



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:54 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 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/ValidationPDFNotes.html>

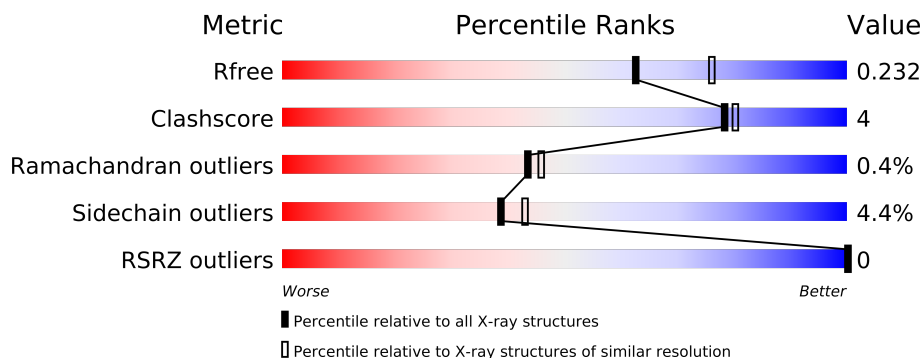
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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 hydrogen and 0 are deuterium.

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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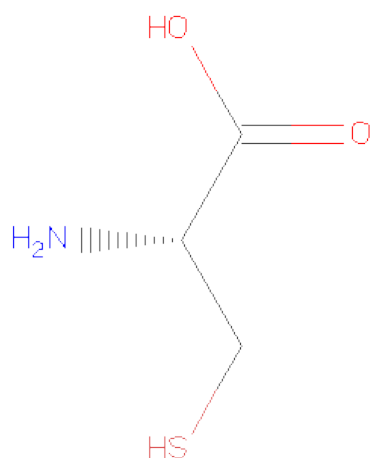
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	HIS	-	EXPRESSION TAG	UNP Q5F5B5
A	17	MET	-	EXPRESSION TAG	UNP Q5F5B5
A	23	ALA	CYS	ENGINEERED MUTATION	UNP Q5F5B5
B	-6	MET	-	EXPRESSION TAG	UNP Q5F5B5
B	-5	GLY	-	EXPRESSION TAG	UNP Q5F5B5
B	-4	HIS	-	EXPRESSION TAG	UNP Q5F5B5
B	-3	HIS	-	EXPRESSION TAG	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: $C_3H_7NO_2S$).

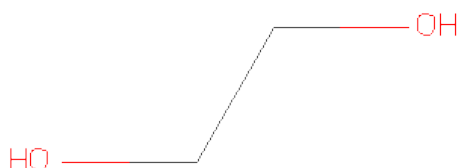


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 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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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	109	Total 110	O 110	0	1

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 0.186 , 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)	0.39 , 29.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1889	0	0	5	0
1	B	1881	0	0	10	0
1	C	1892	0	0	6	0
2	A	7	0	4	0	0
2	B	7	0	4	0	0
2	C	7	0	4	1	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	2	0
5	C	110	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6073	0	48	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:ASP:CB	1:A:254:MET:CE	2.68	0.72
5:A:2014:HOH:O	1:B:51:ARG:NH2	2.24	0.71
1:C:279:GLU:OE1	1:C:279:GLU:N	2.27	0.68
1:C:120[B]:GLN:OE1	5:C:2045:HOH:O	2.12	0.63
1:B:155:LEU:O	1:B:158:GLN:N	2.32	0.63
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: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:183:LYS:NZ	5:B:2076:HOH:O	2.38	0.56
1:C:255:LYS:NZ	1:C:284:GLU:O	2.44	0.51
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:C:51:ARG:CD	5:C:2003:HOH:O	2.60	0.48
1:B:136:LYS:NZ	1:B:279:GLU:O	2.48	0.47
1:B:39:ALA:N	5:B:2001:HOH:O	2.52	0.42
1:A:183:LYS:NZ	5:A:2077:HOH:O	2.53	0.42
1:C:124:ARG:NH1	2:C:350:CYS:O	2.54	0.41
1:A:279:GLU:CD	5:A:2125:HOH:O	2.59	0.41

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%)	43	46
1	B	245/291 (84%)	237 (97%)	7 (3%)	1 (0%)	43	46
1	C	246/291 (84%)	240 (98%)	5 (2%)	1 (0%)	43	46
All	All	737/873 (84%)	716 (97%)	18 (2%)	3 (0%)	43	46

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%)	45	53
1	B	188/228 (82%)	178 (95%)	10 (5%)	32	33
1	C	190/228 (83%)	182 (96%)	8 (4%)	40	46
All	All	568/684 (83%)	543 (96%)	25 (4%)	39	43

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
1	B	137	VAL
1	B	157	ASP

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Mol	Chain	Res	Type
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.81	0	2,2,2	0.37	0
4	EDO	A	1277	-	3,3,3	0.65	0	2,2,2	0.39	0
4	EDO	A	1278	-	3,3,3	0.55	0	2,2,2	1.05	0
2	CYS	A	350	-	6,6,6	0.96	0	7,7,7	0.92	0
4	EDO	B	1270	-	3,3,3	0.48	0	2,2,2	1.40	0
4	EDO	B	1271	-	3,3,3	0.62	0	2,2,2	0.78	0
2	CYS	B	350	-	6,6,6	1.34	1 (16%)	7,7,7	1.42	2 (28%)
4	EDO	C	1272	-	3,3,3	0.63	0	2,2,2	0.24	0
2	CYS	C	350	-	6,6,6	1.29	1 (16%)	7,7,7	1.59	2 (28%)

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	-	-	0/6/6/6	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	-	-	0/6/6/6	0/0/0/0
4	EDO	C	1272	-	-	0/1/1/1	0/0/0/0
2	CYS	C	350	-	-	0/6/6/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	CYS	CB-SG	2.98	1.88	1.81
2	B	350	CYS	OXT-C	-2.14	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	350	CYS	OXT-C-CA	2.61	122.75	116.88
2	C	350	CYS	OXT-C-O	-2.17	119.16	124.07
2	B	350	CYS	OXT-C-O	-2.12	119.28	124.07
2	B	350	CYS	CB-CA-C	-2.06	108.03	111.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.39	0 100 100	13, 23, 37, 48	0
1	B	246/291 (84%)	-0.39	0 100 100	15, 25, 42, 54	0
1	C	246/291 (84%)	-0.37	0 100 100	14, 25, 38, 52	0
All	All	739/873 (84%)	-0.38	0 100 100	13, 25, 40, 54	0

There are no RSRZ outliers to report.

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	B	1270	4/4	0.23	10.30	39,43,43,44	0
4	EDO	A	1277	4/4	0.15	4.11	39,40,42,43	0
4	EDO	A	1278	4/4	0.14	1.24	44,47,48,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	C	1270	1/1	0.11	0.74	26,26,26,26	0
3	ZN	A	1270	1/1	0.11	0.36	22,22,22,22	0
4	EDO	C	1272	4/4	0.15	0.32	51,53,54,55	0
3	ZN	A	1271	1/1	0.11	0.30	25,25,25,25	0
4	EDO	A	1276	4/4	0.12	0.06	28,39,40,41	0
3	ZN	C	1271	1/1	0.09	-0.24	35,35,35,35	0
2	CYS	B	350	7/7	0.10	-0.38	16,16,18,20	0
2	CYS	C	350	7/7	0.09	-0.58	12,14,15,19	0
3	ZN	A	1272	1/1	0.10	-0.76	29,29,29,29	0
4	EDO	B	1271	4/4	0.09	-0.86	27,30,34,39	0
2	CYS	A	350	7/7	0.08	-1.75	13,15,17,19	0
3	ZN	A	1275	1/1	0.04	-3.69	61,61,61,61	0
3	ZN	A	1273	1/1	0.06	-10.33	85,85,85,85	0
3	ZN	A	1274	1/1	0.04	-15.71	85,85,85,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.