J	192	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	203	-	-	-	X
2	SO4	B	201	-	-	-	X
2	SO4	B	202	-	-	-	X
2	SO4	E	201	-	-	-	X
2	SO4	E	203	-	-	-	X
2	SO4	F	202	-	-	-	X
2	SO4	I	201	-	-	-	X
2	SO4	J	202	-	-	-	X
3	GOL	A	204	-	-	-	X
3	GOL	A	205	-	-	-	X
3	GOL	B	204	-	-	-	X
3	GOL	B	205	-	-	-	X
3	GOL	D	203	-	-	-	X
3	GOL	E	205	-	-	-	X
3	GOL	E	206	-	-	-	X
3	GOL	G	203	-	-	-	X
3	GOL	G	204	-	-	-	X
3	GOL	G	205	-	-	-	X
3	GOL	H	204	-	-	-	X
3	GOL	J	203	-	-	-	X
3	GOL	J	205	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13731 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 Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1320	840	219	256	5			
1	B	166	Total	C	N	O	S	0	0	0
			1308	832	217	254	5			
1	C	163	Total	C	N	O	S	0	0	0
			1286	819	214	249	4			
1	D	162	Total	C	N	O	S	0	0	0
			1282	817	213	248	4			
1	E	164	Total	C	N	O	S	0	0	0
			1295	824	215	252	4			
1	F	165	Total	C	N	O	S	0	0	0
			1302	829	216	253	4			
1	G	171	Total	C	N	O	S	0	0	0
			1352	863	225	259	5			
1	H	177	Total	C	N	O	S	0	0	0
			1394	888	231	270	5			
1	I	162	Total	C	N	O	S	0	0	0
			1282	817	213	248	4			
1	J	170	Total	C	N	O	S	0	0	0
			1343	857	223	258	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



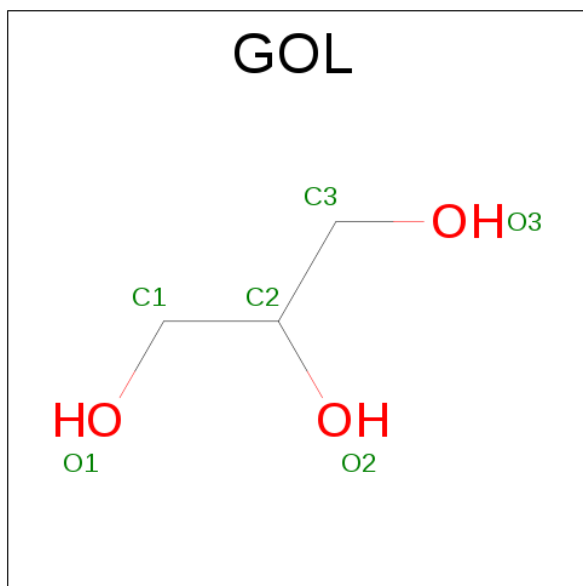
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

- 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	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0
4	B	32	Total 32	O 32	0	0
4	C	29	Total 29	O 29	0	0
4	D	23	Total 23	O 23	0	0
4	E	33	Total 33	O 33	0	0
4	F	40	Total 40	O 40	0	0
4	G	34	Total 34	O 34	0	0
4	H	24	Total 24	O 24	0	0
4	I	32	Total 32	O 32	0	0
4	J	31	Total 31	O 31	0	0

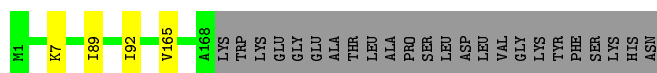


### 3 Residue-property plots [i](#)


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

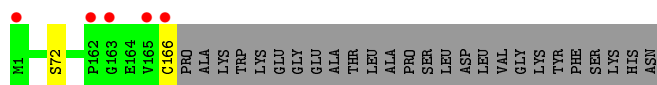
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2

Chain A: 




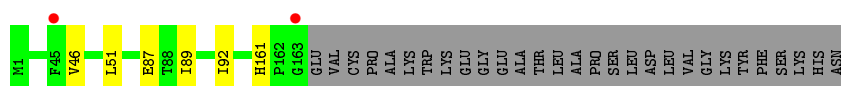
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2

Chain B: 




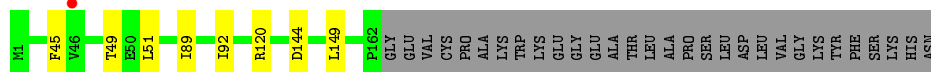
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2

Chain C: 




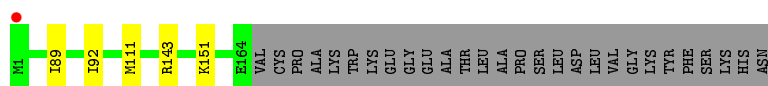
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2

Chain D: 




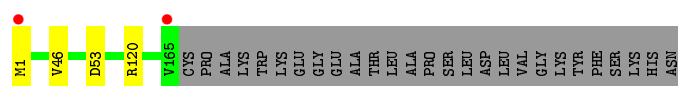
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2

Chain E: 

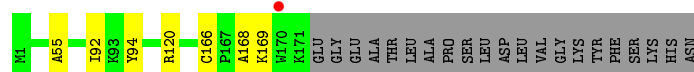
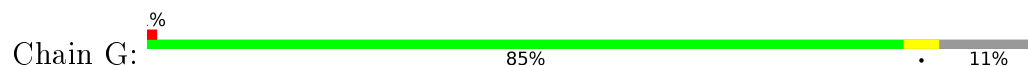


- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2

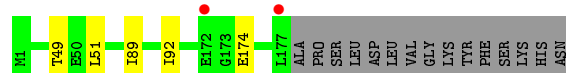
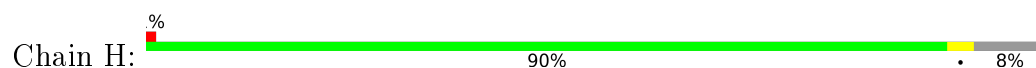
Chain F: 



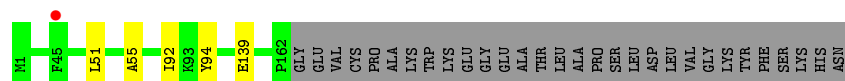
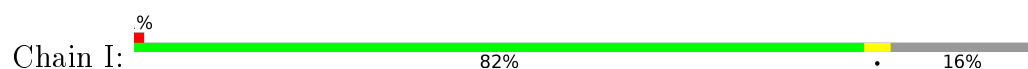
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2



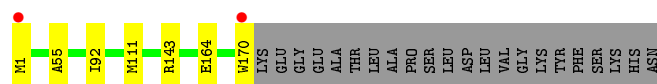
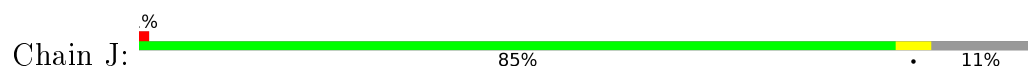
- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2



- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2



- Molecule 1: Alkyl hydroperoxide reductase subunit C,Peroxiredoxin-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.47Å 134.73Å 107.53Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	50.01 – 2.70 29.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.01-2.70) 95.9 (29.32-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.244 , 0.290 0.248 , 0.291	Depositor DCC
$R_{free}$ test set	3356 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 6.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.35	0/1351	0.53	0/1831
1	B	0.34	0/1338	0.51	0/1812
1	C	0.35	0/1316	0.52	0/1782
1	D	0.35	0/1312	0.54	0/1777
1	E	0.34	0/1325	0.54	0/1794
1	F	0.34	0/1332	0.53	0/1804
1	G	0.37	0/1385	0.54	0/1876
1	H	0.34	0/1427	0.52	0/1933
1	I	0.35	0/1312	0.55	0/1777
1	J	0.35	0/1376	0.55	0/1865
All	All	0.35	0/13474	0.53	0/18251

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	168	ALA	Peptide

## 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	1320	0	1274	1	0
1	B	1308	0	1262	0	0
1	C	1286	0	1244	2	0
1	D	1282	0	1241	3	0
1	E	1295	0	1249	1	0
1	F	1302	0	1258	1	0
1	G	1352	0	1311	2	0
1	H	1394	0	1349	2	0
1	I	1282	0	1240	2	0
1	J	1343	0	1298	1	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	20	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	D	18	0	24	1	0
3	E	18	0	24	0	0
3	F	6	0	8	0	0
3	G	18	0	24	0	0
3	H	12	0	16	0	0
3	J	36	0	48	0	0
4	A	42	0	0	0	0
4	B	32	0	0	0	0
4	C	29	0	0	0	0
4	D	23	0	0	0	0
4	E	33	0	0	0	0
4	F	40	0	0	0	0
4	G	34	0	0	0	0
4	H	24	0	0	0	0
4	I	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	31	0	0	0	0
All	All	13731	0	12902	15	0

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 1.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ILE:HG23	1:C:92:ILE:HD12	1.93	0.51
1:D:51:LEU:HB3	1:D:92:ILE:HD11	1.93	0.50
1:J:55:ALA:HB2	1:J:92:ILE:HG22	1.94	0.48
1:G:92:ILE:HD12	1:G:94:TYR:CZ	2.48	0.48
1:G:55:ALA:HB2	1:G:92:ILE:HD13	1.96	0.47
1:I:92:ILE:HD12	1:I:94:TYR:CZ	2.49	0.47
1:H:51:LEU:HB3	1:H:92:ILE:HD11	1.97	0.46
1:E:89:ILE:HG23	1:E:92:ILE:HD12	1.99	0.45
1:H:89:ILE:HG23	1:H:92:ILE:HD12	1.99	0.44
1:C:51:LEU:HB3	1:C:92:ILE:HD11	1.99	0.44
1:I:55:ALA:HB2	1:I:92:ILE:HD13	2.01	0.42
1:A:89:ILE:HG23	1:A:92:ILE:HD12	2.01	0.42
1:F:46:VAL:HG11	1:F:120:ARG:NH2	2.34	0.42
1:D:89:ILE:HG23	1:D:92:ILE:HD12	2.02	0.41
1:D:120:ARG:NH2	3:D:205:GOL:O2	2.53	0.40

There are no symmetry-related clashes.

## 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	166/192 (86%)	161 (97%)	5 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	164/192 (85%)	160 (98%)	4 (2%)	0	100	100
1	C	161/192 (84%)	156 (97%)	5 (3%)	0	100	100
1	D	160/192 (83%)	156 (98%)	4 (2%)	0	100	100
1	E	162/192 (84%)	159 (98%)	3 (2%)	0	100	100
1	F	163/192 (85%)	158 (97%)	5 (3%)	0	100	100
1	G	169/192 (88%)	165 (98%)	4 (2%)	0	100	100
1	H	175/192 (91%)	168 (96%)	7 (4%)	0	100	100
1	I	160/192 (83%)	156 (98%)	4 (2%)	0	100	100
1	J	168/192 (88%)	164 (98%)	4 (2%)	0	100	100
All	All	1648/1920 (86%)	1603 (97%)	45 (3%)	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	140/160 (88%)	138 (99%)	2 (1%)	74	92
1	B	139/160 (87%)	137 (99%)	2 (1%)	74	92
1	C	136/160 (85%)	133 (98%)	3 (2%)	60	86
1	D	136/160 (85%)	132 (97%)	4 (3%)	50	80
1	E	137/160 (86%)	134 (98%)	3 (2%)	60	86
1	F	138/160 (86%)	136 (99%)	2 (1%)	74	92
1	G	143/160 (89%)	140 (98%)	3 (2%)	61	87
1	H	147/160 (92%)	145 (99%)	2 (1%)	74	92
1	I	136/160 (85%)	134 (98%)	2 (2%)	72	91
1	J	142/160 (89%)	137 (96%)	5 (4%)	43	74
All	All	1394/1600 (87%)	1366 (98%)	28 (2%)	63	87

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	165	VAL
1	B	72	SER
1	B	166	CYS
1	C	46	VAL
1	C	87	GLU
1	C	161	HIS
1	D	45	PHE
1	D	49	THR
1	D	144	ASP
1	D	149	LEU
1	E	111	MET
1	E	143	ARG
1	E	151	LYS
1	F	1	MET
1	F	53	ASP
1	G	120	ARG
1	G	166	CYS
1	G	169	LYS
1	H	49	THR
1	H	174	GLU
1	I	51	LEU
1	I	139	GLU
1	J	1	MET
1	J	111	MET
1	J	143	ARG
1	J	164	GLU
1	J	170	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

45 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	SO4	A	201	-	4,4,4	0.35	0	6,6,6	0.13	0
2	SO4	A	202	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	A	203	-	4,4,4	0.33	0	6,6,6	0.07	0
3	GOL	A	204	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	A	205	-	5,5,5	0.31	0	5,5,5	0.26	0
2	SO4	B	201	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	B	202	-	4,4,4	0.31	0	6,6,6	0.15	0
2	SO4	B	203	-	4,4,4	0.36	0	6,6,6	0.21	0
3	GOL	B	204	-	5,5,5	0.25	0	5,5,5	0.20	0
3	GOL	B	205	-	5,5,5	0.31	0	5,5,5	0.19	0
2	SO4	C	201	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	D	201	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	D	202	-	4,4,4	0.35	0	6,6,6	0.06	0
3	GOL	D	203	-	5,5,5	0.41	0	5,5,5	0.32	0
3	GOL	D	204	-	5,5,5	0.25	0	5,5,5	0.20	0
3	GOL	D	205	-	5,5,5	0.24	0	5,5,5	0.29	0
2	SO4	E	201	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	E	202	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	E	203	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	E	204	-	4,4,4	0.35	0	6,6,6	0.07	0
3	GOL	E	205	-	5,5,5	0.27	0	5,5,5	0.14	0
3	GOL	E	206	-	5,5,5	0.19	0	5,5,5	0.18	0
3	GOL	E	207	-	5,5,5	0.29	0	5,5,5	0.26	0
2	SO4	F	201	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	F	202	-	4,4,4	0.34	0	6,6,6	0.06	0
3	GOL	F	203	-	5,5,5	0.28	0	5,5,5	0.16	0
2	SO4	G	201	-	4,4,4	0.33	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	G	202	-	4,4,4	0.34	0	6,6,6	0.07	0
3	GOL	G	203	-	5,5,5	0.31	0	5,5,5	0.32	0
3	GOL	G	204	-	5,5,5	0.23	0	5,5,5	0.16	0
3	GOL	G	205	-	5,5,5	0.29	0	5,5,5	0.34	0
2	SO4	H	201	-	4,4,4	0.32	0	6,6,6	0.06	0
2	SO4	H	202	-	4,4,4	0.34	0	6,6,6	0.06	0
3	GOL	H	203	-	5,5,5	0.25	0	5,5,5	0.12	0
3	GOL	H	204	-	5,5,5	0.28	0	5,5,5	0.37	0
2	SO4	I	201	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	I	202	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	J	201	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	J	202	-	4,4,4	0.34	0	6,6,6	0.06	0
3	GOL	J	203	-	5,5,5	0.27	0	5,5,5	0.28	0
3	GOL	J	204	-	5,5,5	0.28	0	5,5,5	0.18	0
3	GOL	J	205	-	5,5,5	0.27	0	5,5,5	0.15	0
3	GOL	J	206	-	5,5,5	0.26	0	5,5,5	0.18	0
3	GOL	J	207	-	5,5,5	0.26	0	5,5,5	0.20	0
3	GOL	J	208	-	5,5,5	0.30	0	5,5,5	0.25	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
2	SO4	A	201	-	-	0/0/0/0	0/0/0/0
2	SO4	A	202	-	-	0/0/0/0	0/0/0/0
2	SO4	A	203	-	-	0/0/0/0	0/0/0/0
3	GOL	A	204	-	-	0/4/4/4	0/0/0/0
3	GOL	A	205	-	-	0/4/4/4	0/0/0/0
2	SO4	B	201	-	-	0/0/0/0	0/0/0/0
2	SO4	B	202	-	-	0/0/0/0	0/0/0/0
2	SO4	B	203	-	-	0/0/0/0	0/0/0/0
3	GOL	B	204	-	-	0/4/4/4	0/0/0/0
3	GOL	B	205	-	-	0/4/4/4	0/0/0/0
2	SO4	C	201	-	-	0/0/0/0	0/0/0/0
2	SO4	D	201	-	-	0/0/0/0	0/0/0/0
2	SO4	D	202	-	-	0/0/0/0	0/0/0/0
3	GOL	D	203	-	-	0/4/4/4	0/0/0/0
3	GOL	D	204	-	-	0/4/4/4	0/0/0/0
3	GOL	D	205	-	-	0/4/4/4	0/0/0/0
2	SO4	E	201	-	-	0/0/0/0	0/0/0/0
2	SO4	E	202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	203	-	-	0/0/0/0	0/0/0/0
2	SO4	E	204	-	-	0/0/0/0	0/0/0/0
3	GOL	E	205	-	-	0/4/4/4	0/0/0/0
3	GOL	E	206	-	-	0/4/4/4	0/0/0/0
3	GOL	E	207	-	-	0/4/4/4	0/0/0/0
2	SO4	F	201	-	-	0/0/0/0	0/0/0/0
2	SO4	F	202	-	-	0/0/0/0	0/0/0/0
3	GOL	F	203	-	-	0/4/4/4	0/0/0/0
2	SO4	G	201	-	-	0/0/0/0	0/0/0/0
2	SO4	G	202	-	-	0/0/0/0	0/0/0/0
3	GOL	G	203	-	-	0/4/4/4	0/0/0/0
3	GOL	G	204	-	-	0/4/4/4	0/0/0/0
3	GOL	G	205	-	-	0/4/4/4	0/0/0/0
2	SO4	H	201	-	-	0/0/0/0	0/0/0/0
2	SO4	H	202	-	-	0/0/0/0	0/0/0/0
3	GOL	H	203	-	-	0/4/4/4	0/0/0/0
3	GOL	H	204	-	-	0/4/4/4	0/0/0/0
2	SO4	I	201	-	-	0/0/0/0	0/0/0/0
2	SO4	I	202	-	-	0/0/0/0	0/0/0/0
2	SO4	J	201	-	-	0/0/0/0	0/0/0/0
2	SO4	J	202	-	-	0/0/0/0	0/0/0/0
3	GOL	J	203	-	-	0/4/4/4	0/0/0/0
3	GOL	J	204	-	-	0/4/4/4	0/0/0/0
3	GOL	J	205	-	-	0/4/4/4	0/0/0/0
3	GOL	J	206	-	-	0/4/4/4	0/0/0/0
3	GOL	J	207	-	-	0/4/4/4	0/0/0/0
3	GOL	J	208	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	205	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	168/192 (87%)	-0.00	0	100	100	23, 31, 41, 52	0
1	B	166/192 (86%)	-0.03	5 (3%)	54	54	20, 29, 40, 62	0
1	C	163/192 (84%)	0.17	2 (1%)	81	81	25, 35, 47, 59	0
1	D	162/192 (84%)	0.15	1 (0%)	90	91	22, 34, 49, 60	0
1	E	164/192 (85%)	-0.05	1 (0%)	90	91	19, 27, 36, 46	0
1	F	165/192 (85%)	-0.08	2 (1%)	81	81	20, 27, 36, 46	0
1	G	171/192 (89%)	-0.07	1 (0%)	90	91	20, 28, 39, 68	0
1	H	177/192 (92%)	0.05	2 (1%)	82	83	23, 30, 47, 63	0
1	I	162/192 (84%)	-0.01	1 (0%)	90	91	21, 30, 38, 47	0
1	J	170/192 (88%)	-0.08	2 (1%)	81	81	21, 29, 40, 57	0
All	All	1668/1920 (86%)	0.00	17 (1%)	84	85	19, 29, 43, 68	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	VAL	4.5
1	J	170	TRP	3.9
1	C	163	GLY	3.4
1	B	162	PRO	3.1
1	B	163	GLY	3.1
1	B	166	CYS	3.0
1	D	46	VAL	2.9
1	H	172	GLU	2.7
1	H	177	LEU	2.6
1	C	45	PHE	2.5
1	F	1	MET	2.5
1	G	170	TRP	2.4
1	J	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	165	VAL	2.1
1	B	1	MET	2.1
1	E	1	MET	2.1
1	I	45	PHE	2.1

## 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	E	206	6/6	0.76	0.38	6.90	32,32,32,32	0
2	SO4	B	202	5/5	0.95	0.29	6.81	45,46,46,46	0
3	GOL	J	203	6/6	0.87	0.32	6.14	36,36,36,37	0
3	GOL	J	205	6/6	0.76	0.34	6.06	46,46,46,47	0
3	GOL	G	203	6/6	0.81	0.31	5.32	35,35,36,36	0
3	GOL	B	205	6/6	0.81	0.37	5.06	36,36,36,36	0
2	SO4	E	201	5/5	0.93	0.25	5.04	53,53,53,54	0
2	SO4	F	202	5/5	0.94	0.28	4.10	64,65,65,65	0
3	GOL	H	204	6/6	0.83	0.29	4.05	29,30,30,30	0
2	SO4	B	201	5/5	0.94	0.25	3.99	69,69,69,70	0
2	SO4	J	202	5/5	0.84	0.29	3.67	70,70,71,71	0
3	GOL	G	204	6/6	0.87	0.33	3.54	30,30,30,30	0
2	SO4	E	203	5/5	0.95	0.30	3.50	61,61,62,62	0
2	SO4	A	203	5/5	0.85	0.31	3.19	78,78,79,79	0
2	SO4	I	201	5/5	0.93	0.26	2.98	49,49,49,50	0
3	GOL	D	203	6/6	0.75	0.27	2.71	31,31,31,31	0
3	GOL	B	204	6/6	0.93	0.22	2.49	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	204	6/6	0.89	0.25	2.36	28,28,29,29	0
3	GOL	A	205	6/6	0.87	0.24	2.34	29,29,29,29	0
3	GOL	G	205	6/6	0.91	0.27	2.34	31,31,31,31	0
3	GOL	E	205	6/6	0.88	0.22	2.32	27,27,28,28	0
3	GOL	J	208	6/6	0.84	0.25	1.84	40,40,40,40	0
3	GOL	J	207	6/6	0.89	0.20	1.24	34,34,34,34	0
3	GOL	J	204	6/6	0.88	0.26	1.14	34,34,34,35	0
3	GOL	D	205	6/6	0.78	0.26	0.92	29,29,29,30	0
3	GOL	J	206	6/6	0.82	0.26	0.90	39,40,40,40	0
2	SO4	H	202	5/5	0.94	0.25	0.87	49,49,49,49	0
3	GOL	E	207	6/6	0.79	0.24	0.55	31,31,31,31	0
2	SO4	A	201	5/5	0.91	0.20	0.20	44,45,45,45	0
2	SO4	C	201	5/5	0.82	0.21	-0.26	73,73,74,74	0
3	GOL	D	204	6/6	0.77	0.24	-0.27	40,40,41,41	0
2	SO4	E	202	5/5	0.85	0.18	-0.30	58,58,59,59	0
3	GOL	H	203	6/6	0.86	0.17	-0.30	36,36,36,36	0
2	SO4	F	201	5/5	0.95	0.16	-0.65	42,42,43,43	0
2	SO4	D	201	5/5	0.94	0.16	-0.84	70,70,71,71	0
2	SO4	B	203	5/5	0.89	0.31	-	48,48,49,49	0
2	SO4	G	202	5/5	0.93	0.29	-	61,62,62,63	0
2	SO4	I	202	5/5	0.85	0.22	-	89,89,89,89	0
2	SO4	A	202	5/5	0.93	0.22	-	70,71,72,72	0
2	SO4	J	201	5/5	0.93	0.18	-	60,60,61,61	0
3	GOL	F	203	6/6	0.86	0.25	-	43,43,43,43	0
2	SO4	G	201	5/5	0.96	0.19	-	50,51,51,51	0
2	SO4	E	204	5/5	0.82	0.48	-	86,86,86,87	0
2	SO4	H	201	5/5	0.95	0.14	-	55,55,56,56	0
2	SO4	D	202	5/5	0.87	0.25	-	68,68,69,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.