



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 09:59 am BST

PDB ID : 5FSE  
Title : 2.07 Å resolution 1,4-Benzoquinone inhibited *Sporosarcina pasteurii* urease  
Authors : Mazzei, L.; Cianci, M.; Musiani, F.; Ciurli, S.  
Deposited on : 2016-01-04  
Resolution : 2.07 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

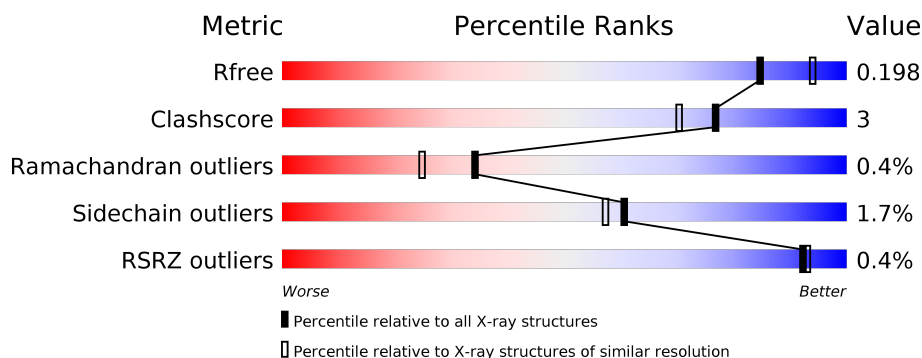
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	100	 93% 7%
2	B	126	 89% 8% 3% 2%
3	C	570	 91% 8% 1%

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
4	EDO	C	1573	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6799 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 UREASE SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	6	0
			824	519	140	158	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	LEU	conflict	UNP P41022
A	22	LYS	ARG	conflict	UNP P41022

- Molecule 2 is a protein called UREASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	2	0
			969	599	174	195	1			

- Molecule 3 is a protein called UREASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	570	Total	C	N	O	S	0	16	0
			4438	2785	763	864	26			

There are 10 discrepancies between the modelled and reference sequences:

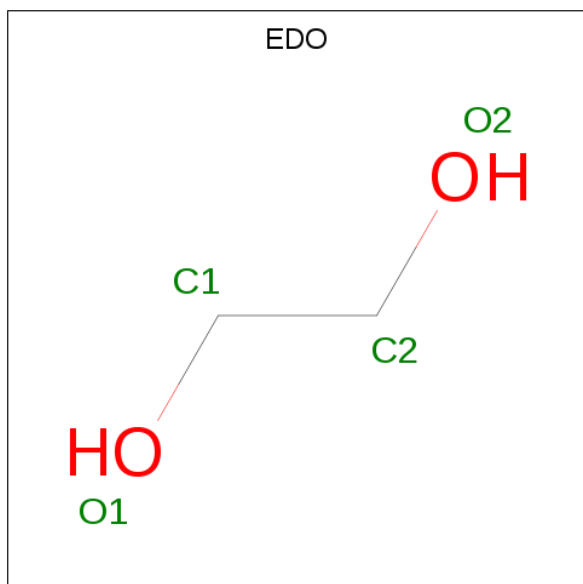
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	GLN	ARG	conflict	UNP P41020
C	28	TRP	GLY	conflict	UNP P41020
C	29	ILE	-	insertion	UNP P41020
C	36	THR	TYR	conflict	UNP P41020
C	37	THR	TYR	conflict	UNP P41020
C	38	TYR	LEU	conflict	UNP P41020
C	42	ALA	VAL	conflict	UNP P41020
C	263	LEU	VAL	conflict	UNP P41020

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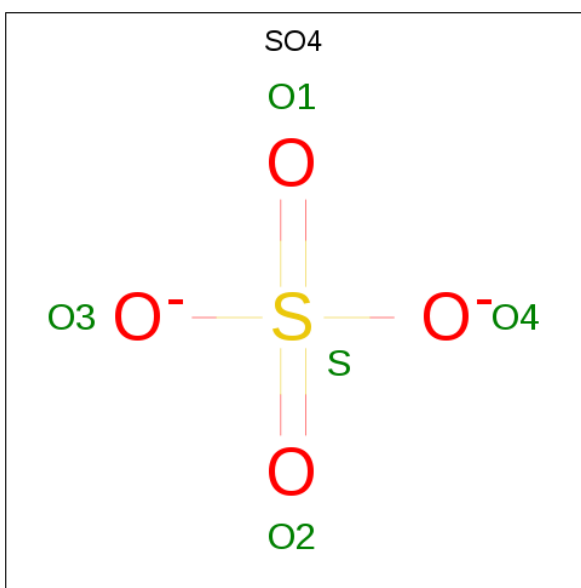
Chain	Residue	Modelled	Actual	Comment	Reference
C	403	ALA	LEU	conflict	UNP P41020
C	420	ILE	MET	conflict	UNP P41020

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

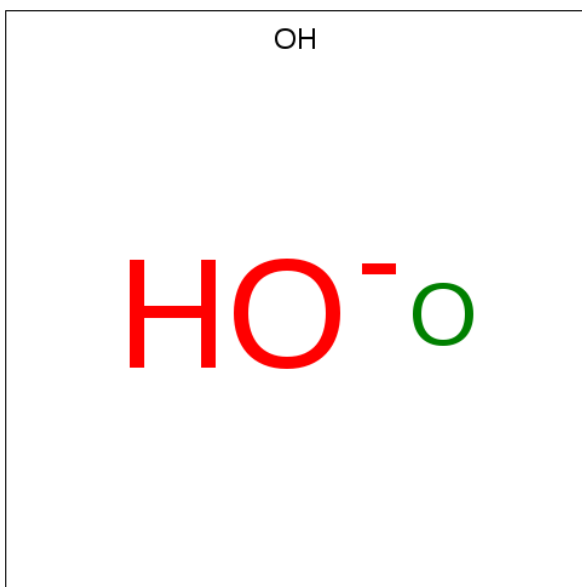


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

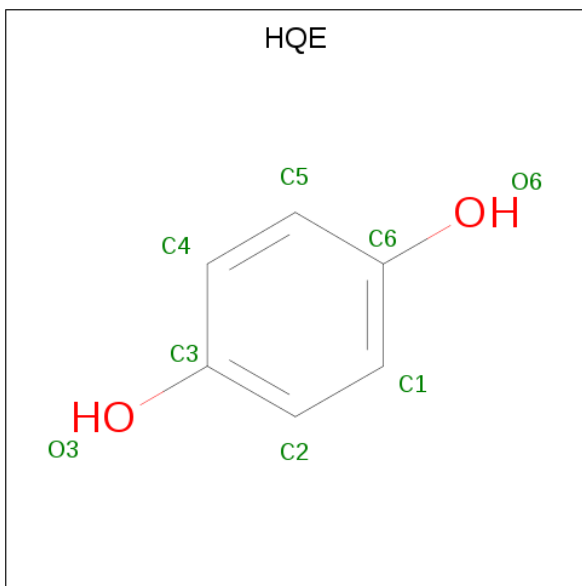
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Ni	0	0
			2	2		

- Molecule 7 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O		0	0
			1	1			

- Molecule 8 is benzene-1,4-diol (three-letter code: HQE) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			8	6	2		
8	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is water.

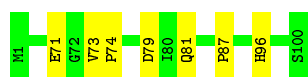
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	70	Total 70	O 70	0	0
9	B	93	Total 93	O 93	0	0
9	C	301	Total 301	O 301	0	0

### 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 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: UREASE SUBUNIT GAMMA

Chain A: 



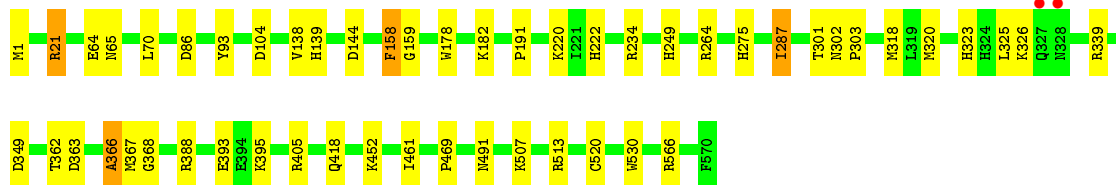
#### • Molecule 2: UREASE SUBUNIT BETA

Chain B: 



#### • Molecule 3: UREASE SUBUNIT ALPHA

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.83Å 131.83Å 188.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.17 – 2.07 114.17 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.4 (114.17-2.07) 98.4 (114.17-2.07)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.145 , 0.192 0.158 , 0.198	Depositor DCC
$R_{free}$ test set	2944 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6799	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 2.67% 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: NI, OH, EDO, KCX, SO4, HQE, CXM

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	0.86	0/831	0.90	0/1117
2	B	0.85	1/981 (0.1%)	0.94	1/1320 (0.1%)
3	C	0.83	2/4519 (0.0%)	0.94	14/6121 (0.2%)
All	All	0.84	3/6331 (0.0%)	0.93	15/8558 (0.2%)

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
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	520	CYS	CB-SG	-6.22	1.71	1.82
2	B	33	SER	CB-OG	-5.78	1.34	1.42
3	C	530	TRP	CB-CG	-5.10	1.41	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	566	ARG	NE-CZ-NH2	-8.05	116.27	120.30
3	C	388	ARG	NE-CZ-NH1	7.91	124.25	120.30
3	C	405	ARG	NE-CZ-NH2	-7.00	116.80	120.30
3	C	520	CYS	CB-CA-C	-6.46	97.49	110.40
3	C	339	ARG	NE-CZ-NH2	-6.31	117.14	120.30
3	C	234	ARG	CG-CD-NE	-5.96	99.28	111.80
3	C	21	ARG	NE-CZ-NH1	5.87	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	349	ASP	CB-CG-OD1	5.81	123.53	118.30
3	C	566	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	B	37	ASP	CB-CG-OD1	5.46	123.22	118.30
3	C	339	ARG	NE-CZ-NH1	5.37	122.99	120.30
3	C	318	MET	CG-SD-CE	5.32	108.72	100.20
3	C	21	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	C	144	ASP	CB-CG-OD2	5.16	122.94	118.30
3	C	264	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	366[A]	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	824	0	840	3	0
2	B	969	0	949	4	0
3	C	4438	0	4407	32	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	32	0	48	7	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	C	35	0	0	1	0
6	C	2	0	0	0	0
7	C	1	0	0	0	0
8	C	16	0	8	1	0
9	A	70	0	0	0	0
9	B	93	0	0	1	0
9	C	301	0	0	3	1
All	All	6799	0	6264	38	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 3.

All (38) 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)
3:C:64[B]:GLU:HG2	4:C:1573:EDO:H11	1.68	0.75
3:C:64[B]:GLU:HG2	4:C:1573:EDO:C1	2.18	0.74
3:C:507[A]:LYS:HD3	9:C:2250:HOH:O	1.93	0.69
3:C:93:TYR:OH	4:C:1578:EDO:H12	1.92	0.69
3:C:452[B]:LYS:HE2	3:C:491:ASN:OD1	1.94	0.67
1:A:79[B]:ASP:OD2	1:A:96[B]:HIS:ND1	2.28	0.67
3:C:287[A]:ILE:HD13	3:C:287[A]:ILE:O	1.99	0.61
3:C:452[B]:LYS:NZ	9:C:2230:HOH:O	2.33	0.61
1:A:71:GLU:N	5:A:1102:SO4:O3	2.28	0.58
3:C:323:HIS:NE2	5:C:1579:SO4:O4	2.37	0.58
3:C:301:THR:CG2	3:C:363:ASP:HB2	2.36	0.55
3:C:191:PRO:O	3:C:452[B]:LYS:HE3	2.09	0.53
3:C:64[B]:GLU:HG2	4:C:1573:EDO:H12	1.88	0.52
3:C:220:KCX:CX	3:C:222:HIS:HD2	2.24	0.49
8:C:1584:HQE:H5	9:C:2110:HOH:O	2.12	0.49
3:C:303:PRO:HG3	3:C:368:GLY:HA2	1.93	0.49
3:C:64[B]:GLU:CG	4:C:1573:EDO:H11	2.40	0.49
3:C:513:ARG:HD3	4:C:1578:EDO:H11	1.97	0.47
3:C:301:THR:HG21	3:C:363:ASP:HB2	1.95	0.47
3:C:158:PHE:CE2	3:C:418[A]:GLN:CG	2.98	0.47
3:C:139:HIS:CD2	3:C:366[B]:ALA:HB2	2.51	0.46
3:C:70:LEU:HD11	3:C:86:ASP:HB3	1.98	0.45
3:C:64[A]:GLU:O	3:C:65:ASN:HB2	2.16	0.45
3:C:138:VAL:O	3:C:159:GLY:HA3	2.15	0.45
3:C:513:ARG:HD3	4:C:1578:EDO:C1	2.46	0.45
2:B:111[B]:GLU:HG2	9:B:2086:HOH:O	2.17	0.43
3:C:287[A]:ILE:HD13	3:C:287[A]:ILE:C	2.38	0.43
3:C:362:THR:O	3:C:368:GLY:HA3	2.18	0.43
3:C:178:TRP:O	3:C:182:LYS:HG2	2.19	0.42
3:C:302:ASN:N	3:C:303:PRO:CD	2.82	0.42
3:C:320:MET:HA	3:C:325:LEU:HD12	2.02	0.42
3:C:320:MET:HA	3:C:325:LEU:HB2	2.03	0.41
1:A:73:VAL:N	1:A:74:PRO:CD	2.84	0.41
2:B:10:GLY:HA2	3:C:21:ARG:O	2.21	0.40
3:C:220:KCX:CX	3:C:222:HIS:CD2	3.04	0.40
3:C:461:ILE:HD11	3:C:469:PRO:HB3	2.04	0.40
2:B:118:LYS:HB2	2:B:125:VAL:HG11	2.03	0.40
2:B:95:GLU:O	3:C:104:ASP:HB3	2.21	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)
9:C:2051:HOH:O	9:C:2051:HOH:O[11_555]	1.92	0.28

## 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	104/100 (104%)	104 (100%)	0	0	100	100
2	B	122/126 (97%)	117 (96%)	4 (3%)	1 (1%)	19	9
3	C	583/570 (102%)	562 (96%)	19 (3%)	2 (0%)	41	32
All	All	809/796 (102%)	783 (97%)	23 (3%)	3 (0%)	34	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	367	MET
2	B	99	ILE
3	C	275	HIS

### 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	89/83 (107%)	86 (97%)	3 (3%)	37	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	103/105 (98%)	101 (98%)	2 (2%)	57	53
3	C	473/458 (103%)	464 (98%)	9 (2%)	57	53
All	All	665/646 (103%)	651 (98%)	14 (2%)	60	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81[A]	GLN
1	A	81[B]	GLN
1	A	87	PRO
2	B	18	GLU
2	B	110	LYS
3	C	1	MET
3	C	158	PHE
3	C	249	HIS
3	C	287[A]	ILE
3	C	287[B]	ILE
3	C	326	LYS
3	C	393[A]	GLU
3	C	393[B]	GLU
3	C	395	LYS

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 ⓘ

2 non-standard protein/DNA/RNA residues 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
3	KCX	C	220	3,6	7,11,12	0.85	0	4,12,14	1.06	0
1	CXM	A	1	1	6,10,11	0.61	0	5,11,13	1.09	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	KCX	C	220	3,6	-	0/7/10/12	-
1	CXM	A	1	1	-	0/7/10/12	-

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	220	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	1128	-	4,4,4	0.40	0	6,6,6	0.48	0
4	EDO	C	1576	-	3,3,3	0.43	0	2,2,2	0.74	0
5	SO4	C	1588	-	4,4,4	0.41	0	6,6,6	0.28	0
4	EDO	C	1571	-	3,3,3	0.37	0	2,2,2	0.49	0
4	EDO	A	1101	-	3,3,3	0.35	0	2,2,2	0.40	0
5	SO4	C	1581	-	4,4,4	0.48	0	6,6,6	0.57	0
8	HQE	C	1584	3	8,8,8	2.45	1 (12%)	10,10,10	1.30	1 (10%)
5	SO4	C	1587	-	4,4,4	0.53	0	6,6,6	0.71	0
5	SO4	C	1585	-	4,4,4	0.60	0	6,6,6	0.42	0
5	SO4	C	1582	-	4,4,4	0.56	0	6,6,6	0.90	0
4	EDO	B	1127	-	3,3,3	0.91	0	2,2,2	0.31	0
5	SO4	C	1586	-	4,4,4	0.40	0	6,6,6	0.47	0
4	EDO	C	1574	-	3,3,3	0.38	0	2,2,2	1.30	0
5	SO4	C	1579	-	4,4,4	0.80	0	6,6,6	0.59	0
4	EDO	C	1578	-	3,3,3	0.90	0	2,2,2	0.10	0
4	EDO	C	1573	-	3,3,3	0.32	0	2,2,2	0.54	0
8	HQE	C	1583	3	8,8,8	2.66	3 (37%)	10,10,10	1.22	1 (10%)
4	EDO	C	1572	-	3,3,3	0.38	0	2,2,2	0.60	0
4	EDO	C	1577	-	3,3,3	0.47	0	2,2,2	0.63	0
5	SO4	A	1102	-	4,4,4	0.61	0	6,6,6	0.55	0
4	EDO	C	1575	-	3,3,3	0.32	0	2,2,2	0.43	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
8	HQE	C	1583	3	-	-	0/1/1/1
4	EDO	C	1571	-	-	0/1/1/1	-
4	EDO	A	1101	-	-	0/1/1/1	-
4	EDO	C	1578	-	-	0/1/1/1	-
4	EDO	C	1575	-	-	0/1/1/1	-
4	EDO	B	1127	-	-	1/1/1/1	-
4	EDO	C	1574	-	-	1/1/1/1	-
4	EDO	C	1573	-	-	0/1/1/1	-
4	EDO	C	1572	-	-	1/1/1/1	-
4	EDO	C	1577	-	-	1/1/1/1	-
8	HQE	C	1584	3	-	-	0/1/1/1
4	EDO	C	1576	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1583	HQE	C5-C6	6.60	1.51	1.38
8	C	1584	HQE	C2-C3	6.25	1.50	1.38
8	C	1583	HQE	C2-C3	2.34	1.43	1.38
8	C	1583	HQE	C4-C3	2.19	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1584	HQE	C2-C1-C6	2.29	122.38	119.88
8	C	1583	HQE	C4-C5-C6	-2.12	117.55	119.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1574	EDO	O1-C1-C2-O2
4	C	1572	EDO	O1-C1-C2-O2
4	C	1577	EDO	O1-C1-C2-O2
4	B	1127	EDO	O1-C1-C2-O2
4	C	1576	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1584	HQE	1	0
5	C	1579	SO4	1	0
4	C	1578	EDO	3	0
4	C	1573	EDO	4	0
5	A	1102	SO4	1	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	99/100 (99%)	-0.57	0	100   100	21, 27, 36, 61	0
2	B	122/126 (96%)	-0.52	1 (0%)	86   87	23, 29, 45, 81	0
3	C	569/570 (99%)	-0.53	2 (0%)	92   93	20, 26, 49, 78	1 (0%)
All	All	790/796 (99%)	-0.54	3 (0%)	92   93	20, 27, 48, 81	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	327	GLN	3.2
2	B	126	GLU	2.8
3	C	328	ASN	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains

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	KCX	C	220	12/13	0.97	0.10	21,23,27,28	0
1	CXM	A	1	11/12	0.98	0.09	26,31,36,41	0

### 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. 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
5	SO4	C	1581	5/5	0.69	0.29	66,94,101,106	0
5	SO4	A	1102	5/5	0.78	0.22	85,91,94,107	0
4	EDO	C	1572	4/4	0.82	0.33	54,56,58,63	0
5	SO4	C	1582	5/5	0.84	0.21	73,77,78,81	0
4	EDO	C	1577	4/4	0.86	0.21	63,63,65,65	0
8	HQE	C	1584	8/8	0.86	0.20	54,67,71,75	0
5	SO4	C	1586	5/5	0.87	0.24	85,101,112,118	0
4	EDO	C	1578	4/4	0.88	0.14	43,43,43,49	0
4	EDO	B	1127	4/4	0.88	0.20	43,48,49,57	0
5	SO4	C	1579	5/5	0.90	0.18	63,68,79,95	0
5	SO4	C	1587	5/5	0.91	0.34	71,86,93,94	0
4	EDO	C	1573	4/4	0.91	0.18	46,48,48,49	0
5	SO4	B	1128	5/5	0.92	0.14	71,79,82,85	0
4	EDO	C	1574	4/4	0.93	0.13	41,42,42,48	0
4	EDO	C	1576	4/4	0.93	0.13	42,48,50,52	0
5	SO4	C	1588	5/5	0.94	0.23	83,84,93,108	0
5	SO4	C	1585	5/5	0.95	0.16	54,55,68,75	0
8	HQE	C	1583	8/8	0.96	0.17	38,40,43,44	0
4	EDO	C	1571	4/4	0.97	0.16	38,43,44,49	0
4	EDO	C	1575	4/4	0.97	0.09	41,41,43,43	0
4	EDO	A	1101	4/4	0.98	0.08	30,33,33,34	0
7	OH	C	1580	1/1	1.00	0.07	31,31,31,31	0
6	NI	C	600	1/1	1.00	0.10	35,35,35,35	0
6	NI	C	601	1/1	1.00	0.09	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.