

Full wwPDB X-ray Structure Validation Report (i)

Dec 11, 2022 – 02:33 AM EST

PDB ID	:	1F9G
Title	:	CRYSTAL STRUCTURE OF STREPTOCOCCUS PNEUMONIAE
		HYALURONATE LYASE COCRYSTALLIZED WITH ASCORBIC ACID
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Deposited on	:	2000-07-10
Resolution	:	2.00 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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		
			4%		
1	А	731	74%	21%	• •

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
2	ASC	А	950	X	-	-	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6059 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	А	721	Total 5781	C 3637	N 965	O 1157	S 22	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	731	VAL	GLY	conflict	UNP Q54873
А	893	HIS	-	expression tag	UNP Q54873
А	894	HIS	-	expression tag	UNP Q54873
А	895	HIS	-	expression tag	UNP Q54873
А	896	HIS	-	expression tag	UNP Q54873
А	897	HIS	-	expression tag	UNP Q54873
A	898	HIS	-	expression tag	UNP Q54873

• Molecule 2 is ASCORBIC ACID (three-letter code: ASC) (formula: $C_6H_8O_6$).





Mol	Chain	Residues	es Atoms			ZeroOcc	AltConf
2	А	1	Total 12	$\begin{array}{c} \mathrm{C} \\ \mathrm{6} \end{array}$	O 6	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	266	Total O 266 266	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	84.26Å 102.67Å 103.25Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	45.00 - 2.00	Depositor
Resolution (A)	46.12 - 2.00	EDS
% Data completeness	89.1 (45.00-2.00)	Depositor
(in resolution range)	88.6 (46.12-2.00)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.33 (at 2.00 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.851	Depositor
B B.	0.216 , 0.252	Depositor
II, II, <i>free</i>	0.203 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38, 63.7	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6059	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ASC

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/5900	0.60	0/7970	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	А	5781	0	5591	114	0
2	А	12	0	7	0	0
3	А	266	0	0	5	0
All	All	6059	0	5598	114	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 10.

All (114) 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:613:ASN:H	1:A:698:GLN:HE22	1.09	0.96



Interatomic Clas						
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:A:749:LYS:HE3	1:A:749:LYS:H	1.40	0.85			
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.45	0.81			
1:A:424:GLN:HE22	1:A:430:ILE:H	1.29	0.80			
1:A:423:ILE:HG22	1:A:424:GLN:HE21	1.50	0.75			
1:A:319:LYS:HB2	1:A:319:LYS:NZ	2.02	0.73			
1:A:424:GLN:HE22	1:A:430:ILE:N	1.86	0.72			
1:A:224:TYR:N	1:A:224:TYR:HD1	1.88	0.70			
1:A:224:TYR:N	1:A:224:TYR:CD1	2.59	0.67			
1:A:274:GLU:HG2	1:A:321:TYR:OH	1.95	0.67			
1:A:832:GLN:HE21	1:A:862:ARG:HH22	1.41	0.67			
1:A:613:ASN:N	1:A:698:GLN:HE22	1.90	0.65			
1:A:708:LYS:HE2	1:A:715:GLU:OE1	1.97	0.65			
1:A:355:ARG:HG3	1:A:419:LEU:CD2	2.27	0.65			
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.80	0.63			
1:A:499:SER:O	1:A:503:THR:HG22	1.98	0.63			
1:A:291:TRP:O	1:A:295:GLU:HG3	1.99	0.62			
1:A:708:LYS:HD3	1:A:710:TYR:OH	2.00	0.62			
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.84	0.60			
1:A:521:LYS:HB2	3:A:1138:HOH:O	2.01	0.60			
1:A:171:LYS:H	1:A:175:THR:HG21	1.67	0.60			
1:A:239:THR:HG22	1:A:298:THR:OG1	2.02	0.59			
1:A:433:ASP:O	1:A:436:GLN:HB2	2.02	0.59			
1:A:424:GLN:NE2	1:A:430:ILE:H	1.99	0.58			
1:A:319:LYS:HB2	1:A:319:LYS:HZ2	1.69	0.57			
1:A:822:GLU:HG2	1:A:823:THR:HG23	1.85	0.57			
1:A:468:ASN:HB2	3:A:1056:HOH:O	2.02	0.57			
1:A:326:GLU:HA	1:A:326:GLU:OE1	2.04	0.57			
1:A:621:THR:C	1:A:622:GLU:HG2	2.25	0.56			
1:A:423:ILE:HG22	1:A:424:GLN:NE2	2.19	0.56			
1:A:610:PRO:HG3	1:A:763:TRP:CE2	2.42	0.55			
1:A:685:GLN:HA	1:A:789:ASN:HD22	1.73	0.54			
1:A:424:GLN:NE2	1:A:424:GLN:HA	2.21	0.54			
1:A:190:TYR:CE2	1:A:521:LYS:HG2	2.43	0.54			
1:A:290:ASN:HD22	1:A:292:TRP:HB3	1.73	0.54			
1:A:661:ASN:C	1:A:661:ASN:HD22	2.11	0.54			
1:A:350:LEU:HD21	1:A:379:GLN:HB2	1.90	0.53			
1:A:426:THR:O	1:A:429:PRO:HD3	2.09	0.53			
1:A:293:ASP:O	1:A:298:THR:HB	2.09	0.53			
1:A:623:THR:HA	1:A:691:THR:O	2.09	0.53			
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.24	0.53			
1:A:302:ILE:O	1:A:306:LEU:HG	2.09	0.53			



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:613:ASN:H	1:A:698:GLN:NE2	1.92	0.52
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.58	0.52
1:A:287:ILE:HD12	1:A:339:THR:HG23	1.92	0.51
1:A:840:TYR:O	1:A:856:ARG:HD2	2.11	0.51
1:A:170:VAL:HG13	1:A:170:VAL:O	2.09	0.51
1:A:476:VAL:O	1:A:480:ARG:HG2	2.11	0.50
1:A:760:LYS:HD2	1:A:774:GLU:OE1	2.12	0.50
1:A:832:GLN:HE21	1:A:862:ARG:NH2	2.08	0.50
1:A:286:SER:O	1:A:288:VAL:HG23	2.11	0.50
1:A:295:GLU:HB3	1:A:329:VAL:HG22	1.93	0.50
1:A:355:ARG:HA	1:A:419:LEU:HD21	1.93	0.50
1:A:380:VAL:HG21	1:A:412:LEU:HD21	1.95	0.49
1:A:337:LYS:HA	1:A:342:PRO:HB3	1.94	0.48
1:A:287:ILE:HD12	1:A:339:THR:CG2	2.42	0.48
1:A:290:ASN:HD22	1:A:292:TRP:CB	2.27	0.48
1:A:224:TYR:HD2	1:A:230:SER:HB3	1.78	0.48
1:A:224:TYR:HD1	1:A:224:TYR:H	1.60	0.48
1:A:263:GLU:HB3	3:A:1161:HOH:O	2.13	0.47
1:A:722:GLU:HG2	1:A:753:SER:OG	2.14	0.47
1:A:607:GLY:C	1:A:610:PRO:HD2	2.35	0.47
1:A:380:VAL:CG2	1:A:412:LEU:HD21	2.45	0.46
1:A:819:GLU:HG3	1:A:820:ASN:N	2.30	0.46
1:A:661:ASN:ND2	1:A:663:THR:OG1	2.49	0.46
1:A:852:GLN:OE1	1:A:888:LYS:HD3	2.14	0.46
1:A:291:TRP:HB2	1:A:295:GLU:OE1	2.15	0.46
1:A:681:GLY:HA3	1:A:793:TYR:CE2	2.50	0.46
1:A:317:GLU:O	1:A:321:TYR:CD2	2.69	0.46
1:A:282:ASN:HD21	1:A:285:LYS:HG2	1.81	0.46
1:A:669:SER:OG	1:A:825:GLN:NE2	2.49	0.46
1:A:671:PHE:HD2	1:A:836:GLY:HA3	1.81	0.45
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.50	0.45
1:A:569:PHE:CE2	1:A:575:ASN:HB3	2.51	0.45
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.81	0.45
1:A:749:LYS:H	1:A:749:LYS:CE	2.19	0.45
1:A:543:TYR:HA	1:A:648:ASP:HB2	1.98	0.45
1:A:392:GLN:O	1:A:392:GLN:HG2	2.16	0.45
1:A:444:LYS:HE2	3:A:1001:HOH:O	2.16	0.45
1:A:431:ASP:HB2	1:A:434:LYS:HZ2	1.82	0.45
1:A:820:ASN:ND2	1:A:825:GLN:HG2	2.23	0.45
1:A:323:ASP:O	1:A:326:GLU:HB2	2.17	0.44
1:A:626:LYS:HG2	1:A:627:ARG:N	2.32	0.44



A + 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:235:SER:HB2	1:A:290:ASN:H	1.81	0.43
1:A:295:GLU:HB3	1:A:329:VAL:CG2	2.48	0.43
1:A:357:LYS:HB2	1:A:373:THR:HG21	2.00	0.43
1:A:420:LEU:HD22	1:A:435:MET:CE	2.48	0.42
1:A:664:LEU:HA	1:A:685:GLN:O	2.19	0.42
1:A:177:ARG:HG2	1:A:177:ARG:NH1	2.34	0.42
1:A:239:THR:HG22	1:A:298:THR:N	2.35	0.42
1:A:767:ASN:HB3	1:A:770:GLN:CG	2.49	0.42
1:A:292:TRP:CD1	1:A:296:ILE:HD12	2.54	0.42
1:A:399:HIS:O	1:A:400:THR:HB	2.20	0.42
1:A:580:ASN:O	1:A:581:LYS:HB2	2.20	0.42
1:A:659:ASN:HD21	1:A:661:ASN:HD21	1.68	0.42
1:A:540:ARG:HE	1:A:540:ARG:HB3	1.78	0.42
1:A:413:ILE:HG23	1:A:414:ASP:N	2.35	0.41
1:A:708:LYS:HD3	1:A:710:TYR:CZ	2.55	0.41
1:A:560:LYS:HE2	3:A:1194:HOH:O	2.18	0.41
1:A:355:ARG:HG3	1:A:419:LEU:HD22	2.01	0.41
1:A:661:ASN:ND2	1:A:661:ASN:H	2.18	0.41
1:A:661:ASN:C	1:A:661:ASN:ND2	2.72	0.41
1:A:754:MET:HB3	1:A:754:MET:HE2	1.91	0.41
1:A:476:VAL:HG11	1:A:516:ASN:HB3	2.02	0.41
1:A:224:TYR:HD2	1:A:227:GLU:HA	1.85	0.41
1:A:291:TRP:HE3	1:A:295:GLU:CD	2.25	0.41
1:A:323:ASP:OD2	1:A:364:ARG:NH2	2.48	0.41
1:A:424:GLN:NE2	1:A:424:GLN:CA	2.84	0.41
1:A:416:LEU:O	1:A:420:LEU:HG	2.21	0.40
1:A:172:ASP:HB2	1:A:173:THR:H	1.74	0.40
1:A:458:MET:HE1	1:A:566:LEU:N	2.37	0.40
1:A:570:SER:HA	1:A:636:LEU:HB3	2.03	0.40
1:A:290:ASN:ND2	1:A:292:TRP:HB2	2.36	0.40
1:A:296:ILE:C	1:A:299:PRO:HD2	2.41	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	А	719/731~(98%)	675~(94%)	43 (6%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	221	ASP

5.3.2 Protein sidechains (i)

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	А	638/649~(98%)	567~(89%)	71 (11%)	6 3		

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	171	LYS
1	А	196	ASP
1	А	200	LYS
1	А	217	SER
1	А	218	SER
1	А	224	TYR
1	А	233	LYS
1	А	235	SER
1	А	238	LEU
1	А	243	ARG
1	А	252	VAL
1	А	254	ASN
1	А	263	GLU
1	А	282	ASN
1	А	286	SER
1	А	316	GLU
1	А	319	LYS
1	А	327	LYS



Mol	Chain	Res	Type
1	А	337	LYS
1	А	338	THR
1	А	355	ARG
1	А	368	GLN
1	А	375	ARG
1	А	378	GLU
1	А	385	ASP
1	А	392	GLN
1	А	397	ILE
1	А	404	TYR
1	А	405	THR
1	А	412	LEU
1	А	419	LEU
1	А	433	ASP
1	А	434	LYS
1	А	435	MET
1	А	444	LYS
1	А	458	MET
1	А	483	HIS
1	А	489	SER
1	А	490	GLU
1	А	492	GLU
1	А	495	GLN
1	А	518	LYS
1	А	521	LYS
1	А	528	SER
1	А	529	LEU
1	А	540	ARG
1	А	560	LYS
1	А	661	ASN
1	А	676	LYS
1	А	701	LEU
1	А	703	SER
1	А	715	GLU
1	А	717	SER
1	А	721	GLN
1	А	724	ASP
1	A	727	GLU
1	А	739	LYS
1	А	749	LYS
1	А	750	SER
1	A	753	SER



Mol	Chain	Res	Type
1	А	758	LEU
1	А	760	LYS
1	А	773	LYS
1	А	774	GLU
1	А	812	GLU
1	А	814	GLU
1	А	853	VAL
1	А	854	LEU
1	А	855	LYS
1	А	864	GLU
1	А	869	LYS

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

Mol	Chain	Res	Type
1	А	189	GLN
1	А	202	ASN
1	А	237	ASN
1	А	254	ASN
1	А	261	GLN
1	А	282	ASN
1	А	290	ASN
1	А	303	ASN
1	А	349	ASN
1	А	386	GLN
1	А	424	GLN
1	А	428	ASN
1	А	436	GLN
1	А	661	ASN
1	А	667	HIS
1	А	698	GLN
1	А	729	GLN
1	А	759	GLN
1	А	789	ASN
1	А	820	ASN
1	А	825	GLN
1	А	832	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	Ros Link		Bond lengths		Bond angles					
		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	ASC	А	950	-	12,12,12	1.73	3 (25%)	17,17,17	2.68	5 (29%)

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	ASC	А	950	-	1/1/5/5	4/6/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	950	ASC	C2-C1	3.36	1.53	1.45
2	А	950	ASC	O3-C3	-2.38	1.25	1.33
2	А	950	ASC	O4-C1	2.10	1.39	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	950	ASC	C6-C5-C4	7.91	125.47	111.86



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	950	ASC	O6-C6-C5	-4.25	101.82	111.07
2	А	950	ASC	O4-C4-C3	3.17	106.98	103.71
2	А	950	ASC	O4-C1-C2	-2.94	107.25	109.86
2	А	950	ASC	O4-C4-C5	2.50	118.20	110.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	А	950	ASC	C5

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	950	ASC	C4-C5-C6-O6
2	А	950	ASC	O4-C4-C5-O5
2	А	950	ASC	O5-C5-C6-O6
2	А	950	ASC	O4-C4-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	А	721/731~(98%)	0.31	31 (4%) 35 34	15, 31, 64, 90	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	427	LYS	6.0
1	А	170	VAL	5.4
1	А	171	LYS	4.5
1	А	338	THR	4.0
1	А	704	SER	3.7
1	А	174	TYR	3.3
1	А	721	GLN	3.3
1	А	223	ILE	3.0
1	А	172	ASP	3.0
1	А	366	ASP	2.9
1	А	435	MET	2.8
1	А	758	LEU	2.8
1	А	340	ASP	2.7
1	А	173	THR	2.7
1	А	368	GLN	2.6
1	А	553	THR	2.5
1	А	289	GLY	2.3
1	А	335	PHE	2.2
1	А	431	ASP	2.2
1	А	220	ALA	2.2
1	А	375	ARG	2.2
1	А	288	VAL	2.2
1	А	428	ASN	2.2
1	А	196	ASP	2.2
1	А	328	PHE	2.2
1	А	233	LYS	2.1
1	А	221	ASP	2.1



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Mol	Chain	Res	Type	RSRZ
1	А	554	ALA	2.1
1	А	719	THR	2.1
1	А	772	ASP	2.1
1	А	339	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	ASC	А	950	12/12	0.64	0.26	58,62,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.

