



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:04 AM GMT

PDB ID : 1OJN  
Title : SPECIFICITY AND MECHANISM OF STREPTOCOCCUS PNEUMONIAE HYALURONATE LYASE: COMPLEX OF THE TYR408PHE MUTANT WITH 6-SULPHATED CHONDROITIN DISACCHARIDE  
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Deposited on : 2003-07-11  
Resolution : 1.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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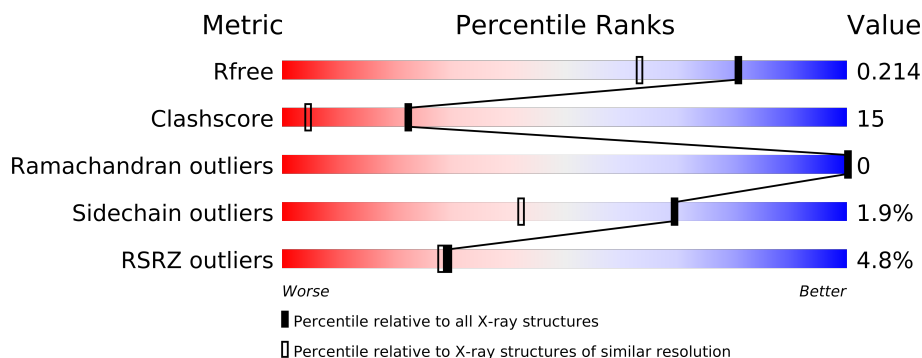
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.60 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	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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. 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	731	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1200	-	X
3	SO4	A	1201	-	X
3	SO4	A	1203	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6651 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 HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	723	5963	3750	1003	1188	22	0	19	1

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	893	HIS	-	EXPRESSION TAG	UNP Q54873
A	894	HIS	-	EXPRESSION TAG	UNP Q54873
A	895	HIS	-	EXPRESSION TAG	UNP Q54873
A	896	HIS	-	EXPRESSION TAG	UNP Q54873
A	897	HIS	-	EXPRESSION TAG	UNP Q54873
A	898	HIS	-	EXPRESSION TAG	UNP Q54873
A	173	THR	ALA	CONFLICT	UNP Q54873
A	196	ASP	GLU	CONFLICT	UNP Q54873
A	223	ILE	THR	CONFLICT	UNP Q54873
A	408	PHE	TYR	CONFLICT	UNP Q54873
A	496	ARG	CYS	CONFLICT	UNP Q54873
A	541	THR	PRO	CONFLICT	UNP Q54873
A	704	SER	GLY	CONFLICT	UNP Q54873
A	736	SER	PHE	CONFLICT	UNP Q54873
A	790	GLY	ARG	CONFLICT	UNP Q54873

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	2	30	14	1	14	1	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	893	HIS	-	EXPRESSION TAG	UNP Q54873

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Chain	Residue	Modelled	Actual	Comment	Reference
A	894	HIS	-	EXPRESSION TAG	UNP Q54873
A	895	HIS	-	EXPRESSION TAG	UNP Q54873
A	896	HIS	-	EXPRESSION TAG	UNP Q54873
A	897	HIS	-	EXPRESSION TAG	UNP Q54873
A	898	HIS	-	EXPRESSION TAG	UNP Q54873
A	173	THR	ALA	CONFLICT	UNP Q54873
A	196	ASP	GLU	CONFLICT	UNP Q54873
A	223	ILE	THR	CONFLICT	UNP Q54873
A	408	PHE	TYR	CONFLICT	UNP Q54873
A	496	ARG	CYS	CONFLICT	UNP Q54873
A	541	THR	PRO	CONFLICT	UNP Q54873
A	704	SER	GLY	CONFLICT	UNP Q54873
A	736	SER	PHE	CONFLICT	UNP Q54873
A	790	GLY	ARG	CONFLICT	UNP Q54873

- 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 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

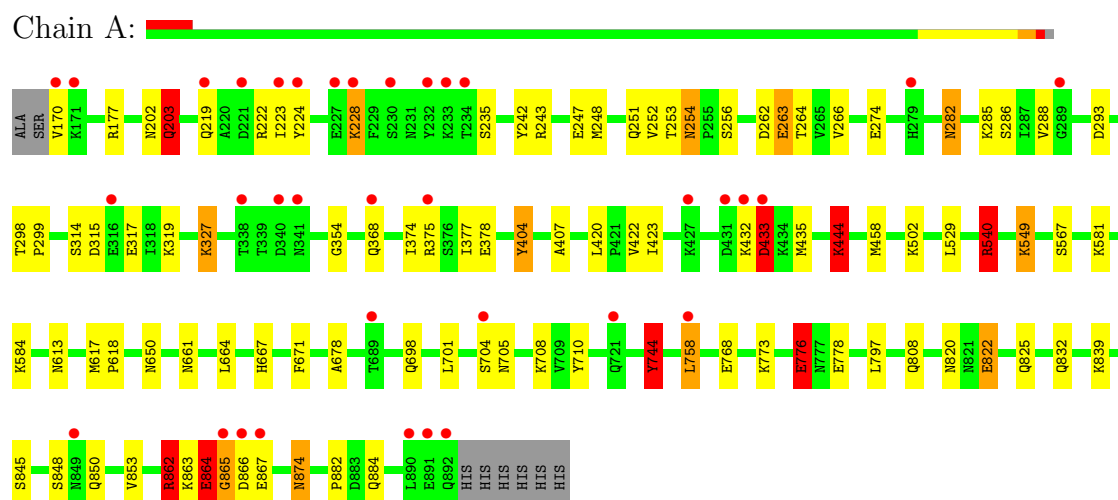
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	638	Total 638	O 638	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 ( $\text{RSRZ} > 2$ ). 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: HYALURONATE LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.91Å 104.20Å 101.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.08 – 1.60 40.57 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.08-1.60) 87.7 (40.57-1.45)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 1.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.194 , 0.209 0.202 , 0.214	Depositor DCC
$R_{free}$ test set	6870 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 40.5	EDS
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 139586 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NG6, GCD, SO4

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	5.29	38/6084 (0.6%)	3.28	61/8209 (0.7%)

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	7

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	776[A]	GLU	CD-OE1	179.73	3.23	1.25
1	A	776[B]	GLU	CD-OE1	179.73	3.23	1.25
1	A	203[A]	GLN	CD-NE2	130.08	4.58	1.32
1	A	203[B]	GLN	CD-NE2	130.08	4.58	1.32
1	A	862[A]	ARG	NE-CZ	103.38	2.67	1.33
1	A	862[B]	ARG	NE-CZ	103.38	2.67	1.33
1	A	432[A]	LYS	CD-CE	78.04	3.46	1.51
1	A	432[B]	LYS	CD-CE	78.04	3.46	1.51
1	A	744[A]	TYR	CD1-CE1	65.44	2.37	1.39
1	A	744[B]	TYR	CD1-CE1	65.44	2.37	1.39
1	A	744[A]	TYR	CG-CD1	55.78	2.11	1.39
1	A	744[B]	TYR	CG-CD1	55.78	2.11	1.39
1	A	433[A]	ASP	CG-OD2	54.79	2.51	1.25
1	A	433[B]	ASP	CG-OD2	54.79	2.51	1.25
1	A	776[A]	GLU	CD-OE2	53.88	1.84	1.25
1	A	776[B]	GLU	CD-OE2	53.88	1.84	1.25
1	A	203[A]	GLN	CG-CD	44.35	2.53	1.51
1	A	203[B]	GLN	CG-CD	44.35	2.53	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758[A]	LEU	CG-CD2	32.44	2.71	1.51
1	A	758[B]	LEU	CG-CD2	32.44	2.71	1.51
1	A	540[A]	ARG	NE-CZ	28.41	1.70	1.33
1	A	540[B]	ARG	NE-CZ	28.41	1.70	1.33
1	A	744[A]	TYR	CG-CD2	-23.80	1.08	1.39
1	A	744[B]	TYR	CG-CD2	-23.80	1.08	1.39
1	A	865[A]	GLY	CA-C	23.55	1.89	1.51
1	A	865[B]	GLY	CA-C	23.55	1.89	1.51
1	A	744[A]	TYR	CD2-CE2	15.71	1.62	1.39
1	A	744[B]	TYR	CD2-CE2	15.71	1.62	1.39
1	A	263[A]	GLU	CB-CG	-13.24	1.26	1.52
1	A	263[B]	GLU	CB-CG	-13.24	1.26	1.52
1	A	444[A]	LYS	CG-CD	10.81	1.89	1.52
1	A	444[B]	LYS	CG-CD	10.81	1.89	1.52
1	A	549[A]	LYS	CD-CE	9.35	1.74	1.51
1	A	549[B]	LYS	CD-CE	9.35	1.74	1.51
1	A	865[A]	GLY	N-CA	-6.20	1.36	1.46
1	A	865[B]	GLY	N-CA	-6.20	1.36	1.46
1	A	228[A]	LYS	CB-CG	5.26	1.66	1.52
1	A	228[B]	LYS	CB-CG	5.26	1.66	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	744[A]	TYR	CB-CG-CD2	78.14	167.89	121.00
1	A	744[B]	TYR	CB-CG-CD2	78.14	167.89	121.00
1	A	744[A]	TYR	CG-CD1-CE1	-70.15	65.18	121.30
1	A	744[B]	TYR	CG-CD1-CE1	-70.15	65.18	121.30
1	A	776[A]	GLU	OE1-CD-OE2	-68.68	40.88	123.30
1	A	776[B]	GLU	OE1-CD-OE2	-68.68	40.88	123.30
1	A	862[A]	ARG	NE-CZ-NH1	-59.67	90.47	120.30
1	A	862[B]	ARG	NE-CZ-NH1	-59.67	90.47	120.30
1	A	433[A]	ASP	CB-CG-OD2	-56.74	67.24	118.30
1	A	433[B]	ASP	CB-CG-OD2	-56.74	67.24	118.30
1	A	744[A]	TYR	CB-CG-CD1	-54.91	88.05	121.00
1	A	744[B]	TYR	CB-CG-CD1	-54.91	88.05	121.00
1	A	744[A]	TYR	CZ-CE2-CD2	-54.44	70.81	119.80
1	A	744[B]	TYR	CZ-CE2-CD2	-54.44	70.81	119.80
1	A	540[A]	ARG	NE-CZ-NH2	-46.01	97.29	120.30
1	A	540[B]	ARG	NE-CZ-NH2	-46.01	97.29	120.30
1	A	862[A]	ARG	CD-NE-CZ	-45.15	60.39	123.60
1	A	862[B]	ARG	CD-NE-CZ	-45.15	60.39	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540[A]	ARG	NE-CZ-NH1	44.27	142.43	120.30
1	A	540[B]	ARG	NE-CZ-NH1	44.27	142.43	120.30
1	A	203[A]	GLN	CG-CD-NE2	-39.50	21.89	116.70
1	A	203[B]	GLN	CG-CD-NE2	-39.50	21.89	116.70
1	A	758[A]	LEU	CB-CG-CD2	-26.68	65.65	111.00
1	A	758[B]	LEU	CB-CG-CD2	-26.68	65.65	111.00
1	A	203[A]	GLN	CG-CD-OE1	-26.10	69.39	121.60
1	A	203[B]	GLN	CG-CD-OE1	-26.10	69.39	121.60
1	A	203[A]	GLN	OE1-CD-NE2	-25.25	63.81	121.90
1	A	203[B]	GLN	OE1-CD-NE2	-25.25	63.81	121.90
1	A	862[A]	ARG	NE-CZ-NH2	25.13	132.87	120.30
1	A	862[B]	ARG	NE-CZ-NH2	25.13	132.87	120.30
1	A	744[A]	TYR	CD1-CE1-CZ	24.73	142.06	119.80
1	A	744[B]	TYR	CD1-CE1-CZ	24.73	142.06	119.80
1	A	744[A]	TYR	CD1-CG-CD2	-24.15	91.33	117.90
1	A	744[B]	TYR	CD1-CG-CD2	-24.15	91.33	117.90
1	A	433[A]	ASP	OD1-CG-OD2	21.87	164.85	123.30
1	A	433[B]	ASP	OD1-CG-OD2	21.87	164.85	123.30
1	A	540[A]	ARG	CD-NE-CZ	-21.61	93.34	123.60
1	A	540[B]	ARG	CD-NE-CZ	-21.61	93.34	123.60
1	A	758[A]	LEU	CD1-CG-CD2	-20.27	49.68	110.50
1	A	758[B]	LEU	CD1-CG-CD2	-20.27	49.68	110.50
1	A	444[A]	LYS	CG-CD-CE	17.61	164.73	111.90
1	A	444[B]	LYS	CG-CD-CE	17.61	164.73	111.90
1	A	203[A]	GLN	CB-CG-CD	-14.86	72.98	111.60
1	A	203[B]	GLN	CB-CG-CD	-14.86	72.98	111.60
1	A	776[A]	GLU	CG-CD-OE1	-13.45	91.39	118.30
1	A	776[B]	GLU	CG-CD-OE1	-13.45	91.39	118.30
1	A	865[A]	GLY	CA-C-O	12.36	142.85	120.60
1	A	865[B]	GLY	CA-C-O	12.36	142.85	120.60
1	A	865[A]	GLY	CA-C-N	-11.42	92.08	117.20
1	A	865[B]	GLY	CA-C-N	-11.42	92.08	117.20
1	A	263[A]	GLU	CA-CB-CG	7.00	128.80	113.40
1	A	263[B]	GLU	CA-CB-CG	7.00	128.80	113.40
1	A	432[A]	LYS	CD-CE-NZ	-6.76	96.16	111.70
1	A	432[B]	LYS	CD-CE-NZ	-6.76	96.16	111.70
1	A	776[A]	GLU	CG-CD-OE2	-6.33	105.63	118.30
1	A	776[B]	GLU	CG-CD-OE2	-6.33	105.63	118.30
1	A	444[A]	LYS	CB-CG-CD	-6.18	95.52	111.60
1	A	444[B]	LYS	CB-CG-CD	-6.18	95.52	111.60
1	A	744[A]	TYR	CG-CD2-CE2	5.70	125.86	121.30
1	A	744[B]	TYR	CG-CD2-CE2	5.70	125.86	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	864	GLU	C-N-CA	5.65	134.17	122.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203[A]	GLN	Sidechain
1	A	433[A]	ASP	Sidechain
1	A	540[A]	ARG	Sidechain
1	A	744[A]	TYR	Sidechain
1	A	776[A]	GLU	Sidechain
1	A	862[A]	ARG	Sidechain
1	A	864	GLU	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	5963	0	5779	177	0
2	A	30	0	19	0	0
3	A	20	0	0	1	0
4	A	638	0	0	7	0
All	All	6651	0	5798	177	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 15.

All (177) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:549[A]:LYS:CD	1:A:549[A]:LYS:CE	1.74	1.64
1:A:444[B]:LYS:CG	1:A:444[B]:LYS:CD	1.78	1.61
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:HD13	1.26	1.56
1:A:540[A]:ARG:NE	1:A:540[A]:ARG:CZ	1.70	1.55
1:A:758[A]:LEU:HD13	1:A:758[A]:LEU:CD2	1.32	1.53
1:A:444[A]:LYS:CD	1:A:444[A]:LYS:CG	1.89	1.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:865[B]:GLY:N	1:A:865[B]:GLY:CA	1.70	1.48
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:CD1	2.00	1.39
1:A:865[A]:GLY:CA	1:A:865[A]:GLY:C	1.89	1.38
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:CG	2.10	1.38
1:A:744[A]:TYR:CG	1:A:744[A]:TYR:CD1	2.11	1.38
1:A:865[B]:GLY:C	1:A:865[B]:GLY:CA	1.93	1.36
1:A:758[A]:LEU:CD1	1:A:758[A]:LEU:CD2	2.08	1.29
1:A:862[A]:ARG:HD3	1:A:862[A]:ARG:CZ	1.63	1.28
1:A:540[B]:ARG:NE	1:A:540[B]:ARG:CZ	2.02	1.22
1:A:203[B]:GLN:HG2	1:A:203[B]:GLN:NE2	1.51	1.22
1:A:203[A]:GLN:NE2	1:A:203[A]:GLN:HG2	1.57	1.17
1:A:758[A]:LEU:HD11	1:A:776[A]:GLU:HG2	1.21	1.15
1:A:776[A]:GLU:OE2	1:A:776[A]:GLU:CD	1.84	1.14
1:A:744[A]:TYR:CE1	1:A:744[A]:TYR:CD1	2.37	1.13
1:A:744[B]:TYR:CD1	1:A:744[B]:TYR:CD2	2.39	1.10
1:A:758[A]:LEU:HD13	1:A:758[A]:LEU:HD21	1.23	1.09
1:A:540[A]:ARG:CD	1:A:540[A]:ARG:CZ	2.30	1.09
1:A:744[A]:TYR:CD2	1:A:744[A]:TYR:CD1	2.39	1.09
1:A:758[B]:LEU:HD21	1:A:758[B]:LEU:HD13	1.15	1.08
1:A:862[A]:ARG:CZ	1:A:862[A]:ARG:CD	2.33	1.07
1:A:758[A]:LEU:HB2	1:A:758[A]:LEU:CD2	1.86	1.06
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:CE2	2.46	1.04
1:A:444[B]:LYS:CD	1:A:444[B]:LYS:CB	2.37	1.03
1:A:758[A]:LEU:HD11	1:A:776[A]:GLU:CG	1.93	0.98
1:A:613:ASN:H	1:A:698:GLN:HE22	1.03	0.98
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:HB3	1.93	0.98
1:A:444[B]:LYS:HB3	1:A:444[B]:LYS:HD2	1.46	0.95
1:A:744[A]:TYR:CB	1:A:744[A]:TYR:CD1	2.53	0.92
1:A:744[B]:TYR:CB	1:A:744[B]:TYR:CD2	2.52	0.92
1:A:203[B]:GLN:HB3	1:A:203[B]:GLN:CD	1.91	0.91
1:A:433[A]:ASP:OD2	1:A:433[A]:ASP:HB3	1.69	0.91
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:CB	2.49	0.90
1:A:758[A]:LEU:HG	1:A:776[A]:GLU:CD	1.92	0.90
1:A:865[A]:GLY:CA	1:A:866:ASP:N	2.35	0.90
1:A:864:GLU:C	1:A:865[B]:GLY:CA	2.40	0.89
1:A:758[A]:LEU:CB	1:A:758[A]:LEU:CD2	2.50	0.88
1:A:444[B]:LYS:HD2	1:A:444[B]:LYS:CB	2.02	0.88
1:A:865[B]:GLY:CA	1:A:866:ASP:N	2.37	0.88
1:A:444[A]:LYS:CD	1:A:444[A]:LYS:CB	2.53	0.85
1:A:540[A]:ARG:HD3	1:A:540[A]:ARG:CZ	2.05	0.84
1:A:433[B]:ASP:HB2	1:A:433[B]:ASP:OD2	1.76	0.83
1:A:758[A]:LEU:CD1	1:A:776[A]:GLU:HG2	2.05	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:865[B]:GLY:N	1:A:865[B]:GLY:C	2.33	0.81
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:HD1	1.97	0.81
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:NE2	2.42	0.81
1:A:444[A]:LYS:HB2	1:A:444[A]:LYS:HD2	1.62	0.81
1:A:862[B]:ARG:HD2	1:A:862[B]:ARG:CZ	2.11	0.80
1:A:540[A]:ARG:NH2	1:A:540[A]:ARG:NE	2.28	0.80
1:A:549[A]:LYS:CE	1:A:549[A]:LYS:CG	2.59	0.80
1:A:744[B]:TYR:HB3	1:A:744[B]:TYR:CD2	2.15	0.79
1:A:758[A]:LEU:CG	1:A:776[A]:GLU:CD	2.51	0.79
1:A:758[A]:LEU:CD1	1:A:776[A]:GLU:CG	2.60	0.77
1:A:203[A]:GLN:CB	1:A:203[A]:GLN:CD	2.52	0.77
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:CD	2.53	0.77
1:A:203[A]:GLN:HB2	1:A:203[A]:GLN:CD	2.05	0.76
1:A:203[B]:GLN:CB	1:A:203[B]:GLN:CD	2.53	0.76
1:A:444[B]:LYS:HB3	1:A:444[B]:LYS:CD	2.10	0.76
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:NE2	2.42	0.74
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:CG	2.65	0.74
1:A:744[A]:TYR:HB2	1:A:744[A]:TYR:CD1	2.20	0.74
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.04	0.72
1:A:862[B]:ARG:NE	1:A:862[B]:ARG:CZ	2.52	0.72
1:A:444[B]:LYS:CG	1:A:444[B]:LYS:HD3	2.11	0.72
1:A:433[A]:ASP:OD2	1:A:433[A]:ASP:CB	2.38	0.71
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:OE1	2.39	0.70
1:A:433[B]:ASP:CB	1:A:433[B]:ASP:OD2	2.40	0.70
1:A:862[B]:ARG:CD	1:A:862[B]:ARG:CZ	2.70	0.70
1:A:248:MET:O	1:A:252[A]:VAL:HG23	1.91	0.69
1:A:444[A]:LYS:CB	1:A:444[A]:LYS:HD2	2.21	0.69
1:A:758[A]:LEU:CG	1:A:758[A]:LEU:CD2	2.71	0.68
1:A:540[B]:ARG:HG2	1:A:540[B]:ARG:HH11	1.59	0.68
1:A:444[A]:LYS:HD3	1:A:444[A]:LYS:CG	2.19	0.67
1:A:708:LYS:HE3	1:A:710:TYR:OH	1.95	0.67
1:A:744[A]:TYR:HD2	1:A:744[A]:TYR:CD1	2.06	0.66
1:A:540[B]:ARG:HG2	1:A:540[B]:ARG:NH1	2.11	0.65
1:A:433[B]:ASP:OD2	1:A:433[B]:ASP:CG	2.36	0.64
1:A:529:LEU:HD23	1:A:529:LEU:C	2.18	0.64
1:A:549[A]:LYS:CD	1:A:549[A]:LYS:NZ	2.56	0.64
1:A:862[B]:ARG:NE	1:A:862[B]:ARG:HH11	1.97	0.63
1:A:701:LEU:HD12	1:A:778:GLU:HG2	1.81	0.62
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:CD	2.67	0.62
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:HD12	2.23	0.62
1:A:874:ASN:HD22	1:A:874:ASN:C	2.03	0.61
1:A:862[B]:ARG:NE	1:A:862[B]:ARG:NH1	2.49	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:315:ASP:O	1:A:319[A]:LYS:HG3	2.01	0.60
1:A:776[B]:GLU:OE2	1:A:776[B]:GLU:OE1	2.20	0.60
1:A:776[A]:GLU:OE1	1:A:776[A]:GLU:OE2	2.20	0.60
1:A:865[A]:GLY:N	1:A:865[A]:GLY:C	2.53	0.60
1:A:584:LYS:NZ	1:A:768:GLU:HG2	2.18	0.59
1:A:444[A]:LYS:CD	1:A:444[A]:LYS:HB2	2.23	0.59
1:A:243:ARG:O	1:A:247:GLU:HG3	2.04	0.58
1:A:758[A]:LEU:CG	1:A:776[A]:GLU:CG	2.82	0.58
1:A:282:ASN:HD22	1:A:282:ASN:C	2.06	0.58
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.86	0.57
1:A:223:ILE:HG13	1:A:224:TYR:CD2	2.39	0.57
1:A:882:PRO:HB2	1:A:884:GLN:HE22	1.69	0.57
1:A:862[A]:ARG:NE	1:A:862[A]:ARG:CZ	2.67	0.57
1:A:758[A]:LEU:HD23	1:A:758[A]:LEU:HB2	1.81	0.56
1:A:808[A]:GLN:HG3	4:A:2573:HOH:O	2.05	0.55
1:A:264:THR:HG22	4:A:2082:HOH:O	2.05	0.55
1:A:822:GLU:CD	1:A:822:GLU:H	2.09	0.55
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.54	0.55
1:A:865[A]:GLY:C	1:A:867:GLU:H	2.10	0.54
1:A:864:GLU:O	1:A:865[A]:GLY:C	2.45	0.54
1:A:704[A]:SER:C	1:A:705:ASN:HD22	2.12	0.54
1:A:758[A]:LEU:HD22	1:A:778:GLU:HB2	1.90	0.53
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:OE1	2.56	0.53
1:A:327:LYS:HD3	1:A:327:LYS:C	2.29	0.53
1:A:882:PRO:HB2	1:A:884:GLN:NE2	2.23	0.53
1:A:254:ASN:HD22	1:A:254:ASN:C	2.12	0.53
1:A:540[A]:ARG:HD3	1:A:540[A]:ARG:NH1	2.23	0.53
1:A:758[B]:LEU:HD23	1:A:758[B]:LEU:HB3	1.83	0.53
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.73	0.53
1:A:704[B]:SER:C	1:A:705:ASN:HD22	2.13	0.52
1:A:864:GLU:O	1:A:865[A]:GLY:O	2.27	0.52
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.91	0.52
1:A:502:LYS:HB2	1:A:529:LEU:HD21	1.91	0.52
1:A:248:MET:O	1:A:252[B]:VAL:HG13	2.09	0.51
1:A:502:LYS:CB	1:A:529:LEU:HD21	2.41	0.51
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.93	0.51
1:A:298:THR:HB	1:A:299:PRO:HD3	1.93	0.50
1:A:862[A]:ARG:NH1	1:A:862[A]:ARG:CD	2.73	0.50
1:A:433[A]:ASP:OD2	1:A:433[A]:ASP:CG	2.51	0.49
1:A:863:LYS:HE2	1:A:865[B]:GLY:O	2.12	0.49
1:A:584:LYS:HE2	3:A:1200:SO4:O1	2.14	0.48
1:A:420:LEU:HD13	1:A:435:MET:CE	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:374:ILE:HD13	1:A:423:ILE:HG23	1.96	0.47
1:A:235:SER:HB2	1:A:293:ASP:HB2	1.97	0.47
1:A:671:PHE:HB2	1:A:678:ALA:HB3	1.97	0.47
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.95	0.47
1:A:314:SER:OG	1:A:317:GLU:HG3	2.16	0.46
1:A:420:LEU:HD13	1:A:435:MET:HE3	1.98	0.46
1:A:864:GLU:O	1:A:865[B]:GLY:CA	2.63	0.46
1:A:848:SER:O	1:A:850:GLN:HG3	2.16	0.46
1:A:286:SER:O	1:A:288:VAL:HG23	2.16	0.45
1:A:458:MET:HE2	1:A:567:SER:HB2	1.98	0.45
1:A:242:TYR:CD2	1:A:298:THR:HG23	2.52	0.45
1:A:758[A]:LEU:HD12	1:A:758[A]:LEU:CD2	2.31	0.45
1:A:254:ASN:ND2	1:A:256:SER:H	2.15	0.44
1:A:374:ILE:O	1:A:378:GLU:HG3	2.18	0.44
1:A:758[A]:LEU:HD11	1:A:776[A]:GLU:CD	2.39	0.44
1:A:549[A]:LYS:HE3	4:A:2612:HOH:O	2.18	0.43
1:A:808[A]:GLN:HG2	4:A:2566:HOH:O	2.18	0.43
1:A:375:ARG:HD3	4:A:2182:HOH:O	2.18	0.43
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.54	0.43
1:A:664:LEU:C	1:A:664:LEU:HD23	2.39	0.43
1:A:170:VAL:HG23	1:A:315:ASP:OD2	2.18	0.43
1:A:422:VAL:HA	4:A:2009:HOH:O	2.18	0.43
1:A:254:ASN:C	1:A:254:ASN:ND2	2.72	0.42
1:A:540[B]:ARG:HG2	1:A:540[B]:ARG:CZ	2.49	0.42
1:A:650:ASN:ND2	1:A:862[A]:ARG:NH2	2.68	0.42
1:A:882:PRO:CB	1:A:884:GLN:HE22	2.31	0.42
1:A:581:LYS:HD3	1:A:768:GLU:HG3	2.02	0.42
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.49	0.42
1:A:252[B]:VAL:HG23	1:A:253:THR:HG23	2.01	0.42
1:A:228[B]:LYS:HG2	1:A:228[B]:LYS:O	2.19	0.42
1:A:282:ASN:HD21	1:A:285:LYS:HG2	1.81	0.41
1:A:222:ARG:HG2	1:A:222:ARG:H	1.61	0.41
1:A:744[A]:TYR:CZ	1:A:797:LEU:HD13	2.55	0.41
1:A:584:LYS:HZ2	1:A:768:GLU:HG2	1.84	0.41
1:A:667:HIS:HD2	4:A:2583:HOH:O	2.03	0.41
1:A:617:MET:HA	1:A:618[B]:PRO:HD3	1.95	0.41
1:A:865[A]:GLY:O	1:A:867:GLU:N	2.54	0.40
1:A:274:GLU:OE1	1:A:274:GLU:HA	2.21	0.40
1:A:671:PHE:CD1	1:A:671:PHE:N	2.89	0.40
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.18	0.40
1:A:458:MET:HE2	1:A:458:MET:HB3	1.82	0.40
1:A:177:ARG:NE	1:A:177:ARG:HA	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:ASP:O	1:A:266:VAL:HG23	2.20	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	740/731 (101%)	715 (97%)	25 (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	659/649 (102%)	645 (98%)	14 (2%)	66	37

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	254	ASN
1	A	263[A]	GLU
1	A	263[B]	GLU
1	A	282	ASN
1	A	327	LYS
1	A	368	GLN
1	A	404	TYR
1	A	444[A]	LYS

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Mol	Chain	Res	Type
1	A	444[B]	LYS
1	A	661	ASN
1	A	773	LYS
1	A	822	GLU
1	A	874	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	231	ASN
1	A	237	ASN
1	A	254	ASN
1	A	261	GLN
1	A	277	HIS
1	A	282	ASN
1	A	368	GLN
1	A	386	GLN
1	A	392	GLN
1	A	418	GLN
1	A	580	ASN
1	A	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	759	GLN
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	ASN

### 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 ⓘ

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GCD	A	900	2	10,11,12	5.32	4 (40%)	11,15,17	3.43	8 (72%)
2	NG6	A	901	2	19,19,19	2.33	7 (36%)	28,28,28	4.65	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GCD	A	900	2	-	0/4/17/20	0/1/1/1
2	NG6	A	901	2	-	0/10/30/30	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	GCD	O5-C5	15.77	1.55	1.37
2	A	901	NG6	C2-N	4.87	1.54	1.45
2	A	901	NG6	O5-C1	4.76	1.52	1.43
2	A	900	GCD	C3-C4	4.00	1.55	1.50
2	A	901	NG6	O5-C5	3.70	1.53	1.44
2	A	901	NG6	C4-C3	2.96	1.60	1.52
2	A	901	NG6	O6-S	-2.80	1.47	1.57
2	A	901	NG6	C7-N	2.64	1.45	1.34
2	A	900	GCD	C4-C5	2.36	1.37	1.33
2	A	901	NG6	C1-C2	2.30	1.55	1.53
2	A	900	GCD	O6A-C6	2.26	1.29	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NG6	C6-O6-S	23.00	146.34	116.76
2	A	900	GCD	O3-C3-C2	-6.67	102.22	111.03
2	A	901	NG6	O6-C6-C5	6.65	120.46	107.81
2	A	900	GCD	C2-C3-C4	4.54	120.04	111.68
2	A	900	GCD	O3-C3-C4	4.18	119.58	109.67
2	A	900	GCD	O5-C5-C4	-3.75	118.19	122.91
2	A	900	GCD	O5-C5-C6	3.27	116.91	111.75
2	A	900	GCD	O6B-C6-O6A	2.92	130.54	123.62
2	A	900	GCD	C3-C4-C5	-2.48	117.61	121.82
2	A	901	NG6	O4-C4-C5	2.39	115.58	109.28
2	A	901	NG6	O4-C4-C3	-2.37	105.03	110.35
2	A	900	GCD	O2-C2-C3	-2.28	108.03	111.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	1200	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	A	1201	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	A	1202	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	A	1203	-	4,4,4	0.39	0	6,6,6	0.08	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	1200	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1201	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1202	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1203	-	-	0/0/0/0	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.

## 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, 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	723/731 (98%)	0.07	35 (4%) 29 28	11, 21, 39, 56	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	892	GLN	11.2
1	A	221	ASP	6.2
1	A	340	ASP	5.5
1	A	891	GLU	5.3
1	A	427	LYS	4.8
1	A	375	ARG	3.6
1	A	279	HIS	3.5
1	A	224	TYR	3.4
1	A	866	ASP	3.4
1	A	316	GLU	3.3
1	A	171	LYS	3.3
1	A	234	THR	3.2
1	A	223	ILE	3.2
1	A	865[A]	GLY	3.2
1	A	233	LYS	3.1
1	A	368	GLN	3.1
1	A	341	ASN	3.0
1	A	170	VAL	2.9
1	A	230	SER	2.9
1	A	689	THR	2.6
1	A	721	GLN	2.6
1	A	704[A]	SER	2.5
1	A	849	ASN	2.5
1	A	431	ASP	2.4
1	A	219	GLN	2.3
1	A	867	GLU	2.3
1	A	338	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	432[A]	LYS	2.3
1	A	227	GLU	2.2
1	A	232	TYR	2.2
1	A	433[A]	ASP	2.1
1	A	228[A]	LYS	2.1
1	A	890	LEU	2.1
1	A	289	GLY	2.0
1	A	758[A]	LEU	2.0

## 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NG6	A	901	19/19	0.17	2.04	23,31,49,52	0
2	GCD	A	900	11/12	0.15	1.50	25,32,37,38	0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1201	5/5	0.12	9.58	29,35,42,43	0
3	SO4	A	1203	5/5	0.29	5.22	62,63,63,65	0
3	SO4	A	1200	5/5	0.22	2.10	39,47,53,53	0
3	SO4	A	1202	5/5	0.17	1.74	53,54,55,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.