



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:31 PM UTC

PDB ID : 2YJP / pdb_00002yjp
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 Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

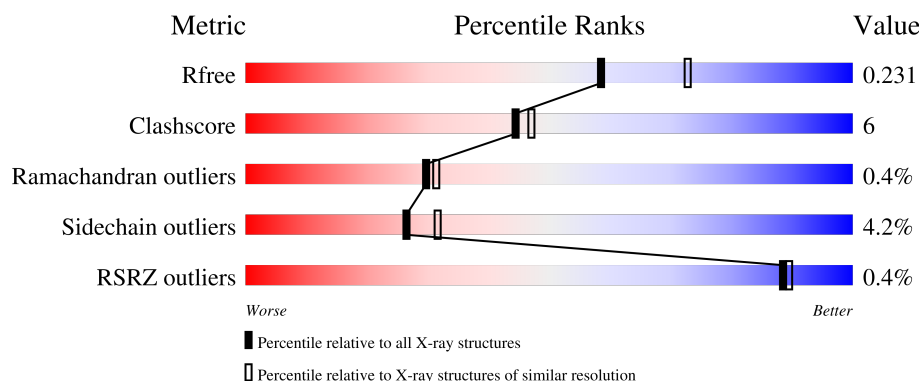
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	291	
1	B	291	
1	C	291	

2 Entry composition

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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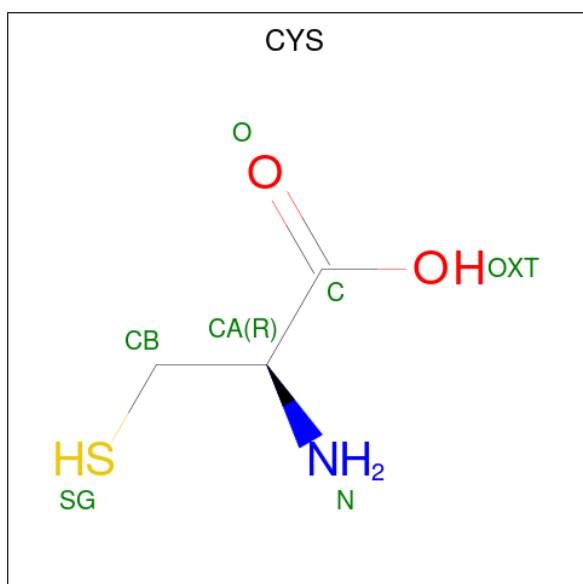
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	HIS	-	expression tag	UNP Q5F5B5
A	17	MET	-	expression tag	UNP Q5F5B5
A	23	ALA	CYS	engineered mutation	UNP Q5F5B5
B	-6	MET	-	expression tag	UNP Q5F5B5
B	-5	GLY	-	expression tag	UNP Q5F5B5
B	-4	HIS	-	expression tag	UNP Q5F5B5
B	-3	HIS	-	expression tag	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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

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

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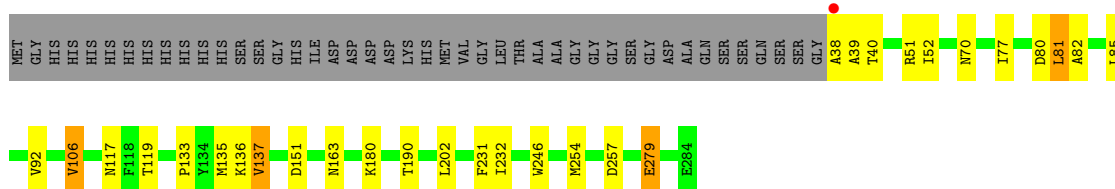
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	109	Total	O	0	1
			110	110		

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.

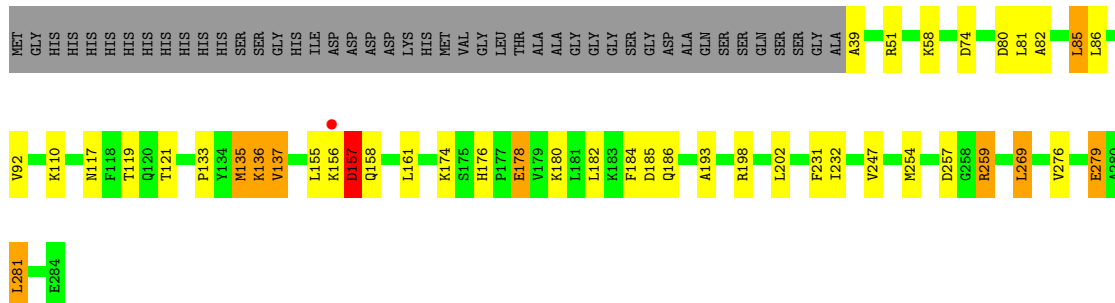
- Molecule 1: PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain A: 75% 9% • 15%



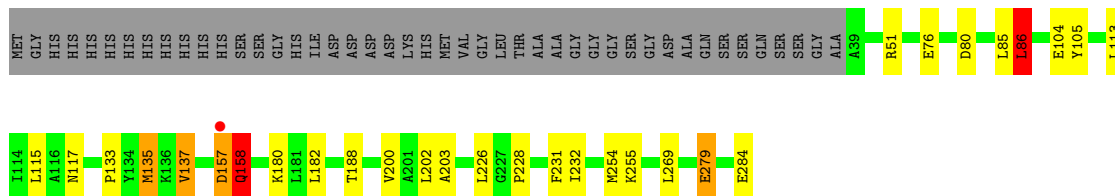
- Molecule 1: PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain B:  69% 12% • 15%



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

Chain C: 74% 8% .. 15%



4 Data and refinement statistics

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) 97.8 (47.18-2.26)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.233 0.184 , 0.231	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)	0.37 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	1.21	6/1926 (0.3%)	1.13	6/2613 (0.2%)
1	B	1.27	8/1918 (0.4%)	1.17	6/2603 (0.2%)
1	C	1.25	9/1929 (0.5%)	1.18	9/2616 (0.3%)
All	All	1.24	23/5773 (0.4%)	1.16	21/7832 (0.3%)

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	ARG	CZ-NH1	-9.60	1.19	1.32
1	B	269	LEU	CG-CD1	-6.61	1.30	1.52
1	C	113	LEU	CG-CD2	-5.97	1.32	1.52
1	C	86	LEU	CG-CD2	-5.97	1.32	1.52
1	C	105	TYR	CG-CD2	-5.95	1.26	1.39
1	C	105	TYR	CG-CD1	-5.93	1.26	1.39
1	A	70	ASN	CG-ND2	-5.92	1.20	1.33
1	C	113	LEU	CG-CD1	-5.79	1.33	1.52
1	A	106	VAL	CB-CG2	-5.74	1.33	1.52
1	B	121	THR	CA-CB	5.68	1.60	1.53
1	B	184	PHE	C-O	-5.63	1.16	1.23
1	C	182	LEU	CG-CD2	-5.56	1.34	1.52
1	C	105	TYR	CE1-CZ	-5.51	1.25	1.38
1	A	81	LEU	CG-CD1	-5.47	1.34	1.52
1	A	137	VAL	CA-CB	5.46	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	ASN	CG-OD1	-5.43	1.13	1.23
1	B	247	VAL	CA-CB	5.39	1.61	1.54
1	B	186	GLN	C-O	-5.38	1.17	1.23
1	C	105	TYR	CE2-CZ	-5.35	1.25	1.38
1	C	226	LEU	C-O	5.32	1.29	1.23
1	B	58	LYS	N-CA	-5.29	1.41	1.46
1	B	137	VAL	CB-CG2	-5.18	1.35	1.52
1	A	151	ASP	CG-OD1	-5.15	1.15	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	LEU	CD1-CG-CD2	-10.65	87.37	110.80
1	B	259	ARG	NE-CZ-NH2	10.36	128.53	119.20
1	B	137	VAL	CG1-CB-CG2	-9.61	89.66	110.80
1	A	81	LEU	CD1-CG-CD2	-9.50	89.90	110.80
1	C	113	LEU	CD1-CG-CD2	-9.18	90.61	110.80
1	A	106	VAL	CG1-CB-CG2	-8.62	91.83	110.80
1	C	86	LEU	CD1-CG-CD2	-7.60	94.08	110.80
1	C	158	GLN	N-CA-C	7.44	120.23	109.14
1	A	151	ASP	OD1-CG-OD2	-7.41	105.12	122.90
1	B	81	LEU	CD1-CG-CD2	-7.00	95.39	110.80
1	A	257	ASP	OD1-CG-OD2	-6.88	106.40	122.90
1	B	185	ASP	N-CA-C	6.21	120.12	112.54
1	B	269	LEU	CD1-CG-CD2	-6.12	97.35	110.80
1	B	259	ARG	NH1-CZ-NH2	-5.82	111.74	119.30
1	C	269	LEU	CA-C-N	-5.72	113.78	119.56
1	C	269	LEU	C-N-CA	-5.72	113.78	119.56
1	A	52	ILE	N-CA-C	5.71	116.08	107.75
1	C	137	VAL	CG1-CB-CG2	-5.47	98.76	110.80
1	A	257	ASP	CB-CG-OD1	5.35	130.71	118.40
1	C	76	GLU	OE1-CD-OE2	-5.14	110.55	122.90
1	C	104	GLU	OE1-CD-OE2	-5.03	110.82	122.90

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 ⓘ

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	28	0
1	C	1892	0	1889	21	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	2	0
All	All	6073	0	5699	69	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.

All (69) 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:C:80:ASP:HB3	1:C:254:MET:HE2	1.61	0.82
1:B:80:ASP:HB3	1:B:254:MET:HE2	1.66	0.76
1:C:80:ASP:CB	1:C:254:MET:HE2	2.15	0.76
1:A:80:ASP:HB3	1:A:254:MET:HE2	1.68	0.76
1:A:80:ASP:CB	1:A:254:MET:CE	2.68	0.71
5:A:2014:HOH:O	1:B:51:ARG:NH2	2.24	0.71
1:C:228:PRO:HA	5:C:2100:HOH:O	1.90	0.70
1:B:80:ASP:CB	1:B:254:MET:HE2	2.21	0.70
1:B:80:ASP:HB3	1:B:254:MET:CE	2.23	0.69
1:C:80:ASP:HB3	1:C:254:MET:CE	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:CB	1:A:254:MET:HE2	2.23	0.67
1:C:157:ASP:HB3	1:C:158:GLN:OE1	1.94	0.66
1:B:51:ARG:NH1	1:B:110:LYS:O	2.34	0.61
1:B:279:GLU:N	1:B:279:GLU:OE1	2.34	0.60
1:B:80:ASP:CB	1:B:254:MET:CE	2.79	0.60
1:B:193:ALA:HA	1:B:198[A]:ARG:HE	1.67	0.60
1:A:279:GLU:N	1:A:279:GLU:OE1	2.35	0.59
1:A:38:ALA:N	1:A:39:ALA:CA	2.66	0.58
1:C:85:LEU:C	1:C:86:LEU:HD23	2.29	0.57
1:B:85:LEU:HB3	1:B:86:LEU:HD22	1.86	0.57
1:C:80:ASP:CB	1:C:254:MET:CE	2.81	0.57
1:C:135:MET:HG2	1:C:232:ILE:HB	1.87	0.57
1:A:133:PRO:HB3	1:A:231:PHE:HB3	1.88	0.56
1:B:133:PRO:HB3	1:B:231:PHE:HB3	1.89	0.54
1:A:119:THR:HG1	2:A:350:CYS:N	2.06	0.53
1:A:202:LEU:C	1:A:202:LEU:HD23	2.34	0.53
1:C:133:PRO:HB3	1:C:231:PHE:HB3	1.90	0.53
1:A:38:ALA:HB3	1:A:40:THR:H	1.74	0.52
1:C:202:LEU:C	1:C:202:LEU:HD23	2.34	0.52
1:A:279:GLU:CD	1:A:279:GLU:H	2.17	0.51
1:A:51[A]:ARG:HD3	5:A:2004:HOH:O	2.11	0.51
1:B:82:ALA:HB2	1:B:92:VAL:HG22	1.93	0.50
1:B:279:GLU:H	1:B:279:GLU:CD	2.19	0.50
1:B:155:LEU:O	1:B:157:ASP:N	2.44	0.50
1:B:257:ASP:OD2	1:B:259:ARG:NH1	2.45	0.49
1:A:82:ALA:HB2	1:A:92:VAL:HG22	1.95	0.49
1:C:86:LEU:HD23	1:C:86:LEU:N	2.27	0.49
1:B:135:MET:HG2	1:B:232:ILE:HB	1.94	0.49
1:B:85:LEU:CD1	1:B:86:LEU:HD22	2.43	0.48
1:B:276:VAL:CG1	1:B:281:LEU:HD22	2.43	0.48
1:A:77:ILE:O	1:A:81:LEU:HG	2.15	0.46
1:B:136:LYS:NZ	1:B:279:GLU:O	2.48	0.46
1:C:255:LYS:NZ	1:C:284:GLU:O	2.44	0.46
1:A:279:GLU:CD	5:A:2125:HOH:O	2.59	0.45
1:C:279:GLU:OE1	1:C:279:GLU:N	2.27	0.45
1:C:158:GLN:HG2	1:C:200:VAL:HG11	1.98	0.45
1:B:80:ASP:HB2	1:B:254:MET:CE	2.47	0.44
1:B:161:LEU:HD23	1:B:182:LEU:HB3	2.00	0.44
1:A:190:THR:HG22	1:A:202:LEU:HD11	1.98	0.43
1:B:85:LEU:HD13	1:B:86:LEU:HD22	2.00	0.43
1:B:119:THR:HG1	2:B:350:CYS:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:O	1:B:158:GLN:N	2.32	0.43
1:C:85:LEU:HG	1:C:86:LEU:HD23	2.01	0.43
1:C:85:LEU:HD23	1:C:86:LEU:HD21	2.00	0.43
1:B:202:LEU:C	1:B:202:LEU:HD23	2.44	0.43
1:B:39:ALA:N	5:B:2001:HOH:O	2.52	0.42
1:B:74:ASP:OD2	1:B:117:ASN:HB2	2.19	0.42
1:B:276:VAL:HG11	1:B:281:LEU:HD22	2.02	0.42
1:B:176:HIS:HA	1:B:178:GLU:OE2	2.19	0.42
1:A:190:THR:HG22	1:A:202:LEU:CD1	2.48	0.42
1:A:135:MET:HG2	1:A:232:ILE:HB	2.01	0.42
1:C:80:ASP:HB2	1:C:254:MET:CE	2.49	0.41
1:A:85:LEU:HB2	1:A:246:TRP:CH2	2.56	0.41
1:C:279:GLU:H	1:C:279:GLU:CD	2.20	0.41
1:C:202:LEU:HD23	1:C:203:ALA:N	2.36	0.40
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.97	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	246/291 (84%)	239 (97%)	6 (2%)	1 (0%)	30	31
1	B	245/291 (84%)	237 (97%)	7 (3%)	1 (0%)	30	31
1	C	246/291 (84%)	240 (98%)	5 (2%)	1 (0%)	30	31
All	All	737/873 (84%)	716 (97%)	18 (2%)	3 (0%)	30	31

All (3) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	C	117	ASN

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	190/228 (83%)	185 (97%)	5 (3%)	40	50
1	B	188/228 (82%)	177 (94%)	11 (6%)	18	18
1	C	190/228 (83%)	182 (96%)	8 (4%)	26	31
All	All	568/684 (83%)	544 (96%)	24 (4%)	26	31

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	136	LYS
1	A	137	VAL
1	A	180	LYS
1	A	279	GLU
1	B	85	LEU
1	B	135	MET
1	B	136	LYS
1	B	137	VAL
1	B	157	ASP
1	B	174	LYS
1	B	178	GLU
1	B	180	LYS
1	B	269	LEU
1	B	279	GLU
1	B	281	LEU
1	C	86	LEU
1	C	135	MET
1	C	137	VAL
1	C	157	ASP
1	C	158	GLN

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Mol	Chain	Res	Type
1	C	180	LYS
1	C	188	THR
1	C	279	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	245	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 oligosaccharides 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	$\# Z > 2$
4	EDO	A	1278	-	3,3,3	0.44	0	2,2,2	0.99	0
4	EDO	B	1270	-	3,3,3	0.35	0	2,2,2	1.32	0
2	CYS	B	350	-	5,6,6	1.73	2 (40%)	3,7,7	1.99	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	1276	-	3,3,3	0.73	0	2,2,2	0.36	0
4	EDO	C	1272	-	3,3,3	0.52	0	2,2,2	0.25	0
2	CYS	A	350	-	5,6,6	1.26	1 (20%)	3,7,7	0.97	0
4	EDO	A	1277	-	3,3,3	0.56	0	2,2,2	0.39	0
4	EDO	B	1271	-	3,3,3	0.48	0	2,2,2	0.75	0
2	CYS	C	350	-	5,6,6	1.59	1 (20%)	3,7,7	1.49	1 (33%)

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
4	EDO	A	1278	-	-	0/1/1/1	-
4	EDO	B	1270	-	-	0/1/1/1	-
2	CYS	B	350	-	-	0/6/6/6	-
4	EDO	A	1276	-	-	1/1/1/1	-
4	EDO	C	1272	-	-	1/1/1/1	-
2	CYS	A	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	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	CYS	CB-SG	3.30	1.88	1.81
2	B	350	CYS	OXT-C	-2.52	1.22	1.30
2	B	350	CYS	CB-CA	2.39	1.55	1.53
2	A	350	CYS	OXT-C	-2.13	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	350	CYS	OXT-C-O	-2.17	119.16	124.08
2	B	350	CYS	OXT-C-O	-2.12	119.28	124.08

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	A	247/291 (84%)	-0.46	1 (0%) 88 89	13, 23, 37, 48	1 (0%)
1	B	246/291 (84%)	-0.42	1 (0%) 88 89	14, 25, 42, 54	1 (0%)
1	C	246/291 (84%)	-0.40	1 (0%) 88 89	10, 25, 38, 52	2 (0%)
All	All	739/873 (84%)	-0.42	3 (0%) 88 89	10, 24, 40, 54	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	2.7
1	C	157	ASP	2.3
1	B	156	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	EDO	B	1270	4/4	0.71	0.20	39,43,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	1276	4/4	0.82	0.15	28,39,40,41	0
4	EDO	A	1278	4/4	0.84	0.18	44,47,48,49	0
4	EDO	B	1271	4/4	0.87	0.15	27,30,34,39	0
4	EDO	A	1277	4/4	0.88	0.16	39,40,42,43	0
4	EDO	C	1272	4/4	0.89	0.20	51,53,54,55	0
3	ZN	A	1273	1/1	0.92	0.07	85,85,85,85	0
3	ZN	A	1274	1/1	0.93	0.06	85,85,85,85	0
2	CYS	A	350	7/7	0.98	0.05	13,15,17,19	0
3	ZN	A	1275	1/1	0.99	0.06	61,61,61,61	0
3	ZN	C	1271	1/1	0.99	0.03	35,35,35,35	0
2	CYS	B	350	7/7	0.99	0.04	16,16,18,20	0
2	CYS	C	350	7/7	0.99	0.04	12,14,15,19	0
3	ZN	C	1270	1/1	1.00	0.01	26,26,26,26	0
3	ZN	A	1270	1/1	1.00	0.01	22,22,22,22	0
3	ZN	A	1271	1/1	1.00	0.01	25,25,25,25	0
3	ZN	A	1272	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.