



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:41 PM GMT

PDB ID : 4YU9  
Title : Crystal Structure of double mutant Y115E Y117E human Glutaminyl Cyclase  
Authors : Di Pisa, F.; Pozzi, C.; Benvenuti, M.; Mangani, S.  
Deposited on : 2015-03-18  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

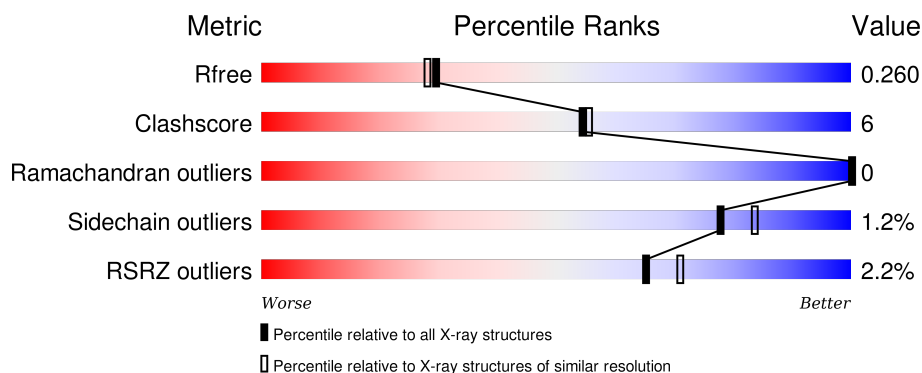
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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	329	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	B	329	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	C	329	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>

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	404	-	-	-	X
4	EDO	A	406	-	-	-	X
4	EDO	A	407	-	-	X	-
4	EDO	A	409	-	-	-	X
4	EDO	B	402	-	-	-	X
4	EDO	B	403	-	-	-	X
4	EDO	C	403	-	-	-	X
4	EDO	C	405	-	-	-	X
4	EDO	C	406	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8775 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	3	0
			2591	1660	443	479	9			
1	B	324	Total	C	N	O	S	0	4	0
			2599	1668	447	475	9			
1	C	325	Total	C	N	O	S	0	1	0
			2568	1645	440	474	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLU	TYR	engineered mutation	UNP Q16769
A	117	GLU	TYR	engineered mutation	UNP Q16769
B	115	GLU	TYR	engineered mutation	UNP Q16769
B	117	GLU	TYR	engineered mutation	UNP Q16769
C	115	GLU	TYR	engineered mutation	UNP Q16769
C	117	GLU	TYR	engineered mutation	UNP Q16769

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

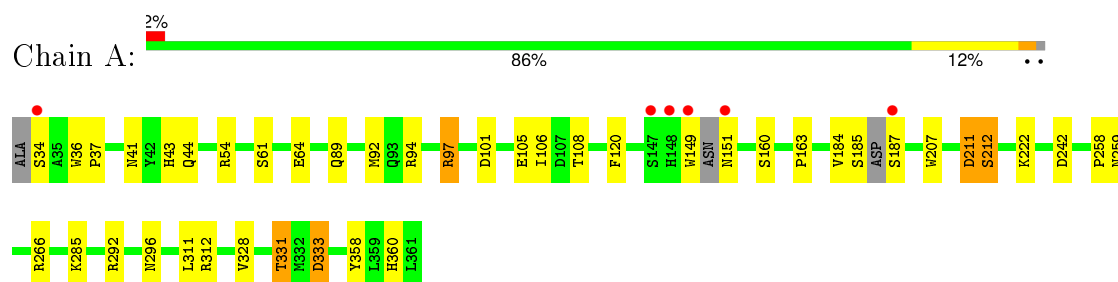
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	332	Total O 332 332	0	0
5	B	312	Total O 312 312	0	0
5	C	295	Total O 295 295	0	0

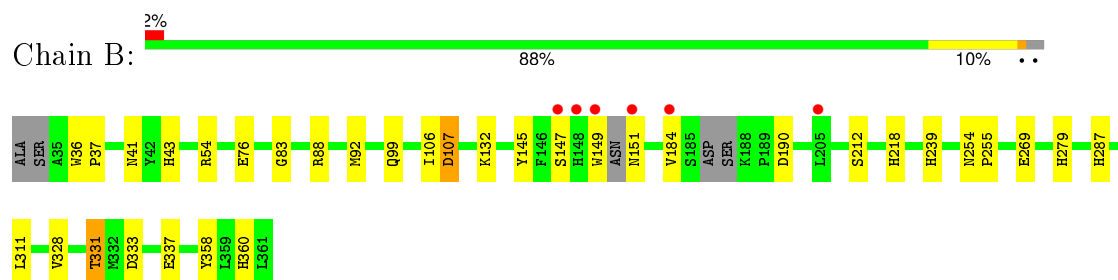
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

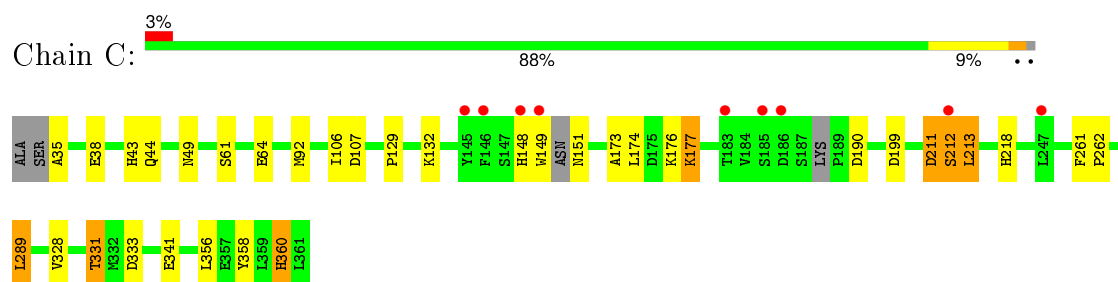
- Molecule 1: Glutaminyl-peptide cyclotransferase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.38 Å 149.63 Å 96.30 Å 90.00° 96.68° 90.00°	Depositor
Resolution (Å)	95.65 – 2.10 31.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.6 (95.65-2.10) 92.6 (31.88-2.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.211 , 0.254 0.220 , 0.260	Depositor DCC
$R_{free}$ test set	3350 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	5.9	Xtriage
Anisotropy	0.969	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 65419 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	8775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.88	2/2670 (0.1%)	0.93	7/3632 (0.2%)
1	B	0.85	1/2682 (0.0%)	0.89	3/3650 (0.1%)
1	C	0.91	2/2641 (0.1%)	0.88	6/3594 (0.2%)
All	All	0.88	5/7993 (0.1%)	0.90	16/10876 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	212	SER	C-N	17.84	1.75	1.34
1	C	211	ASP	C-N	-8.78	1.13	1.34
1	A	211	ASP	C-N	-7.25	1.17	1.34
1	A	212	SER	C-N	6.65	1.49	1.34
1	B	212	SER	C-N	6.10	1.48	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	97	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	97	ARG	NE-CZ-NH1	7.44	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	O-C-N	-7.35	110.94	122.70
1	B	107	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	88	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	C	211	ASP	O-C-N	-6.72	111.94	122.70
1	A	212	SER	CB-CA-C	6.17	121.83	110.10
1	C	213	LEU	N-CA-CB	-6.00	98.41	110.40
1	A	312	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	199	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	199	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	333	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	212	SER	CB-CA-C	5.35	120.27	110.10
1	C	212	SER	CB-CA-C	5.35	120.26	110.10
1	C	213	LEU	N-CA-C	5.28	125.27	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	ASP	Mainchain
1	C	211	ASP	Mainchain

## 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	2591	0	2511	38	0
1	B	2599	0	2530	27	0
1	C	2568	0	2470	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	10	0	0	0	0
3	C	5	0	0	0	0
4	A	24	0	36	9	0
4	B	20	0	30	3	0
4	C	16	0	24	6	0
5	A	332	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	312	0	0	13	0
5	C	295	0	0	10	0
All	All	8775	0	7601	99	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 (99) 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:C:212:SER:C	1:C:213:LEU:N	1.75	1.36
1:B:311:LEU:HG	5:B:810:HOH:O	1.54	1.06
1:A:101:ASP:CB	4:A:407:EDO:H11	1.90	1.00
1:A:101:ASP:CB	4:A:407:EDO:C1	2.40	0.99
1:B:99:GLN:HG2	5:B:769:HOH:O	1.60	0.98
1:C:176:LYS:H	4:C:406:EDO:H22	1.44	0.82
1:C:149:TRP:O	1:C:151:ASN:N	2.13	0.82
1:C:148:HIS:CB	5:C:755:HOH:O	2.29	0.79
1:A:101:ASP:CB	4:A:407:EDO:C2	2.61	0.78
1:C:328:VAL:O	1:C:331:THR:HB	1.85	0.76
1:B:92:MET:SD	1:B:106:ILE:HD11	2.26	0.75
1:A:44:GLN:O	1:A:360:HIS:HE1	1.72	0.73
1:A:185:SER:O	1:A:187:SER:N	2.22	0.72
1:B:149:TRP:CB	5:B:760:HOH:O	2.38	0.70
1:B:337:GLU:HA	5:B:785:HOH:O	1.92	0.70
1:C:38:GLU:HG3	5:C:718:HOH:O	1.92	0.68
1:C:43:HIS:HE1	1:C:358:TYR:O	1.77	0.67
1:A:222[B]:LYS:HB3	1:A:222[B]:LYS:HZ3	1.60	0.67
1:C:92:MET:SD	1:C:106:ILE:HD11	2.36	0.66
1:A:92:MET:SD	1:A:106:ILE:HD11	2.36	0.66
1:A:149:TRP:O	1:A:151:ASN:N	2.28	0.66
1:C:43:HIS:HD2	5:C:613:HOH:O	1.78	0.66
1:A:222[B]:LYS:CB	1:A:222[B]:LYS:NZ	2.59	0.66
1:C:173:ALA:O	4:C:406:EDO:H21	1.97	0.65
1:C:176:LYS:N	4:C:406:EDO:H22	2.12	0.64
1:B:149:TRP:O	1:B:151:ASN:N	2.31	0.63
1:C:35:ALA:N	5:C:788:HOH:O	2.31	0.63
1:C:331:THR:HG23	1:C:333:ASP:H	1.64	0.62
1:A:266:ARG:HE	4:A:409:EDO:H21	1.64	0.62
1:A:89:GLN:HG3	5:A:548:HOH:O	1.99	0.62
1:A:328:VAL:O	1:A:331:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:405:EDO:H12	5:B:676:HOH:O	2.01	0.60
1:B:331:THR:HG23	1:B:333:ASP:H	1.64	0.60
1:A:222[B]:LYS:CB	1:A:222[B]:LYS:HZ3	2.14	0.60
1:A:285:LYS:HE3	5:A:752:HOH:O	2.00	0.60
4:C:405:EDO:H21	5:C:692:HOH:O	2.00	0.59
1:A:64:GLU:HG2	5:A:779:HOH:O	2.03	0.58
1:C:44:GLN:O	1:C:360:HIS:HE1	1.87	0.57
1:B:360:HIS:CE1	5:B:720:HOH:O	2.56	0.57
1:A:101:ASP:CB	4:A:407:EDO:H22	2.36	0.54
1:C:212:SER:CA	1:C:213:LEU:N	2.66	0.53
1:B:184:VAL:HG22	5:B:790:HOH:O	2.09	0.53
1:C:43:HIS:CE1	1:C:358:TYR:O	2.61	0.52
1:A:36:TRP:CG	1:A:37:PRO:HD3	2.44	0.52
1:A:292:ARG:HH22	1:A:296:ASN:HD21	1.57	0.52
1:B:337:GLU:CB	5:B:786:HOH:O	2.58	0.52
1:C:289:LEU:HG	5:C:775:HOH:O	2.09	0.52
1:A:34:SER:N	4:A:405:EDO:HO1	2.07	0.52
1:C:331:THR:CG2	1:C:333:ASP:H	2.22	0.52
1:A:184:VAL:HG22	5:A:814:HOH:O	2.09	0.51
1:A:331:THR:HG23	1:A:333:ASP:H	1.74	0.51
1:C:341:GLU:CB	5:C:772:HOH:O	2.58	0.51
1:B:43:HIS:HD2	5:B:570:HOH:O	1.93	0.50
1:B:43:HIS:HE1	1:B:358:TYR:O	1.95	0.49
1:C:132:LYS:HG3	1:C:190:ASP:OD2	2.13	0.49
1:B:107:ASP:OD1	1:B:218:HIS:HE1	1.97	0.48
1:A:43:HIS:HD2	5:A:579:HOH:O	1.97	0.48
1:A:44:GLN:O	1:A:360:HIS:CE1	2.62	0.48
1:A:106:ILE:HG22	1:A:108:THR:OG1	2.13	0.47
4:C:405:EDO:C2	5:C:692:HOH:O	2.62	0.47
1:C:149:TRP:C	1:C:151:ASN:N	2.68	0.47
1:B:269:GLU:HB3	4:B:403:EDO:H21	1.97	0.47
1:C:212:SER:C	1:C:213:LEU:CA	2.75	0.46
4:A:409:EDO:H22	5:A:638:HOH:O	2.15	0.46
1:A:258:PRO:HD2	5:A:734:HOH:O	2.14	0.46
1:A:207:TRP:CZ2	1:A:212:SER:HB2	2.51	0.46
1:C:38:GLU:CG	5:C:718:HOH:O	2.59	0.46
1:A:61:SER:OG	1:A:64:GLU:HB2	2.16	0.46
1:B:41:ASN:ND2	5:B:666:HOH:O	2.48	0.45
1:A:292:ARG:HH22	1:A:296:ASN:ND2	2.14	0.45
1:A:331:THR:CG2	1:A:333:ASP:H	2.29	0.45
1:A:41:ASN:HA	4:A:409:EDO:O2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:O	1:A:97:ARG:HG2	2.18	0.44
1:B:145:TYR:CD1	1:B:145:TYR:C	2.90	0.44
1:B:254:ASN:N	1:B:255:PRO:CD	2.81	0.44
1:A:160[B]:SER:HB2	1:A:163:PRO:HG2	2.00	0.44
1:B:279:HIS:HD2	1:B:287:HIS:ND1	2.16	0.43
1:C:177:LYS:HD2	4:C:406:EDO:O1	2.17	0.43
1:B:328:VAL:O	1:B:331:THR:HB	2.18	0.43
1:B:331:THR:HG21	5:B:766:HOH:O	2.18	0.43
1:B:311:LEU:HD12	5:B:630:HOH:O	2.19	0.43
1:A:108:THR:HA	1:A:120:PHE:O	2.20	0.42
1:B:132:LYS:HG3	1:B:190:ASP:OD2	2.19	0.42
1:C:107:ASP:OD1	1:C:218:HIS:HE1	2.03	0.42
1:B:36:TRP:N	1:B:37:PRO:CD	2.83	0.42
1:B:76:GLU:O	1:B:83:GLY:HA3	2.20	0.41
1:C:49:ASN:OD1	1:C:49:ASN:C	2.59	0.41
1:A:43:HIS:HE1	1:A:358:TYR:O	2.04	0.41
1:C:174:LEU:HD13	1:C:356:LEU:CD2	2.50	0.41
1:A:101:ASP:CB	4:A:407:EDO:O1	2.68	0.41
1:C:61:SER:CB	1:C:64:GLU:HG3	2.51	0.41
1:A:311:LEU:HD23	1:A:311:LEU:C	2.41	0.41
1:B:239:HIS:CD2	4:B:402:EDO:H22	2.56	0.41
1:C:261:PHE:HA	1:C:262:PRO:HD3	1.96	0.41
1:B:54[A]:ARG:HD2	1:B:54[A]:ARG:HH11	1.72	0.41
1:B:147:SER:HB3	5:B:757:HOH:O	2.21	0.40
1:A:36:TRP:N	1:A:37:PRO:CD	2.84	0.40
1:C:177:LYS:NZ	5:C:691:HOH:O	2.55	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	323/329 (98%)	309 (96%)	14 (4%)	0	100	100
1	B	322/329 (98%)	311 (97%)	11 (3%)	0	100	100
1	C	320/329 (97%)	312 (98%)	8 (2%)	0	100	100
All	All	965/987 (98%)	932 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	281/290 (97%)	277 (99%)	4 (1%)	74	80
1	B	282/290 (97%)	281 (100%)	1 (0%)	93	96
1	C	275/290 (95%)	270 (98%)	5 (2%)	66	72
All	All	838/870 (96%)	828 (99%)	10 (1%)	78	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
1	A	242	ASP
1	A	259	ASN
1	A	331	THR
1	B	331	THR
1	C	129	PRO
1	C	177	LYS
1	C	289	LEU
1	C	331	THR
1	C	360	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	HIS
1	A	128	ASN
1	A	194	GLN
1	A	218	HIS
1	A	259	ASN
1	A	272	GLN
1	A	279	HIS
1	A	296	ASN
1	A	338	ASN
1	A	360	HIS
1	B	41	ASN
1	B	43	HIS
1	B	55	GLN
1	B	128	ASN
1	B	194	GLN
1	B	218	HIS
1	B	272	GLN
1	B	276	HIS
1	B	279	HIS
1	B	338	ASN
1	C	41	ASN
1	C	43	HIS
1	C	128	ASN
1	C	218	HIS
1	C	272	GLN
1	C	279	HIS
1	C	338	ASN
1	C	360	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\# Z  > 2$
3	SO4	A	402	-	4,4,4	0.54	0	6,6,6	0.31	0
3	SO4	A	403	-	4,4,4	0.50	0	6,6,6	0.80	0
4	EDO	A	404	-	3,3,3	0.53	0	2,2,2	0.19	0
4	EDO	A	405	-	3,3,3	0.68	0	2,2,2	0.41	0
4	EDO	A	406	-	3,3,3	0.66	0	2,2,2	0.37	0
4	EDO	A	407	-	3,3,3	0.22	0	2,2,2	0.75	0
4	EDO	A	408	-	3,3,3	0.64	0	2,2,2	0.12	0
4	EDO	A	409	-	3,3,3	0.67	0	2,2,2	1.36	0
4	EDO	B	402	-	3,3,3	0.40	0	2,2,2	1.08	0
4	EDO	B	403	-	3,3,3	0.36	0	2,2,2	0.63	0
4	EDO	B	404	-	3,3,3	0.54	0	2,2,2	0.21	0
4	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.18	0
4	EDO	B	406	-	3,3,3	0.28	0	2,2,2	0.96	0
3	SO4	C	402	-	4,4,4	0.65	0	6,6,6	0.78	0
4	EDO	C	403	-	3,3,3	0.67	0	2,2,2	0.45	0
4	EDO	C	404	-	3,3,3	0.52	0	2,2,2	0.25	0
4	EDO	C	405	-	3,3,3	0.38	0	2,2,2	0.98	0
4	EDO	C	406	-	3,3,3	0.34	0	2,2,2	0.76	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
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	EDO	A	405	-	-	0/1/1/1	0/0/0/0
4	EDO	A	406	-	-	0/1/1/1	0/0/0/0
4	EDO	A	407	-	-	0/1/1/1	0/0/0/0
4	EDO	A	408	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	409	-	-	0/1/1/1	0/0/0/0
4	EDO	B	402	-	-	0/1/1/1	0/0/0/0
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	EDO	B	406	-	-	0/1/1/1	0/0/0/0
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	EDO	C	403	-	-	0/1/1/1	0/0/0/0
4	EDO	C	404	-	-	0/1/1/1	0/0/0/0
4	EDO	C	405	-	-	0/1/1/1	0/0/0/0
4	EDO	C	406	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	1	0
4	A	407	EDO	5	0
4	A	409	EDO	3	0
4	B	402	EDO	1	0
4	B	403	EDO	1	0
4	B	405	EDO	1	0
4	C	405	EDO	2	0
4	C	406	EDO	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

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Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	212:SER	C	213:LEU	N	1.75
1	A	211:ASP	C	212:SER	N	1.17
1	C	211:ASP	C	212:SER	N	1.13

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	326/329 (99%)	-0.11	6 (1%) 71 76	6, 11, 25, 56	0
1	B	324/329 (98%)	-0.09	6 (1%) 70 75	6, 11, 25, 61	0
1	C	325/329 (98%)	-0.05	9 (2%) 56 64	7, 13, 26, 56	0
All	All	975/987 (98%)	-0.08	21 (2%) 65 71	6, 12, 26, 61	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	TRP	5.3
1	C	186	ASP	5.0
1	A	149	TRP	4.9
1	A	148	HIS	4.7
1	C	149	TRP	4.4
1	C	148	HIS	3.8
1	B	148	HIS	3.8
1	B	151	ASN	3.4
1	A	34	SER	3.4
1	A	147	SER	3.3
1	B	184	VAL	2.9
1	A	187	SER	2.9
1	C	185	SER	2.6
1	B	205[A]	LEU	2.6
1	B	147	SER	2.4
1	C	247	LEU	2.3
1	C	212	SER	2.3
1	A	151	ASN	2.3
1	C	146	PHE	2.2
1	C	145	TYR	2.1
1	C	183	THR	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 carbohydrates 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. 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	EDO	B	403	4/4	0.82	0.25	12.09	26,32,32,35	0
4	EDO	C	405	4/4	0.86	0.15	8.58	20,22,23,24	0
4	EDO	A	404	4/4	0.83	0.17	7.74	34,36,37,39	0
4	EDO	A	406	4/4	0.74	0.25	4.87	32,35,37,39	0
4	EDO	A	409	4/4	0.88	0.15	4.44	16,17,19,21	0
4	EDO	C	403	4/4	0.87	0.15	4.35	20,20,20,21	0
4	EDO	B	402	4/4	0.89	0.19	4.28	32,32,33,34	0
4	EDO	C	406	4/4	0.88	0.23	2.13	38,41,44,45	0
4	EDO	B	405	4/4	0.95	0.12	1.42	19,20,20,20	0
4	EDO	A	405	4/4	0.85	0.25	1.36	24,30,31,34	0
4	EDO	A	408	4/4	0.87	0.13	0.34	29,29,30,31	0
3	SO4	A	403	5/5	0.98	0.09	-1.35	13,14,14,15	0
2	ZN	B	401	1/1	0.99	0.03	-3.26	12,12,12,12	0
3	SO4	A	402	5/5	0.99	0.07	-3.44	11,12,12,12	0
2	ZN	C	401	1/1	1.00	0.03	-4.67	13,13,13,13	0
2	ZN	A	401	1/1	0.99	0.02	-4.92	13,13,13,13	0
4	EDO	B	406	4/4	0.87	0.27	-	46,46,48,50	0
4	EDO	B	404	4/4	0.73	0.27	-	44,44,44,46	0
4	EDO	C	404	4/4	0.85	0.32	-	36,37,39,39	0
4	EDO	A	407	4/4	0.93	0.20	-	18,20,23,27	0
3	SO4	C	402	5/5	0.99	0.07	-	12,13,13,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.