



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:20 PM GMT

PDB ID : 1OJM
Title : SPECIFICITY AND MECHANISM OF STREPTOCOCCUS PNEUMONIAE HYALURONATE LYASE: COMPLEX WITH UNSULPHATED CHONDROITIN DISACCHARIDE
Authors : Rigden, D.J.; Jedrzejas, M.J.
Deposited on : 2003-07-11
Resolution : 1.78 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

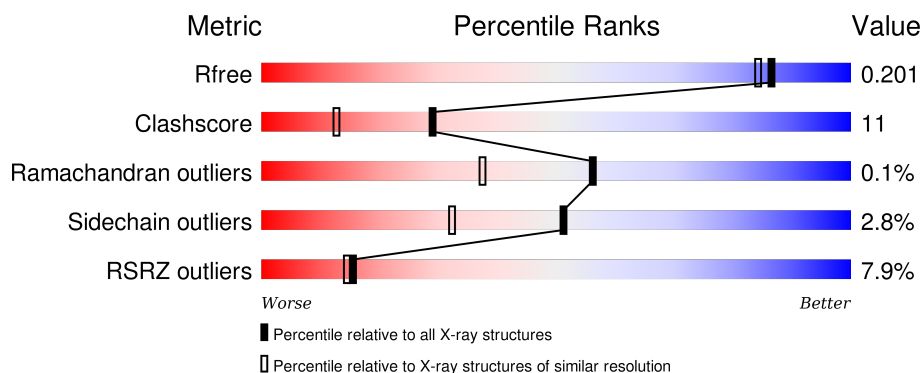
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	729	<div> <div>8%</div> <div>84%</div> <div>12% ...</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6514 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 HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	12	1
			5897	3710	991	1174	22			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	VAL	-	EXPRESSION TAG	UNP Q54873
A	171	LYS	-	EXPRESSION TAG	UNP Q54873
A	172	ASP	-	EXPRESSION TAG	UNP Q54873
A	173	THR	-	EXPRESSION TAG	UNP Q54873
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	196	ASP	GLU	CONFLICT	UNP Q54873
A	223	ILE	THR	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
2	A	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

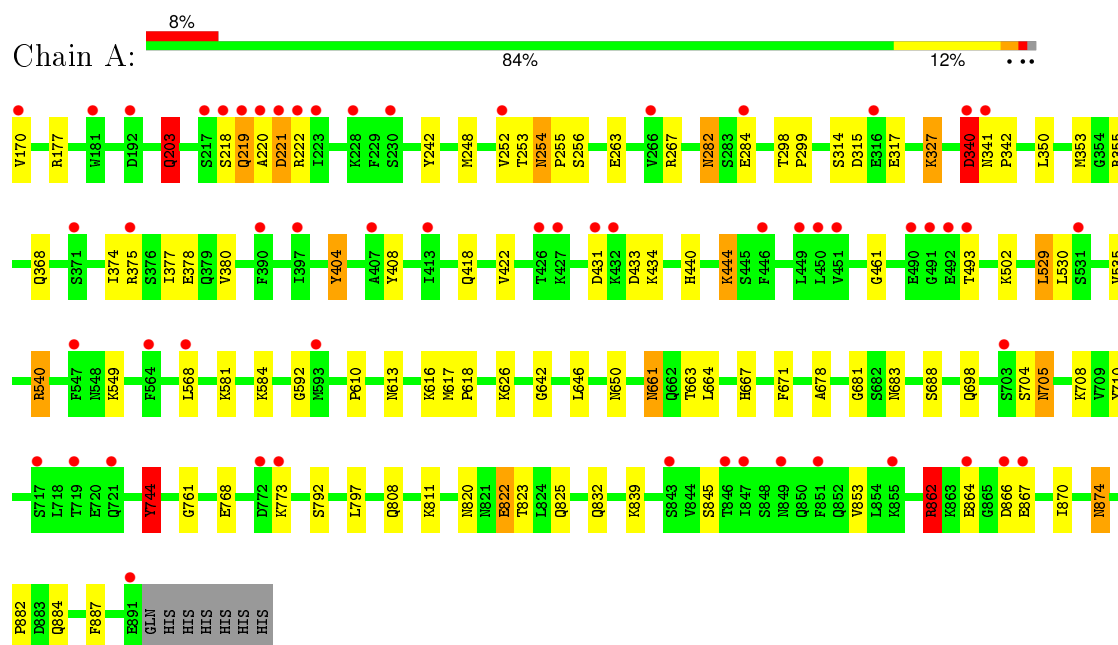
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	571	Total	O	0	0
			571	571		

3 Residue-property plots [i](#)

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: HYALURONATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.66Å 104.27Å 98.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.38 – 1.78 40.38 – 1.77	Depositor EDS
% Data completeness (in resolution range)	84.2 (40.38-1.78) 83.9 (40.38-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.224 0.198 , 0.201	Depositor DCC
R_{free} test set	3551 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.921	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71120 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6514	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

5.1 Standard geometry

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

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	4.11	18/6018 (0.3%)	2.93	28/8125 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203[A]	GLN	CD-NE2	134.01	4.67	1.32
1	A	203[B]	GLN	CD-NE2	134.01	4.67	1.32
1	A	340[A]	ASP	CG-OD1	109.41	3.77	1.25
1	A	340[B]	ASP	CG-OD1	109.41	3.77	1.25
1	A	340[A]	ASP	CG-OD2	87.72	3.27	1.25
1	A	340[B]	ASP	CG-OD2	87.72	3.27	1.25
1	A	744[A]	TYR	CZ-OH	79.06	2.72	1.37
1	A	744[B]	TYR	CZ-OH	79.06	2.72	1.37
1	A	862[A]	ARG	CZ-NH2	53.95	2.03	1.33
1	A	862[B]	ARG	CZ-NH2	53.95	2.03	1.33
1	A	203[A]	GLN	CG-CD	49.09	2.63	1.51
1	A	203[B]	GLN	CG-CD	49.09	2.63	1.51
1	A	444[A]	LYS	CD-CE	32.49	2.32	1.51
1	A	444[B]	LYS	CD-CE	32.49	2.32	1.51
1	A	862[A]	ARG	CZ-NH1	5.60	1.40	1.33
1	A	862[B]	ARG	CZ-NH1	5.60	1.40	1.33
1	A	203[A]	GLN	CB-CG	5.39	1.67	1.52
1	A	203[B]	GLN	CB-CG	5.39	1.67	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	340[A]	ASP	CB-CG-OD1	-109.87	19.42	118.30
1	A	340[B]	ASP	CB-CG-OD1	-109.87	19.42	118.30
1	A	340[A]	ASP	CB-CG-OD2	-83.70	42.97	118.30
1	A	340[B]	ASP	CB-CG-OD2	-83.70	42.97	118.30
1	A	862[A]	ARG	NE-CZ-NH1	-61.54	89.53	120.30
1	A	862[B]	ARG	NE-CZ-NH1	-61.54	89.53	120.30
1	A	862[A]	ARG	NE-CZ-NH2	56.47	148.53	120.30
1	A	862[B]	ARG	NE-CZ-NH2	56.47	148.53	120.30
1	A	340[A]	ASP	OD1-CG-OD2	-46.18	35.56	123.30
1	A	340[B]	ASP	OD1-CG-OD2	-46.18	35.56	123.30
1	A	203[A]	GLN	CG-CD-NE2	-39.56	21.76	116.70
1	A	203[B]	GLN	CG-CD-NE2	-39.56	21.76	116.70
1	A	862[A]	ARG	NH1-CZ-NH2	-34.23	81.75	119.40
1	A	862[B]	ARG	NH1-CZ-NH2	-34.23	81.75	119.40
1	A	744[A]	TYR	OH-CZ-CE2	-27.73	45.22	120.10
1	A	744[B]	TYR	OH-CZ-CE2	-27.73	45.22	120.10
1	A	203[A]	GLN	CG-CD-OE1	-23.68	74.25	121.60
1	A	203[B]	GLN	CG-CD-OE1	-23.68	74.25	121.60
1	A	203[A]	GLN	OE1-CD-NE2	-18.81	78.64	121.90
1	A	203[B]	GLN	OE1-CD-NE2	-18.81	78.64	121.90
1	A	203[A]	GLN	CB-CG-CD	-16.98	67.45	111.60
1	A	203[B]	GLN	CB-CG-CD	-16.98	67.45	111.60
1	A	744[A]	TYR	CE1-CZ-OH	15.22	161.20	120.10
1	A	744[B]	TYR	CE1-CZ-OH	15.22	161.20	120.10
1	A	444[A]	LYS	CG-CD-CE	-11.71	76.78	111.90
1	A	444[B]	LYS	CG-CD-CE	-11.71	76.78	111.90
1	A	540[A]	ARG	CG-CD-NE	-5.24	100.80	111.80
1	A	540[B]	ARG	CG-CD-NE	-5.24	100.80	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203[A]	GLN	Sidechain
1	A	340[A]	ASP	Sidechain
1	A	744[A]	TYR	Sidechain
1	A	862[A]	ARG	Sidechain

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	5897	0	5717	133	0
2	A	26	0	19	2	0
3	A	20	0	0	1	0
4	A	571	0	0	17	0
All	All	6514	0	5736	133	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 11.

All (133) 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:549[B]:LYS:CD	1:A:549[B]:LYS:CE	1.78	1.61
1:A:444[B]:LYS:CG	1:A:444[B]:LYS:CD	1.93	1.47
1:A:862[B]:ARG:NH2	1:A:862[B]:ARG:CZ	1.87	1.37
1:A:744[A]:TYR:HE2	1:A:744[A]:TYR:OH	1.18	1.24
1:A:444[B]:LYS:CD	1:A:444[B]:LYS:CE	2.14	1.23
1:A:203[A]:GLN:HG2	1:A:203[A]:GLN:NE2	1.54	1.22
1:A:862[A]:ARG:NH2	1:A:862[A]:ARG:CZ	2.03	1.21
1:A:744[B]:TYR:HE1	1:A:744[B]:TYR:OH	1.20	1.21
1:A:203[B]:GLN:HG2	1:A:203[B]:GLN:NE2	1.61	1.15
1:A:744[A]:TYR:CE2	1:A:744[A]:TYR:OH	2.00	1.13
1:A:744[B]:TYR:OH	1:A:744[B]:TYR:CE1	2.05	1.09
1:A:444[A]:LYS:CD	1:A:444[A]:LYS:CE	2.32	1.06
1:A:613:ASN:H	1:A:698:GLN:HE22	1.07	0.96
1:A:218:SER:O	1:A:220:ALA:N	1.99	0.94
1:A:444[B]:LYS:CB	1:A:444[B]:LYS:CD	2.51	0.88
1:A:444[A]:LYS:CE	1:A:444[A]:LYS:CG	2.52	0.87
1:A:444[B]:LYS:CG	1:A:444[B]:LYS:CE	2.53	0.87
1:A:340[A]:ASP:OD1	1:A:340[A]:ASP:HB3	1.75	0.87
1:A:203[A]:GLN:CD	1:A:203[A]:GLN:HB3	1.94	0.86
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:CD	2.47	0.82
1:A:340[B]:ASP:OD1	1:A:340[B]:ASP:HB2	1.79	0.81
1:A:444[A]:LYS:CE	1:A:444[A]:LYS:HG3	2.11	0.81
1:A:862[A]:ARG:NH2	1:A:862[A]:ARG:NH1	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:NE2	2.43	0.80
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:NE2	2.43	0.79
1:A:444[B]:LYS:HB2	1:A:444[B]:LYS:CD	2.12	0.79
1:A:203[A]:GLN:CB	1:A:203[A]:GLN:CD	2.52	0.78
1:A:549[B]:LYS:CG	1:A:549[B]:LYS:CE	2.60	0.78
1:A:340[A]:ASP:HB2	1:A:340[A]:ASP:OD2	1.86	0.76
1:A:203[B]:GLN:CB	1:A:203[B]:GLN:CD	2.55	0.74
1:A:444[A]:LYS:HE3	1:A:444[A]:LYS:HG3	1.69	0.74
1:A:340[B]:ASP:HB3	1:A:340[B]:ASP:OD2	1.88	0.73
1:A:493:THR:HG22	4:A:2271:HOH:O	1.87	0.73
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:OE1	2.37	0.72
1:A:761:GLY:C	4:A:2487:HOH:O	2.29	0.71
1:A:340[A]:ASP:OD1	1:A:340[A]:ASP:CB	2.38	0.71
1:A:340[A]:ASP:OD2	1:A:340[A]:ASP:CB	2.39	0.71
1:A:203[B]:GLN:HB2	1:A:203[B]:GLN:CD	2.11	0.70
1:A:340[B]:ASP:CB	1:A:340[B]:ASP:OD1	2.38	0.70
1:A:340[B]:ASP:CB	1:A:340[B]:ASP:OD2	2.40	0.69
1:A:549[B]:LYS:CD	1:A:549[B]:LYS:NZ	2.55	0.69
1:A:248:MET:O	1:A:252[B]:VAL:HG23	1.93	0.68
1:A:444[B]:LYS:HE3	1:A:444[B]:LYS:HG3	1.77	0.66
1:A:529:LEU:HD23	1:A:529:LEU:C	2.14	0.66
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:CD	2.63	0.66
1:A:282:ASN:HD22	1:A:284:GLU:H	1.45	0.65
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.44	0.63
1:A:444[B]:LYS:HG3	1:A:444[B]:LYS:CE	2.28	0.63
1:A:808:GLN:HG3	4:A:2518:HOH:O	1.99	0.62
1:A:882:PRO:HB2	1:A:884:GLN:NE2	2.16	0.61
1:A:440:HIS:NE2	1:A:444[B]:LYS:HD3	2.16	0.61
1:A:254:ASN:C	1:A:254:ASN:HD22	2.02	0.61
1:A:862[B]:ARG:NH2	1:A:862[B]:ARG:NH1	2.29	0.60
1:A:874:ASN:HD22	1:A:874:ASN:C	2.05	0.60
1:A:340[A]:ASP:OD1	1:A:340[A]:ASP:OD2	2.20	0.59
1:A:340[B]:ASP:OD1	1:A:340[B]:ASP:OD2	2.19	0.59
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.82	0.59
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.86	0.58
1:A:540[A]:ARG:HD3	4:A:2312:HOH:O	2.06	0.55
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.89	0.55
1:A:220:ALA:O	1:A:221:ASP:OD1	2.25	0.54
1:A:708:LYS:HE3	1:A:710:TYR:OH	2.09	0.53
1:A:282:ASN:HD22	1:A:282:ASN:C	2.11	0.53
1:A:440:HIS:HE2	1:A:444[B]:LYS:HD3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704[A]:SER:C	1:A:705:ASN:HD22	2.13	0.52
1:A:744[B]:TYR:CE2	1:A:797:LEU:HD13	2.45	0.52
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.73	0.52
1:A:681:GLY:O	1:A:792:SER:HB2	2.10	0.52
1:A:252[A]:VAL:HG23	1:A:253:THR:HG23	1.92	0.51
1:A:822:GLU:HG2	1:A:823:THR:HG23	1.92	0.51
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:OE1	2.59	0.51
1:A:616:LYS:HE2	4:A:2178:HOH:O	2.10	0.51
1:A:374:ILE:O	1:A:378:GLU:HG3	2.12	0.50
1:A:254:ASN:ND2	1:A:256:SER:H	2.10	0.50
1:A:646:LEU:HD21	1:A:862[B]:ARG:HB2	1.94	0.50
1:A:340[B]:ASP:HB2	1:A:340[B]:ASP:OD2	2.12	0.50
1:A:704[B]:SER:C	1:A:705:ASN:HD22	2.15	0.49
1:A:882:PRO:CB	1:A:884:GLN:HE22	2.26	0.49
1:A:314:SER:OG	1:A:317:GLU:HG3	2.13	0.49
1:A:502:LYS:CB	1:A:529:LEU:HD21	2.43	0.49
1:A:282:ASN:ND2	1:A:284:GLU:H	2.10	0.48
1:A:248:MET:O	1:A:252[A]:VAL:HG13	2.13	0.48
1:A:688:SER:HB2	4:A:2431:HOH:O	2.14	0.48
1:A:340[A]:ASP:OD2	1:A:340[A]:ASP:HB3	2.11	0.48
1:A:744[B]:TYR:CZ	1:A:797:LEU:HD13	2.49	0.47
1:A:377:ILE:O	1:A:380:VAL:HG12	2.14	0.47
1:A:646:LEU:HD21	1:A:862[A]:ARG:HB2	1.96	0.47
1:A:341:ASN:N	1:A:342:PRO:HD3	2.29	0.47
1:A:254:ASN:ND2	1:A:254:ASN:C	2.67	0.47
1:A:870:ILE:HD11	1:A:887:PHE:CD2	2.49	0.47
1:A:177:ARG:NE	1:A:177:ARG:HA	2.30	0.46
1:A:327:LYS:HD3	1:A:327:LYS:C	2.35	0.46
1:A:664:LEU:C	1:A:664:LEU:HD23	2.36	0.46
1:A:408:TYR:CE1	2:A:901:NGA:H82	2.51	0.46
1:A:404:TYR:CE1	1:A:461:GLY:HA3	2.51	0.46
1:A:610:PRO:HB2	4:A:2487:HOH:O	2.15	0.46
1:A:862[A]:ARG:NH2	1:A:862[A]:ARG:HH12	2.09	0.46
1:A:221:ASP:CG	1:A:221:ASP:O	2.54	0.46
1:A:254:ASN:HD22	1:A:255:PRO:N	2.14	0.46
1:A:267:ARG:HD3	4:A:2090:HOH:O	2.15	0.45
1:A:811:LYS:HE3	4:A:2514:HOH:O	2.17	0.45
1:A:170:VAL:HG23	1:A:315:ASP:OD2	2.17	0.45
1:A:705:ASN:HD22	1:A:705:ASN:N	2.13	0.45
1:A:242:TYR:CD2	1:A:298:THR:HG23	2.52	0.45
1:A:661:ASN:C	1:A:661:ASN:HD22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:CD1	2:A:901:NGA:H82	2.52	0.45
1:A:431:ASP:OD2	1:A:434:LYS:HE3	2.16	0.45
1:A:617:MET:HA	1:A:618[A]:PRO:HD3	1.86	0.44
1:A:882:PRO:HB2	1:A:884:GLN:HE22	1.80	0.44
1:A:642:GLY:HA2	4:A:2328:HOH:O	2.18	0.44
1:A:422:VAL:HA	4:A:2010:HOH:O	2.17	0.44
1:A:535:VAL:HG22	4:A:2275:HOH:O	2.17	0.44
1:A:350:LEU:O	1:A:353:MET:HB3	2.18	0.44
1:A:502:LYS:HB2	1:A:529:LEU:HD21	1.99	0.43
1:A:375:ARG:HD3	4:A:2184:HOH:O	2.19	0.43
1:A:584:LYS:HE2	3:A:1200:SO4:O1	2.18	0.43
1:A:671:PHE:HB2	1:A:678:ALA:HB3	2.01	0.43
1:A:862[A]:ARG:HD3	1:A:864:GLU:OE1	2.18	0.43
1:A:355:ARG:HH11	1:A:418:GLN:NE2	2.17	0.43
1:A:298:THR:HB	1:A:299:PRO:HD3	2.01	0.42
1:A:667:HIS:HE1	4:A:2418:HOH:O	2.01	0.42
1:A:822:GLU:H	1:A:822:GLU:CD	2.23	0.42
1:A:667:HIS:HD2	4:A:2528:HOH:O	2.02	0.42
1:A:761:GLY:CA	4:A:2487:HOH:O	2.67	0.42
1:A:864:GLU:O	1:A:867:GLU:HB2	2.20	0.42
1:A:203[A]:GLN:HG3	4:A:2030:HOH:O	2.19	0.42
1:A:444[B]:LYS:HB2	1:A:444[B]:LYS:HD2	1.97	0.41
1:A:568:LEU:CD2	1:A:592:GLY:HA2	2.50	0.41
1:A:617:MET:HA	1:A:618[B]:PRO:HD2	1.92	0.41
1:A:219:GLN:HG2	1:A:222:ARG:CZ	2.50	0.41
1:A:661:ASN:ND2	1:A:663:THR:OG1	2.52	0.40
1:A:874:ASN:ND2	1:A:874:ASN:C	2.75	0.40
1:A:529:LEU:HD23	1:A:530:LEU:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	732/729 (100%)	706 (96%)	25 (3%)	1 (0%)	56 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLN

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	652/648 (101%)	633 (97%)	19 (3%)	50 31

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203[A]	GLN
1	A	203[B]	GLN
1	A	221	ASP
1	A	254	ASN
1	A	263	GLU
1	A	282	ASN
1	A	327	LYS
1	A	368	GLN
1	A	404	TYR
1	A	433	ASP
1	A	529	LEU
1	A	626	LYS
1	A	661	ASN
1	A	683	ASN
1	A	705	ASN
1	A	773	LYS
1	A	822	GLU
1	A	866	ASP
1	A	874	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	705	ASN
1	A	759	GLN
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	ASN
1	A	884	GLN

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 ⓘ

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	7,11,12	4.48	4 (57%)	8,15,17	2.77	4 (50%)
2	NGA	A	901	2	15,15,15	2.11	4 (26%)	17,21,21	1.35	2 (11%)

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	-	0/0/17/20	0/1/1/1
2	NGA	A	901	2	-	0/6/26/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NGA	C7-N2	2.41	1.43	1.34
2	A	900	GCD	C4-C5	2.89	1.36	1.32
2	A	900	GCD	C3-C4	3.34	1.54	1.50
2	A	901	NGA	O5-C5	3.51	1.53	1.44
2	A	901	NGA	O5-C1	4.06	1.50	1.43
2	A	901	NGA	C2-N2	4.36	1.53	1.45
2	A	900	GCD	O5-C1	4.88	1.53	1.45
2	A	900	GCD	O5-C5	9.61	1.52	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	GCD	O5-C1-C2	-4.53	105.77	111.06
2	A	900	GCD	O3-C3-C2	-3.35	104.10	109.73
2	A	900	GCD	C1-C2-C3	-2.66	106.39	109.54
2	A	901	NGA	C2-N2-C7	-2.16	117.57	123.10
2	A	901	NGA	O4-C4-C5	2.79	116.64	109.24
2	A	900	GCD	O3-C3-C4	4.30	119.43	109.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NGA	2	0

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	0.34	0	6,6,6	0.09	0
3	SO4	A	1201	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	A	1202	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	A	1203	-	4,4,4	0.40	0	6,6,6	0.09	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1200	SO4	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	722/729 (99%)	0.58	57 (7%) 15 14	15, 23, 39, 57	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	11.1
1	A	218	SER	6.3
1	A	891	GLU	6.2
1	A	375	ARG	5.1
1	A	223	ILE	4.2
1	A	316	GLU	4.0
1	A	341	ASN	3.9
1	A	491	GLY	3.9
1	A	449	LEU	3.8
1	A	866	ASP	3.6
1	A	493	THR	3.5
1	A	371	SER	3.5
1	A	426	THR	3.2
1	A	427	LYS	3.2
1	A	413	ILE	3.1
1	A	446	PHE	3.0
1	A	432	LYS	3.0
1	A	772	ASP	2.9
1	A	864	GLU	2.9
1	A	431	ASP	2.9
1	A	252[A]	VAL	2.9
1	A	490	GLU	2.9
1	A	564	PHE	2.8
1	A	219	GLN	2.8
1	A	867	GLU	2.8
1	A	492	GLU	2.7
1	A	773	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	846	THR	2.6
1	A	228	LYS	2.6
1	A	451	VAL	2.6
1	A	397	ILE	2.6
1	A	721	GLN	2.6
1	A	847	ILE	2.5
1	A	221	ASP	2.5
1	A	230	SER	2.4
1	A	407	ALA	2.4
1	A	717	SER	2.4
1	A	220	ALA	2.3
1	A	390	PHE	2.3
1	A	266	VAL	2.3
1	A	568	LEU	2.3
1	A	284	GLU	2.3
1	A	531	SER	2.3
1	A	855	LYS	2.3
1	A	217	SER	2.3
1	A	851	PHE	2.2
1	A	340[A]	ASP	2.2
1	A	719	THR	2.2
1	A	222	ARG	2.2
1	A	849	ASN	2.1
1	A	703	SER	2.1
1	A	450	LEU	2.1
1	A	547	PHE	2.1
1	A	181	TRP	2.0
1	A	593	MET	2.0
1	A	843	SER	2.0
1	A	192	ASP	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, 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
2	NGA	A	901	15/15	0.95	0.10	-0.62	16,21,22,26	0
2	GCD	A	900	11/12	0.95	0.10	-1.36	21,22,27,28	0

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, 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
3	SO4	A	1203	5/5	0.96	0.21	-	61,61,61,62	0
3	SO4	A	1201	5/5	0.97	0.14	-	33,34,39,39	0
3	SO4	A	1202	5/5	0.88	0.19	-	53,53,56,58	0
3	SO4	A	1200	5/5	0.96	0.12	-	35,36,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.