W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 06:48 PM EDT

PDB ID	:	6WAG
Title	:	Crystal Structure of SmcR S76A from Vibrio Vulnificus
Authors	:	Newman, J.D.; Russell, M.M.; Gonzalez-Gutierrez, G.; van Kessel, J.C.
Deposited on	:	2020-03-25
Resolution	:	2.58 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

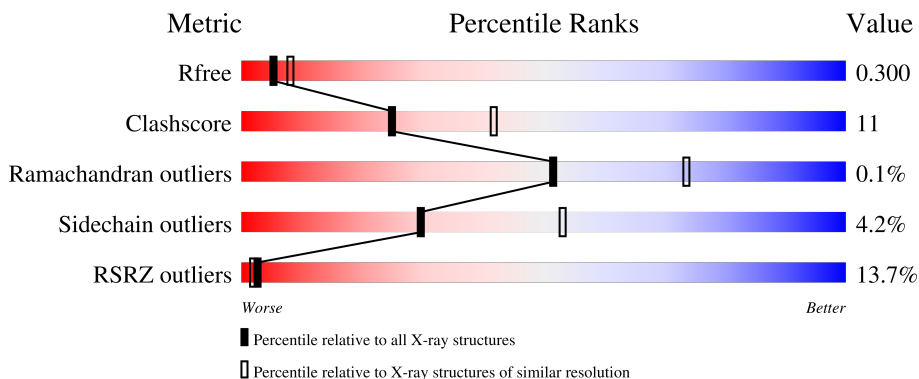|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.58 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	Percentile Ranks	Value
Rfree		0.300
Clashscore		11
Ramachandran outliers		0.1%
Sidechain outliers		4.2%
RSRZ outliers		13.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	225	17% / 64% 22% • 11%
1	B	225	12% / 65% 23% • 10%
1	C	225	7% / 68% 20% • 10%
1	D	225	12% / 64% 24% 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6628 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 LuxR family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total 1633	C 1033	N 291	O 302	S 7	0	0	0
1	B	202	Total 1629	C 1032	N 287	O 303	S 7	0	0	0
1	C	203	Total 1641	C 1039	N 290	O 305	S 7	0	0	0
1	D	199	Total 1603	C 1016	N 283	O 297	S 7	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9L8G8
A	-18	GLY	-	expression tag	UNP Q9L8G8
A	-17	SER	-	expression tag	UNP Q9L8G8
A	-16	SER	-	expression tag	UNP Q9L8G8
A	-15	HIS	-	expression tag	UNP Q9L8G8
A	-14	HIS	-	expression tag	UNP Q9L8G8
A	-13	HIS	-	expression tag	UNP Q9L8G8
A	-12	HIS	-	expression tag	UNP Q9L8G8
A	-11	HIS	-	expression tag	UNP Q9L8G8
A	-10	HIS	-	expression tag	UNP Q9L8G8
A	-9	SER	-	expression tag	UNP Q9L8G8
A	-8	SER	-	expression tag	UNP Q9L8G8
A	-7	GLY	-	expression tag	UNP Q9L8G8
A	-6	LEU	-	expression tag	UNP Q9L8G8
A	-5	VAL	-	expression tag	UNP Q9L8G8
A	-4	PRO	-	expression tag	UNP Q9L8G8
A	-3	ARG	-	expression tag	UNP Q9L8G8
A	-2	GLY	-	expression tag	UNP Q9L8G8
A	-1	SER	-	expression tag	UNP Q9L8G8
A	0	HIS	-	expression tag	UNP Q9L8G8
A	76	ALA	SER	engineered mutation	UNP Q9L8G8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q9L8G8
B	-18	GLY	-	expression tag	UNP Q9L8G8
B	-17	SER	-	expression tag	UNP Q9L8G8
B	-16	SER	-	expression tag	UNP Q9L8G8
B	-15	HIS	-	expression tag	UNP Q9L8G8
B	-14	HIS	-	expression tag	UNP Q9L8G8
B	-13	HIS	-	expression tag	UNP Q9L8G8
B	-12	HIS	-	expression tag	UNP Q9L8G8
B	-11	HIS	-	expression tag	UNP Q9L8G8
B	-10	HIS	-	expression tag	UNP Q9L8G8
B	-9	SER	-	expression tag	UNP Q9L8G8
B	-8	SER	-	expression tag	UNP Q9L8G8
B	-7	GLY	-	expression tag	UNP Q9L8G8
B	-6	LEU	-	expression tag	UNP Q9L8G8
B	-5	VAL	-	expression tag	UNP Q9L8G8
B	-4	PRO	-	expression tag	UNP Q9L8G8
B	-3	ARG	-	expression tag	UNP Q9L8G8
B	-2	GLY	-	expression tag	UNP Q9L8G8
B	-1	SER	-	expression tag	UNP Q9L8G8
B	0	HIS	-	expression tag	UNP Q9L8G8
B	76	ALA	SER	engineered mutation	UNP Q9L8G8
C	-19	MET	-	expression tag	UNP Q9L8G8
C	-18	GLY	-	expression tag	UNP Q9L8G8
C	-17	SER	-	expression tag	UNP Q9L8G8
C	-16	SER	-	expression tag	UNP Q9L8G8
C	-15	HIS	-	expression tag	UNP Q9L8G8
C	-14	HIS	-	expression tag	UNP Q9L8G8
C	-13	HIS	-	expression tag	UNP Q9L8G8
C	-12	HIS	-	expression tag	UNP Q9L8G8
C	-11	HIS	-	expression tag	UNP Q9L8G8
C	-10	HIS	-	expression tag	UNP Q9L8G8
C	-9	SER	-	expression tag	UNP Q9L8G8
C	-8	SER	-	expression tag	UNP Q9L8G8
C	-7	GLY	-	expression tag	UNP Q9L8G8
C	-6	LEU	-	expression tag	UNP Q9L8G8
C	-5	VAL	-	expression tag	UNP Q9L8G8
C	-4	PRO	-	expression tag	UNP Q9L8G8
C	-3	ARG	-	expression tag	UNP Q9L8G8
C	-2	GLY	-	expression tag	UNP Q9L8G8
C	-1	SER	-	expression tag	UNP Q9L8G8
C	0	HIS	-	expression tag	UNP Q9L8G8
C	76	ALA	SER	engineered mutation	UNP Q9L8G8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q9L8G8
D	-18	GLY	-	expression tag	UNP Q9L8G8
D	-17	SER	-	expression tag	UNP Q9L8G8
D	-16	SER	-	expression tag	UNP Q9L8G8
D	-15	HIS	-	expression tag	UNP Q9L8G8
D	-14	HIS	-	expression tag	UNP Q9L8G8
D	-13	HIS	-	expression tag	UNP Q9L8G8
D	-12	HIS	-	expression tag	UNP Q9L8G8
D	-11	HIS	-	expression tag	UNP Q9L8G8
D	-10	HIS	-	expression tag	UNP Q9L8G8
D	-9	SER	-	expression tag	UNP Q9L8G8
D	-8	SER	-	expression tag	UNP Q9L8G8
D	-7	GLY	-	expression tag	UNP Q9L8G8
D	-6	LEU	-	expression tag	UNP Q9L8G8
D	-5	VAL	-	expression tag	UNP Q9L8G8
D	-4	PRO	-	expression tag	UNP Q9L8G8
D	-3	ARG	-	expression tag	UNP Q9L8G8
D	-2	GLY	-	expression tag	UNP Q9L8G8
D	-1	SER	-	expression tag	UNP Q9L8G8
D	0	HIS	-	expression tag	UNP Q9L8G8
D	76	ALA	SER	engineered mutation	UNP Q9L8G8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
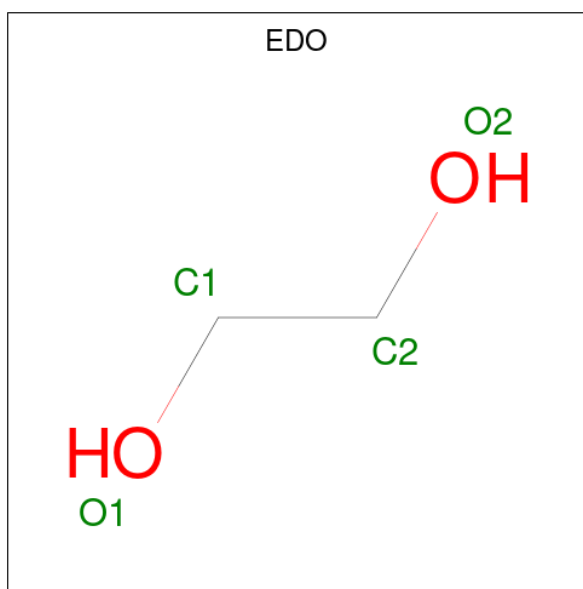
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	33	Total 33	O 33	0	0
4	C	33	Total 33	O 33	0	0
4	D	22	Total 22	O 22	0	0

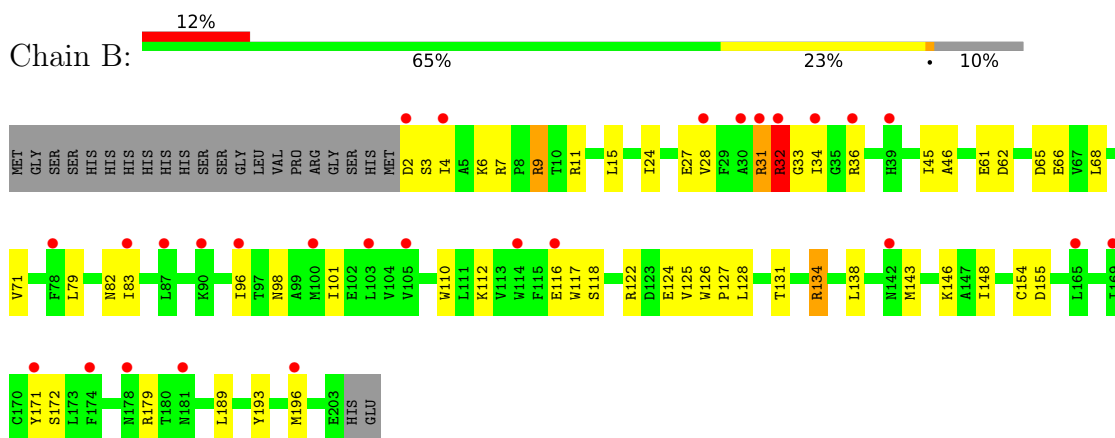# 3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
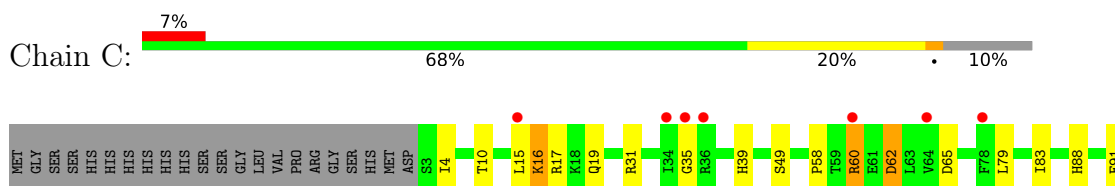
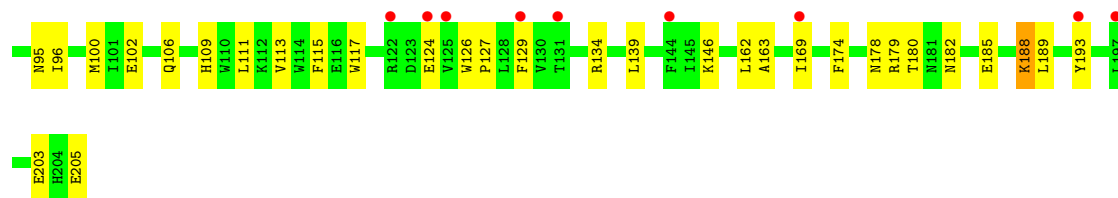• Molecule 1: LuxR family transcriptional regulator

Chain A:

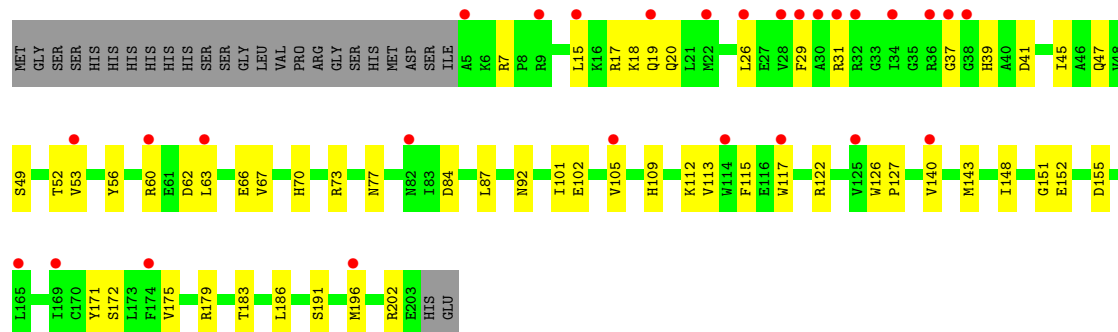
• Molecule 1: LuxR family transcriptional regulator

Chain B:

• Molecule 1: LuxR family transcriptional regulator

Chain C:

N95 I96 M100 I101 E102 Q106 H109 W110 L111 K112 V113 W114 F115 E116 W117 R122 D123 E124 V125 W126 P127 L128 F129 V130 T131 R134 L139 F144 I145 K146 L162 A163 I169 F174 N178 R179 T180 N181 N182 E185 K188 L189 Y193 L197

E203 H204 E205

• Molecule 1: LuxR family transcriptional regulator

Chain D:

12%

64%   24%   12%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ASP SER ILE A5 K6 R7 P8 R9 L15 K16 R17 K18 Q19 Q20 L21 M22 L26 E27 V28 F29 A30 R31 R32 G33 I34 G35 R36 G37 G38 H39 A40 D41 I45 A46 Q47 V48

S49 T52 V53 Y56 R60 E61 D62 L63 E66 V67 H70 R73 N77 N82 I83 D84 L87 N92 I101 E102 V105 H109 K112 V113 W114 F115 E116 W117 R122 V125 W126 P127 V140 M143 I148 G151 E152 D155

L165 I169 C170 Y171 S172 L173 F174 V175 R179 T183 L186 S191 M196 R202 E203 HIS GLU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.04Å 99.04Å 129.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.42 – 2.58 64.84 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.2 (55.42-2.58) 99.4 (64.84-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.15_3459: ???)	Depositor
R, R_{free}	0.245 , 0.299 0.245 , 0.300	Depositor DCC
R_{free} test set	1677 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.00 % 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 6.2491e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, EDO

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	0.30	0/1666	0.44	0/2259
1	B	0.29	0/1661	0.47	1/2255 (0.0%)
1	C	0.28	0/1674	0.41	0/2271
1	D	0.26	0/1635	0.41	0/2221
All	All	0.28	0/6636	0.44	1/9006 (0.0%)

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	3
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	LEU	CA-CB-CG	7.04	131.49	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	HIS	Peptide
1	A	33	GLY	Peptide
1	A	34	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	11	ARG	Peptide
1	B	9	ARG	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	1633	0	1605	42	0
1	B	1629	0	1601	37	0
1	C	1641	0	1610	30	0
1	D	1603	0	1570	40	0
2	A	4	0	6	0	0
2	C	4	0	6	1	0
3	C	5	0	0	0	0
4	A	21	0	0	6	0
4	B	33	0	0	8	0
4	C	33	0	0	6	0
4	D	22	0	0	2	0
All	All	6628	0	6398	140	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 11.

The worst 5 of 140 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLY:O	1:D:202:ARG:NH1	1.92	1.01
1:C:205:GLU:OE1	4:C:401:HOH:O	1.90	0.88
1:A:176:GLN:OE1	1:A:189:LEU:HD21	1.74	0.87
1:D:152:GLU:HG3	1:D:202:ARG:CG	2.05	0.86
1:C:163:ALA:O	4:C:402:HOH:O	1.94	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/225 (88%)	195 (98%)	4 (2%)	0	100	100
1	B	200/225 (89%)	197 (98%)	2 (1%)	1 (0%)	29	50
1	C	201/225 (89%)	197 (98%)	4 (2%)	0	100	100
1	D	197/225 (88%)	194 (98%)	3 (2%)	0	100	100
All	All	797/900 (89%)	783 (98%)	13 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	SER

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	178/200 (89%)	167 (94%)	11 (6%)	18	35
1	B	178/200 (89%)	171 (96%)	7 (4%)	32	56
1	C	179/200 (90%)	171 (96%)	8 (4%)	27	50
1	D	174/200 (87%)	170 (98%)	4 (2%)	50	73
All	All	709/800 (89%)	679 (96%)	30 (4%)	30	53

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	117	TRP
1	D	122	ARG
1	B	172	SER
1	D	191	SER
1	C	115	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	ASN
1	C	95	ASN
1	C	181	ASN
1	D	77	ASN
1	D	157	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	EDO	A	301	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	C	301	-	3,3,3	0.45	0	2,2,2	0.28	0
3	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.08	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	EDO	A	301	-	-	1/1/1/1	-
2	EDO	C	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	EDO	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, 95th 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(Å²)	Q<0.9
1	A	201/225 (89%)	1.07	39 (19%)	1	0	38, 62, 96, 112	0
1	B	202/225 (89%)	0.80	27 (13%)	3	2	31, 54, 85, 111	0
1	C	203/225 (90%)	0.71	16 (7%)	12	10	34, 53, 81, 111	0
1	D	199/225 (88%)	0.95	28 (14%)	2	2	30, 60, 94, 109	0
All	All	805/900 (89%)	0.88	110 (13%)	3	2	30, 56, 92, 112	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	GLY	10.8
1	D	37	GLY	9.7
1	D	36	ARG	6.5
1	A	125	VAL	6.3
1	A	21	LEU	5.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95th 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^2)	Q<0.9
2	EDO	A	301	4/4	0.73	0.38	52,53,55,57	0
3	SO4	C	302	5/5	0.78	0.39	107,108,112,113	0
2	EDO	C	301	4/4	0.88	0.28	41,42,44,46	0

6.5 Other polymers (i)

There are no such residues in this entry.