wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 10:52 am GMT

PDB ID	:	2YJP
Title	:	Crystal structure of the solute receptors for L-cysteine of Neisseria gonorrhoeae
Authors	:	Bulut, H.; Moniot, S.; Scheffel, F.; Gathmann, S.; Licht, A.; Saenger, W.; Schneider, E.
Deposited on	:	2011-05-23
Resolution	:	2.26 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:

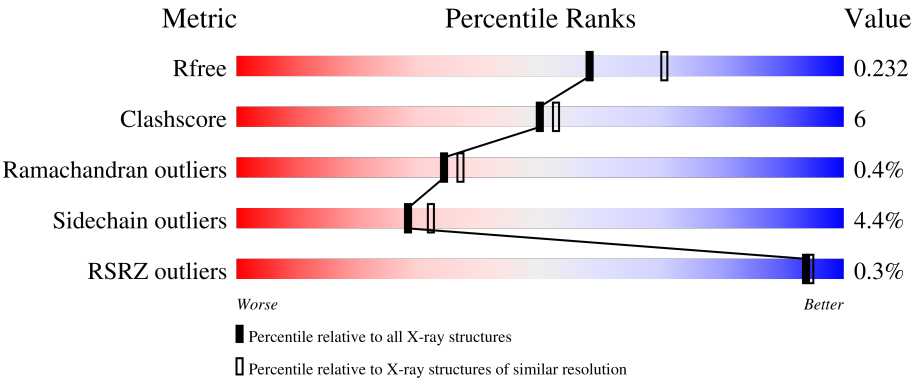
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	291	75% 9% • 15%
1	B	291	70% 10% • • 15%
1	C	291	% 74% 8% •• 15%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6073 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 PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	1	0
			1889	1214	317	355	3			
1	B	246	Total	C	N	O	S	0	1	0
			1881	1208	313	357	3			
1	C	246	Total	C	N	O	S	0	2	0
			1892	1215	317	357	3			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q5F5B5
A	-5	GLY	-	expression tag	UNP Q5F5B5
A	-4	HIS	-	expression tag	UNP Q5F5B5
A	-3	HIS	-	expression tag	UNP Q5F5B5
A	-2	HIS	-	expression tag	UNP Q5F5B5
A	-1	HIS	-	expression tag	UNP Q5F5B5
A	0	HIS	-	expression tag	UNP Q5F5B5
A	1	HIS	-	expression tag	UNP Q5F5B5
A	2	HIS	-	expression tag	UNP Q5F5B5
A	3	HIS	-	expression tag	UNP Q5F5B5
A	4	HIS	-	expression tag	UNP Q5F5B5
A	5	HIS	-	expression tag	UNP Q5F5B5
A	6	SER	-	expression tag	UNP Q5F5B5
A	7	SER	-	expression tag	UNP Q5F5B5
A	8	GLY	-	expression tag	UNP Q5F5B5
A	9	HIS	-	expression tag	UNP Q5F5B5
A	10	ILE	-	expression tag	UNP Q5F5B5
A	11	ASP	-	expression tag	UNP Q5F5B5
A	12	ASP	-	expression tag	UNP Q5F5B5
A	13	ASP	-	expression tag	UNP Q5F5B5
A	14	ASP	-	expression tag	UNP Q5F5B5
A	15	LYS	-	expression tag	UNP Q5F5B5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	16	HIS	-	expression tag	UNP Q5F5B5
A	17	MET	-	expression tag	UNP Q5F5B5
A	23	ALA	CYS	engineered mutation	UNP Q5F5B5
B	-6	MET	-	expression tag	UNP Q5F5B5
B	-5	GLY	-	expression tag	UNP Q5F5B5
B	-4	HIS	-	expression tag	UNP Q5F5B5
B	-3	HIS	-	expression tag	UNP Q5F5B5
B	-2	HIS	-	expression tag	UNP Q5F5B5
B	-1	HIS	-	expression tag	UNP Q5F5B5
B	0	HIS	-	expression tag	UNP Q5F5B5
B	1	HIS	-	expression tag	UNP Q5F5B5
B	2	HIS	-	expression tag	UNP Q5F5B5
B	3	HIS	-	expression tag	UNP Q5F5B5
B	4	HIS	-	expression tag	UNP Q5F5B5
B	5	HIS	-	expression tag	UNP Q5F5B5
B	6	SER	-	expression tag	UNP Q5F5B5
B	7	SER	-	expression tag	UNP Q5F5B5
B	8	GLY	-	expression tag	UNP Q5F5B5
B	9	HIS	-	expression tag	UNP Q5F5B5
B	10	ILE	-	expression tag	UNP Q5F5B5
B	11	ASP	-	expression tag	UNP Q5F5B5
B	12	ASP	-	expression tag	UNP Q5F5B5
B	13	ASP	-	expression tag	UNP Q5F5B5
B	14	ASP	-	expression tag	UNP Q5F5B5
B	15	LYS	-	expression tag	UNP Q5F5B5
B	16	HIS	-	expression tag	UNP Q5F5B5
B	17	MET	-	expression tag	UNP Q5F5B5
B	23	ALA	CYS	engineered mutation	UNP Q5F5B5
C	-6	MET	-	expression tag	UNP Q5F5B5
C	-5	GLY	-	expression tag	UNP Q5F5B5
C	-4	HIS	-	expression tag	UNP Q5F5B5
C	-3	HIS	-	expression tag	UNP Q5F5B5
C	-2	HIS	-	expression tag	UNP Q5F5B5
C	-1	HIS	-	expression tag	UNP Q5F5B5
C	0	HIS	-	expression tag	UNP Q5F5B5
C	1	HIS	-	expression tag	UNP Q5F5B5
C	2	HIS	-	expression tag	UNP Q5F5B5
C	3	HIS	-	expression tag	UNP Q5F5B5
C	4	HIS	-	expression tag	UNP Q5F5B5
C	5	HIS	-	expression tag	UNP Q5F5B5
C	6	SER	-	expression tag	UNP Q5F5B5
C	7	SER	-	expression tag	UNP Q5F5B5

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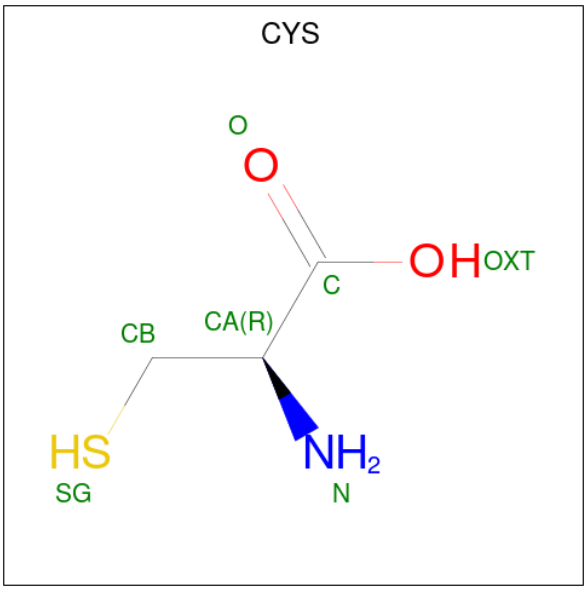
Chain	Residue	Modelled	Actual	Comment	Reference
C	8	GLY	-	expression tag	UNP Q5F5B5
C	9	HIS	-	expression tag	UNP Q5F5B5
C	10	ILE	-	expression tag	UNP Q5F5B5
C	11	ASP	-	expression tag	UNP Q5F5B5
C	12	ASP	-	expression tag	UNP Q5F5B5
C	13	ASP	-	expression tag	UNP Q5F5B5
C	14	ASP	-	expression tag	UNP Q5F5B5
C	15	LYS	-	expression tag	UNP Q5F5B5
C	16	HIS	-	expression tag	UNP Q5F5B5
C	17	MET	-	expression tag	UNP Q5F5B5
C	23	ALA	CYS	engineered mutation	UNP Q5F5B5

- Molecule 2 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).

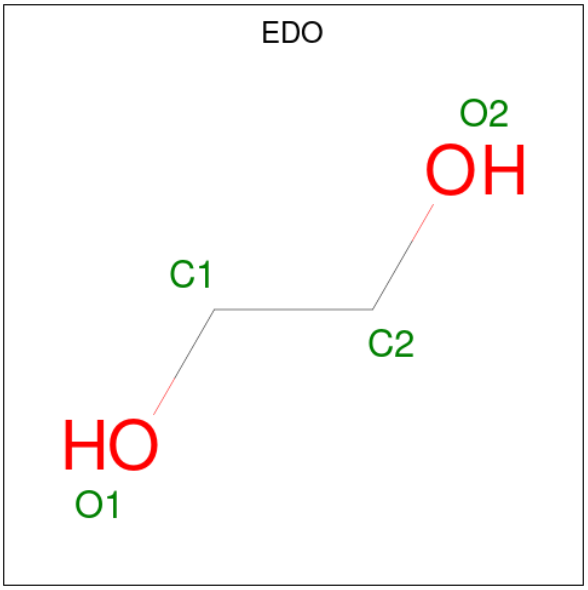


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Zn 6 6	0	0
3	C	2	Total Zn 2 2	0	0

- 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 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 126 126	0	1
5	B	122	Total O 122 122	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	109	Total 110	O 110	0	1

3 Residue-property plots (i)

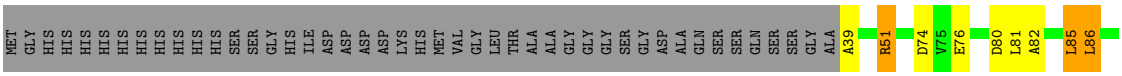
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain A:

• Molecule 1: PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain B:



• Molecule 1: PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.71Å 91.59Å 158.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 2.26 47.18 – 2.26	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.18-2.26) 97.9 (47.18-2.26)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.233 0.183 , 0.232	Depositor DCC
R_{free} test set	1996 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: EDO, ZN

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	1.07	5/1926 (0.3%)	1.03	9/2613 (0.3%)
1	B	1.08	6/1918 (0.3%)	1.06	16/2603 (0.6%)
1	C	1.18	14/1929 (0.7%)	1.03	13/2616 (0.5%)
All	All	1.11	25/5773 (0.4%)	1.04	38/7832 (0.5%)

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	B	0	1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	ARG	CZ-NH1	-10.57	1.19	1.33
1	C	105	TYR	CE1-CZ	-10.40	1.25	1.38
1	C	105	TYR	CE2-CZ	-10.10	1.25	1.38
1	C	105	TYR	CG-CD2	-9.46	1.26	1.39
1	C	105	TYR	CG-CD1	-9.43	1.26	1.39

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	259	ARG	NE-CZ-NH2	16.45	128.53	120.30
1	A	257	ASP	CB-CG-OD1	13.79	130.71	118.30
1	B	137	VAL	CG1-CB-CG2	-13.28	89.66	110.90
1	A	151	ASP	CB-CG-OD2	12.87	129.88	118.30
1	A	106	VAL	CG1-CB-CG2	-11.92	91.83	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	ASP	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	1889	0	1894	20	0
1	B	1881	0	1868	27	0
1	C	1892	0	1889	19	0
2	A	7	0	4	1	0
2	B	7	0	4	1	0
2	C	7	0	4	0	0
3	A	6	0	0	0	0
3	C	2	0	0	0	0
4	A	12	0	18	0	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
5	A	126	0	0	3	0
5	B	122	0	0	1	0
5	C	110	0	0	3	0
All	All	6073	0	5699	66	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 6.

The worst 5 of 66 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:80:ASP:HB3	1:A:254:MET:CE	2.02	0.90
1:A:38:ALA:N	1:A:39:ALA:HA	1.87	0.88
1:C:51:ARG:HD3	5:C:2003:HOH:O	1.71	0.87
1:B:80:ASP:HB3	1:B:254:MET:HE2	1.67	0.77
1:C:80:ASP:HB3	1:C:254:MET:HE2	1.67	0.74

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	246/291 (84%)	239 (97%)	6 (2%)	1 (0%)	34	37
1	B	245/291 (84%)	237 (97%)	7 (3%)	1 (0%)	34	37
1	C	246/291 (84%)	240 (98%)	5 (2%)	1 (0%)	34	37
All	All	737/873 (84%)	716 (97%)	18 (2%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	LYS
1	A	117	ASN
1	C	117	ASN

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	190/228 (83%)	183 (96%)	7 (4%)	34	40
1	B	188/228 (82%)	178 (95%)	10 (5%)	22	23
1	C	190/228 (83%)	182 (96%)	8 (4%)	30	34
All	All	568/684 (83%)	543 (96%)	25 (4%)	28	32

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	269	LEU
1	C	86	LEU
1	C	279	GLU
1	B	281	LEU
1	C	135	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	CYS	B	350	-	5,6,6	1.68	2 (40%)	5,7,7	1.69	1 (20%)
4	EDO	A	1277	-	3,3,3	0.58	0	2,2,2	0.35	0
4	EDO	B	1271	-	3,3,3	0.53	0	2,2,2	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CYS	C	350	-	5,6,6	1.54	1 (20%)	5,7,7	1.76	2 (40%)
2	CYS	A	350	-	5,6,6	1.21	1 (20%)	5,7,7	1.08	0
4	EDO	C	1272	-	3,3,3	0.55	0	2,2,2	0.20	0
4	EDO	B	1270	-	3,3,3	0.39	0	2,2,2	1.33	0
4	EDO	A	1276	-	3,3,3	0.75	0	2,2,2	0.35	0
4	EDO	A	1278	-	3,3,3	0.47	0	2,2,2	0.99	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	CYS	B	350	-	-	0/6/6/6	-
4	EDO	A	1277	-	-	0/1/1/1	-
4	EDO	B	1271	-	-	1/1/1/1	-
2	CYS	C	350	-	-	0/6/6/6	-
2	CYS	A	350	-	-	0/6/6/6	-
4	EDO	C	1272	-	-	1/1/1/1	-
4	EDO	B	1270	-	-	0/1/1/1	-
4	EDO	A	1276	-	-	1/1/1/1	-
4	EDO	A	1278	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	CYS	CB-SG	3.20	1.88	1.81
2	B	350	CYS	OXT-C	-2.42	1.22	1.30
2	B	350	CYS	CB-CA	2.36	1.55	1.53
2	A	350	CYS	OXT-C	-2.04	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	350	CYS	OXT-C-CA	2.75	122.75	113.38
2	C	350	CYS	OXT-C-O	-2.17	119.16	124.09
2	B	350	CYS	OXT-C-O	-2.12	119.28	124.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1271	EDO	O1-C1-C2-O2
4	C	1272	EDO	O1-C1-C2-O2
4	A	1276	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	350	CYS	1	0
2	A	350	CYS	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^{th} 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^2)	Q<0.9
1	A	247/291 (84%)	-0.38	0	100	100	13, 23, 37, 48	0
1	B	246/291 (84%)	-0.35	0	100	100	15, 25, 42, 54	0
1	C	246/291 (84%)	-0.35	2 (0%)	86	87	14, 25, 38, 52	0
All	All	739/873 (84%)	-0.36	2 (0%)	94	94	13, 25, 40, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	ASP	3.2
1	C	228	PRO	2.2

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, 95^{th} 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
3	ZN	A	1273	1/1	0.74	0.06	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	1270	4/4	0.80	0.22	39,43,43,44	0
4	EDO	C	1272	4/4	0.82	0.17	51,53,54,55	0
4	EDO	A	1276	4/4	0.86	0.13	28,39,40,41	0
3	ZN	A	1274	1/1	0.88	0.04	85,85,85,85	0
4	EDO	A	1278	4/4	0.91	0.14	44,47,48,49	0
4	EDO	A	1277	4/4	0.92	0.17	39,40,42,43	0
4	EDO	B	1271	4/4	0.95	0.12	27,30,34,39	0
2	CYS	A	350	7/7	0.97	0.10	13,15,17,19	0
3	ZN	C	1271	1/1	0.98	0.09	35,35,35,35	0
3	ZN	A	1275	1/1	0.99	0.05	61,61,61,61	0
3	ZN	A	1272	1/1	0.99	0.10	29,29,29,29	0
2	CYS	B	350	7/7	0.99	0.12	16,16,18,20	0
2	CYS	C	350	7/7	0.99	0.11	12,14,15,19	0
3	ZN	A	1271	1/1	1.00	0.11	25,25,25,25	0
3	ZN	C	1270	1/1	1.00	0.12	26,26,26,26	0
3	ZN	A	1270	1/1	1.00	0.11	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.