



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

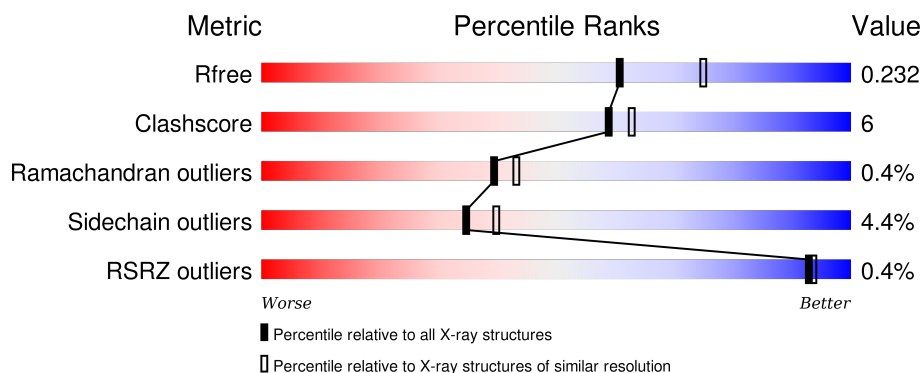
1 Overall quality at a glance ⓘ

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	
1	B	291	
1	C	291	

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	A	1277	-	-	-	X
4	EDO	B	1270	-	-	-	X

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

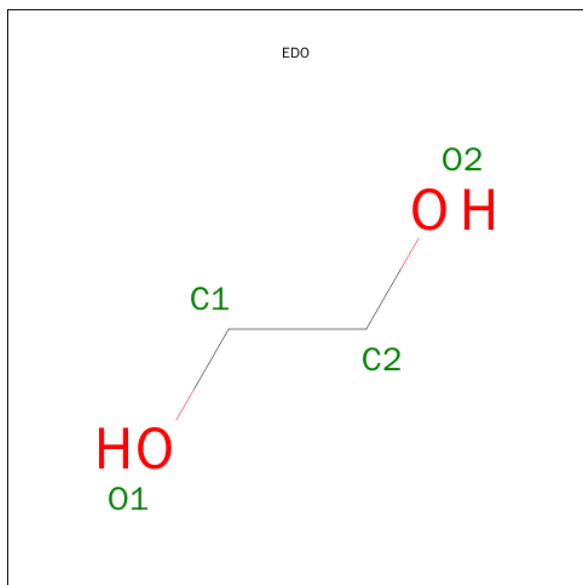
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- Chemical structure of Cysteine (CYS) is shown. The side chain is labeled CB (Carbon Beta) and contains a thiol group (HS) labeled SG (Sulfhydryl Group). The main chain is labeled CA(R) (Carbon Alpha) and contains an amino group (NH₂) labeled N (Nitrogen). The carboxyl group is labeled C (Carbon) and contains a hydroxyl group (OH) labeled OXT (Oxygen). The structure is a 2D representation of the molecule.

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

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- WORLD WIDE
PDB
PROTEIN DATA BANK

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 (three-letter code: 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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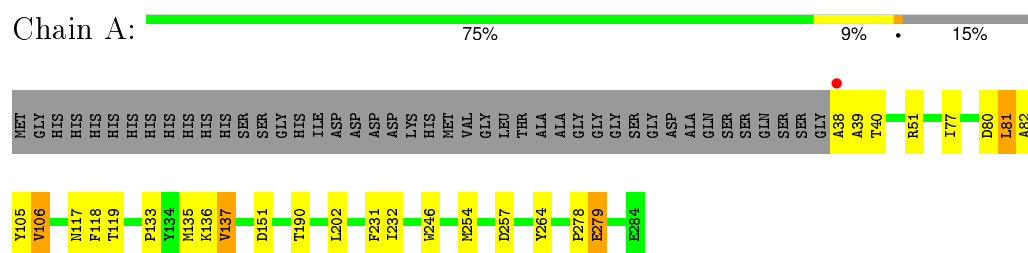
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	109	Total	O	0	1
			110	110		

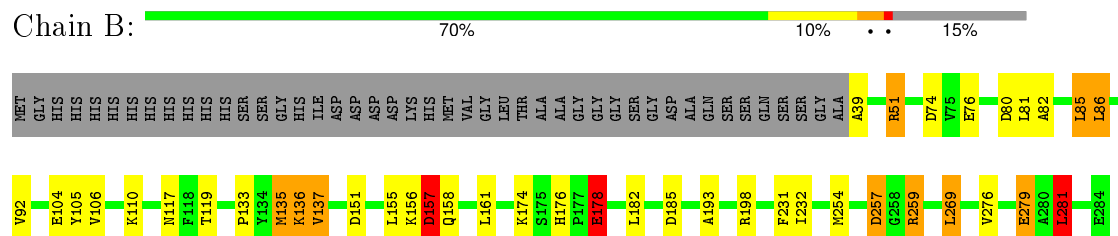
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

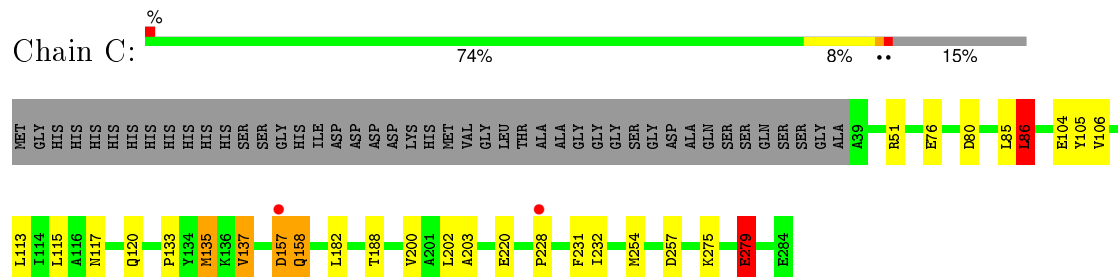
- Molecule 1: PUTATIVE ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID



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



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



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) 97.9 (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 0.183 , 0.232	Depositor DCC
R_{free} test set	1996 reflections (5.26%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 39913 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.07	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

All (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
1	A	106	VAL	CB-CG2	-9.16	1.33	1.52
1	B	137	VAL	CB-CG2	-8.29	1.35	1.52
1	C	76	GLU	CD-OE2	-8.16	1.16	1.25
1	C	220	GLU	CD-OE2	-7.64	1.17	1.25
1	C	220	GLU	CD-OE1	-7.20	1.17	1.25
1	C	76	GLU	CD-OE1	-7.13	1.17	1.25
1	C	137	VAL	CB-CG1	-7.02	1.38	1.52
1	A	105	TYR	CE2-CZ	-6.64	1.29	1.38
1	A	106	VAL	CB-CG1	-6.08	1.40	1.52
1	C	106	VAL	CB-CG1	-6.08	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	VAL	CB-CG1	-5.89	1.40	1.52
1	B	137	VAL	CB-CG1	-5.84	1.40	1.52
1	B	105	TYR	CE2-CZ	-5.78	1.31	1.38
1	B	269	LEU	CG-CD1	-5.70	1.30	1.51
1	C	104	GLU	CD-OE2	-5.61	1.19	1.25
1	C	279	GLU	CD-OE1	-5.57	1.19	1.25
1	A	105	TYR	CG-CD2	-5.28	1.32	1.39
1	C	113	LEU	CG-CD2	-5.14	1.32	1.51
1	C	86	LEU	CG-CD2	-5.13	1.32	1.51
1	B	106	VAL	CB-CG2	-5.03	1.42	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	C	76	GLU	OE1-CD-OE2	-10.62	110.55	123.30
1	C	104	GLU	OE1-CD-OE2	-10.40	110.82	123.30
1	A	151	ASP	OD1-CG-OD2	-9.57	105.12	123.30
1	A	257	ASP	OD1-CG-OD2	-8.89	106.40	123.30
1	C	220	GLU	OE1-CD-OE2	-8.38	113.24	123.30
1	B	257	ASP	CB-CG-OD1	8.38	125.84	118.30
1	C	182	LEU	CD1-CG-CD2	-7.71	87.37	110.50
1	B	269	LEU	CA-CB-CG	7.69	132.98	115.30
1	C	137	VAL	CG1-CB-CG2	-7.59	98.76	110.90
1	B	281	LEU	CA-CB-CG	7.58	132.73	115.30
1	A	151	ASP	CB-CG-OD1	7.40	124.96	118.30
1	C	279	GLU	OE1-CD-OE2	-7.12	114.75	123.30
1	B	259	ARG	NH1-CZ-NH2	-6.97	111.74	119.40
1	B	76	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	C	257	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	81	LEU	CD1-CG-CD2	-6.87	89.90	110.50
1	C	113	LEU	CD1-CG-CD2	-6.63	90.61	110.50
1	A	137	VAL	CG1-CB-CG2	-6.31	100.81	110.90
1	C	105	TYR	CZ-CE2-CD2	5.82	125.04	119.80
1	B	86	LEU	CA-CB-CG	5.73	128.48	115.30
1	B	106	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	C	105	TYR	CD1-CE1-CZ	5.56	124.80	119.80
1	B	185	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	86	LEU	CD1-CG-CD2	-5.47	94.08	110.50
1	C	105	TYR	CB-CG-CD1	5.40	124.24	121.00
1	B	151	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	269	LEU	CB-CG-CD1	5.27	119.96	111.00
1	B	104	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	257	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	81	LEU	CD1-CG-CD2	-5.04	95.39	110.50
1	C	105	TYR	CE1-CZ-CE2	-5.03	111.75	119.80
1	B	178	GLU	CB-CA-C	-5.00	100.40	110.40

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	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.

All (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
1:A:80:ASP:HB3	1:A:254:MET:HE2	1.69	0.74
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:HB3	1:B:254:MET:CE	2.23	0.69
1:A:80:ASP:CB	1:A:254:MET:HE2	2.22	0.68
1:C:80:ASP:HB3	1:C:254:MET:CE	2.25	0.67
1:C:157:ASP:HB3	1:C:158:GLN:OE1	1.94	0.66
1:C:120[B]:GLN:OE1	5:C:2045:HOH:O	2.12	0.63
1:B:51:ARG:NH1	1:B:110:LYS:O	2.34	0.61
1:C:80:ASP:HB2	1:C:254:MET:HE1	1.83	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:C:80:ASP:CB	1:C:254:MET:CE	2.81	0.59
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:B:80:ASP:CB	1:B:254:MET:HE2	2.34	0.57
1:B:85:LEU:HB3	1:B:86:LEU:HD22	1.86	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:80:ASP:HB2	1:B:254:MET:HE1	1.89	0.55
1:A:119:THR:HG1	2:A:350:CYS:N	2.05	0.55
1:B:133:PRO:HB3	1:B:231:PHE:HB3	1.89	0.54
1:C:133:PRO:HB3	1:C:231:PHE:HB3	1.90	0.53
1:C:85:LEU:C	1:C:86:LEU:HD23	2.29	0.52
1:A:38:ALA:HB3	1:A:40:THR:H	1.74	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:N	1:C:86:LEU:HD23	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:202:LEU:HD23	1:A:202:LEU:C	2.34	0.48
1:C:202:LEU:HD23	1:C:202:LEU:C	2.34	0.47
1:A:279:GLU:CD	1:A:279:GLU:H	2.17	0.46
1:B:136:LYS:NZ	1:B:279:GLU:O	2.48	0.46
1:A:77:ILE:O	1:A:81:LEU:HG	2.15	0.46
1:B:279:GLU:H	1:B:279:GLU:CD	2.19	0.45
1:C:279:GLU:N	1:C:279:GLU:OE1	2.27	0.45
1:C:158:GLN:HG2	1:C:200:VAL:HG11	1.98	0.45
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:C:85:LEU:HG	1:C:86:LEU:HD23	2.01	0.43
1:B:155:LEU:O	1:B:158:GLN:N	2.32	0.43
1:B:119:THR:HG1	2:B:350:CYS:N	2.16	0.43
1:C:85:LEU:HD23	1:C:86:LEU:HD21	2.00	0.43
1:B:39:ALA:N	5:B:2001:HOH:O	2.52	0.42
1:B:276:VAL:HG11	1:B:281:LEU:HD22	2.02	0.42
1:B:74:ASP:OD2	1:B:117:ASN:HB2	2.19	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:A:85:LEU:HB2	1:A:246:TRP:CH2	2.56	0.41
1:A:279:GLU:CD	5:A:2125:HOH:O	2.59	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 ⓘ

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	246/291 (84%)	239 (97%)	6 (2%)	1 (0%)	39	43
1	B	245/291 (84%)	237 (97%)	7 (3%)	1 (0%)	39	43
1	C	246/291 (84%)	240 (98%)	5 (2%)	1 (0%)	39	43
All	All	737/873 (84%)	716 (97%)	18 (2%)	3 (0%)	39	43

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 ⓘ

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%)	41	50
1	B	188/228 (82%)	178 (95%)	10 (5%)	28	30
1	C	190/228 (83%)	182 (96%)	8 (4%)	36	42
All	All	568/684 (83%)	543 (96%)	25 (4%)	35	40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	118	PHE
1	A	136	LYS
1	A	137	VAL
1	A	264	TYR
1	A	278	PRO
1	A	279	GLU
1	B	85	LEU
1	B	135	MET
1	B	136	LYS

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Mol	Chain	Res	Type
1	B	137	VAL
1	B	157	ASP
1	B	174	LYS
1	B	178	GLU
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
1	C	188	THR
1	C	275	LYS
1	C	279	GLU

Some 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 carbohydrates 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	1276	-	3,3,3	0.75	0	2,2,2	0.39	0
4	EDO	A	1277	-	3,3,3	0.59	0	2,2,2	0.44	0
4	EDO	A	1278	-	3,3,3	0.48	0	2,2,2	1.08	0
2	CYS	A	350	-	3,6,6	0.28	0	1,7,7	0.11	0
4	EDO	B	1270	-	3,3,3	0.40	0	2,2,2	1.43	0
4	EDO	B	1271	-	3,3,3	0.54	0	2,2,2	0.82	0
2	CYS	B	350	-	3,6,6	1.59	1 (33%)	1,7,7	1.87	0
4	EDO	C	1272	-	3,3,3	0.56	0	2,2,2	0.29	0
2	CYS	C	350	-	3,6,6	1.79	1 (33%)	1,7,7	0.58	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
4	EDO	A	1276	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1277	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1278	-	-	0/1/1/1	0/0/0/0
2	CYS	A	350	-	-	0/2/6/6	0/0/0/0
4	EDO	B	1270	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1271	-	-	0/1/1/1	0/0/0/0
2	CYS	B	350	-	-	0/2/6/6	0/0/0/0
4	EDO	C	1272	-	-	0/1/1/1	0/0/0/0
2	CYS	C	350	-	-	0/2/6/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	CYS	CB-CA	2.22	1.55	1.53
2	C	350	CYS	CB-SG	3.05	1.88	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	CYS	1	0
2	B	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, 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%)	-0.33	1 (0%) 93 93	13, 23, 37, 48	0
1	B	246/291 (84%)	-0.30	0 100 100	15, 25, 42, 54	0
1	C	246/291 (84%)	-0.30	2 (0%) 87 88	14, 25, 38, 52	0
All	All	739/873 (84%)	-0.31	3 (0%) 93 93	13, 25, 40, 54	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	ASP	3.4
1	C	228	PRO	2.3
1	A	38	ALA	2.1

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	B	1270	4/4	0.80	0.22	16.12	39,43,43,44	0
4	EDO	A	1277	4/4	0.92	0.17	10.17	39,40,42,43	0
4	EDO	A	1278	4/4	0.91	0.14	1.82	44,47,48,49	0
2	CYS	B	350	7/7	0.99	0.12	1.14	16,16,18,20	0
2	CYS	C	350	7/7	0.99	0.11	0.77	12,14,15,19	0
3	ZN	C	1270	1/1	1.00	0.12	0.73	26,26,26,26	0
2	CYS	A	350	7/7	0.97	0.10	-0.52	13,15,17,19	0
3	ZN	A	1271	1/1	1.00	0.11	-	25,25,25,25	0
3	ZN	C	1271	1/1	0.98	0.09	-	35,35,35,35	0
3	ZN	A	1272	1/1	0.99	0.10	-	29,29,29,29	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
3	ZN	A	1275	1/1	0.99	0.05	-	61,61,61,61	0
3	ZN	A	1273	1/1	0.74	0.06	-	85,85,85,85	0
3	ZN	A	1270	1/1	1.00	0.11	-	22,22,22,22	0
4	EDO	B	1271	4/4	0.95	0.12	-	27,30,34,39	0
4	EDO	C	1272	4/4	0.82	0.17	-	51,53,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.