



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 AM UTC

PDB ID : 1F9G / pdb_00001f9g
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

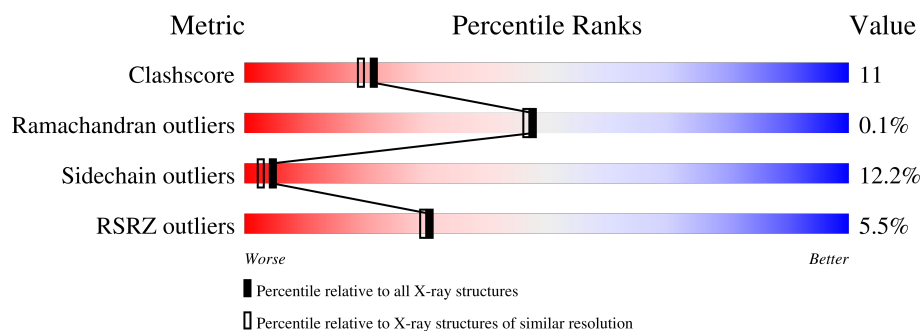
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	731	

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	A	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.

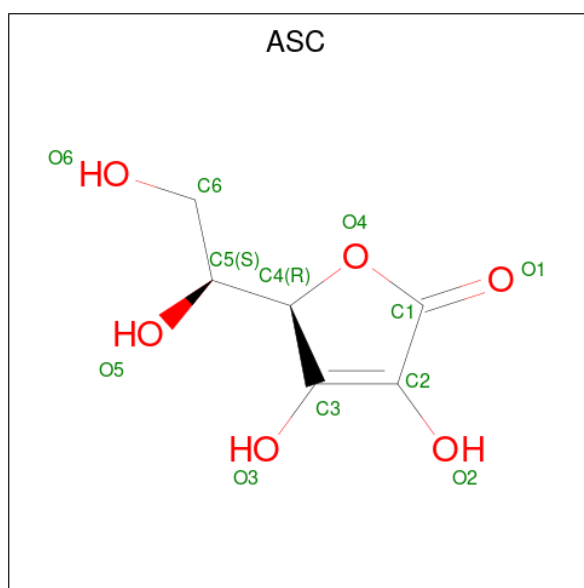
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	721	5781	3637	965	1157	22	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	731	VAL	GLY	conflict	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

- Molecule 2 is ASCORBIC ACID (CCD ID: ASC) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

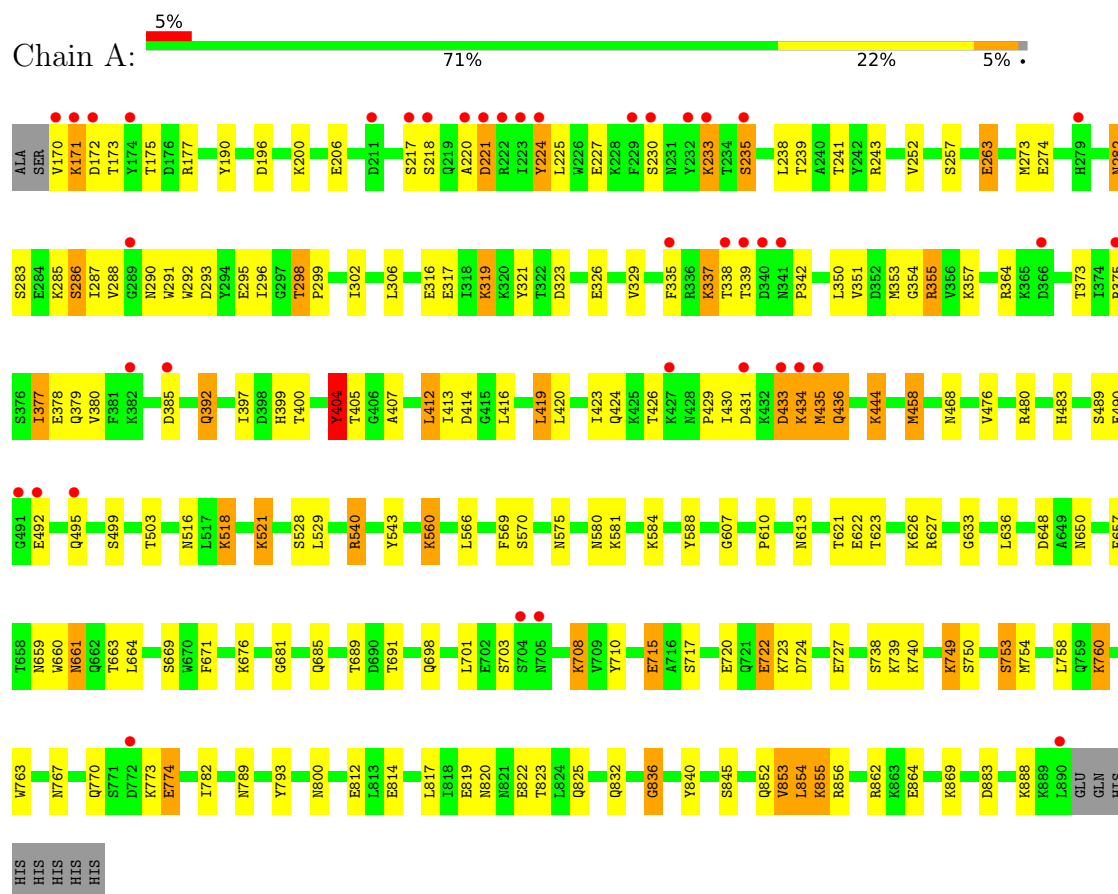
- Molecule 3 is water.

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

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.26Å 102.67Å 103.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.00 45.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (45.00-2.00) 88.6 (45.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.216 , 0.252 0.225 , (Not available)	Depositor 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 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/5900	0.89	14/7970 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	LYS	N-CA-C	7.49	121.26	112.72
1	A	657	PHE	N-CA-C	6.83	120.99	110.20
1	A	233	LYS	N-CA-C	-6.73	105.23	113.50
1	A	800	ASN	N-CA-C	6.25	120.24	112.24
1	A	660	TRP	N-CA-C	6.12	119.59	111.75
1	A	708	LYS	N-CA-C	-5.75	99.14	108.52
1	A	854	LEU	N-CA-C	5.60	121.91	114.12
1	A	720	GLU	N-CA-C	-5.41	105.54	111.82
1	A	633	GLY	N-CA-C	5.41	118.28	112.33
1	A	836	GLY	N-CA-C	-5.15	100.98	113.18
1	A	404	TYR	N-CA-C	5.14	118.59	111.71
1	A	588	TYR	N-CA-C	5.13	118.85	112.59
1	A	855	LYS	N-CA-C	5.11	117.57	109.50
1	A	225	LEU	N-CA-C	-5.07	105.22	111.40

There are no chirality outliers.

There are no planarity outliers.

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	5781	0	5591	124	0
2	A	12	0	7	0	0
3	A	266	0	0	5	0
All	All	6059	0	5598	124	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 (124) 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
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:754:MET:HE3	1:A:782:ILE:HG12	1.68	0.75
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:420:LEU:HD22	1:A:435:MET:HE3	1.71	0.71
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:335:PHE:CZ	1:A:353:MET:HE2	2.33	0.64
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:621:THR:C	1:A:622:GLU:HG2	2.25	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ASN:C	1:A:661:ASN:HD22	2.11	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:274:GLU:HG2	1:A:321:TYR:HH	1.69	0.57
1:A:430:ILE:HB	1:A:435:MET:HE1	1.86	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: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:458:MET:HE1	1:A:566:LEU:C	2.33	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:350:LEU:HD21	1:A:379:GLN:HB2	1.90	0.53
1:A:335:PHE:CE2	1:A:353:MET:HE2	2.44	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:273:MET:HE2	1:A:306:LEU:HD21	1.90	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
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:607:GLY:C	1:A:610:PRO:HD2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLU:HG2	1:A:753:SER:OG	2.14	0.47
1:A:380:VAL:CG2	1:A:412:LEU:HD21	2.45	0.46
1:A:661:ASN:C	1:A:661:ASN:ND2	2.72	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:291:TRP:HE3	1:A:295:GLU:CD	2.25	0.45
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:296:ILE:C	1:A:299:PRO:HD2	2.41	0.45
1:A:820:ASN:ND2	1:A:825:GLN:HG2	2.23	0.45
1:A:220:ALA:O	1:A:221:ASP:C	2.60	0.45
1:A:323:ASP:O	1:A:326:GLU:HB2	2.17	0.44
1:A:206:GLU:OE2	1:A:257:SER:OG	2.32	0.44
1:A:626:LYS:HG2	1:A:627:ARG:N	2.32	0.44
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: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:295:GLU:C	1:A:299:PRO:HG2	2.43	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:431:ASP:HB2	1:A:434:LYS:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:SER:C	1:A:285:LYS:H	2.28	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:738:SER:C	1:A:740:LYS:H	2.28	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: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: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

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	719/731 (98%)	675 (94%)	43 (6%)	1 (0%)	48 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	A	638/649 (98%)	560 (88%)	78 (12%)	5 3

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	A	196	ASP
1	A	200	LYS
1	A	217	SER
1	A	218	SER
1	A	224	TYR
1	A	233	LYS
1	A	235	SER
1	A	238	LEU
1	A	241	THR
1	A	243	ARG
1	A	252	VAL
1	A	263	GLU
1	A	282	ASN
1	A	286	SER
1	A	298	THR
1	A	316	GLU
1	A	319	LYS
1	A	337	LYS
1	A	338	THR
1	A	351	VAL
1	A	355	ARG
1	A	375	ARG
1	A	377	ILE
1	A	378	GLU
1	A	385	ASP
1	A	392	GLN
1	A	397	ILE
1	A	404	TYR
1	A	405	THR
1	A	412	LEU
1	A	419	LEU
1	A	433	ASP
1	A	434	LYS

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Mol	Chain	Res	Type
1	A	435	MET
1	A	436	GLN
1	A	444	LYS
1	A	458	MET
1	A	483	HIS
1	A	489	SER
1	A	490	GLU
1	A	492	GLU
1	A	495	GLN
1	A	518	LYS
1	A	521	LYS
1	A	528	SER
1	A	529	LEU
1	A	540	ARG
1	A	560	LYS
1	A	584	LYS
1	A	661	ASN
1	A	676	LYS
1	A	689	THR
1	A	701	LEU
1	A	703	SER
1	A	715	GLU
1	A	717	SER
1	A	722	GLU
1	A	723	LYS
1	A	724	ASP
1	A	727	GLU
1	A	739	LYS
1	A	749	LYS
1	A	750	SER
1	A	753	SER
1	A	758	LEU
1	A	760	LYS
1	A	773	LYS
1	A	774	GLU
1	A	812	GLU
1	A	814	GLU
1	A	817	LEU
1	A	853	VAL
1	A	854	LEU
1	A	855	LYS
1	A	864	GLU

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Mol	Chain	Res	Type
1	A	869	LYS
1	A	883	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	237	ASN
1	A	251	GLN
1	A	254	ASN
1	A	261	GLN
1	A	282	ASN
1	A	290	ASN
1	A	303	ASN
1	A	349	ASN
1	A	424	GLN
1	A	428	ASN
1	A	498	GLN
1	A	661	ASN
1	A	667	HIS
1	A	698	GLN
1	A	729	GLN
1	A	759	GLN
1	A	789	ASN
1	A	820	ASN
1	A	825	GLN
1	A	832	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ASC	A	950	-	12,12,12	1.65	2 (16%)	17,17,17	2.75	6 (35%)

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	A	950	-	1/1/5/5	4/6/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	950	ASC	C2-C1	3.13	1.53	1.45
2	A	950	ASC	O3-C3	-2.06	1.25	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	ASC	C6-C5-C4	8.08	125.47	111.86
2	A	950	ASC	O6-C6-C5	-4.44	101.82	111.16
2	A	950	ASC	O4-C4-C3	3.22	106.98	103.76
2	A	950	ASC	O4-C1-C2	-2.95	107.25	109.86
2	A	950	ASC	O4-C4-C5	2.61	118.20	110.07
2	A	950	ASC	O2-C2-C1	2.04	127.20	122.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	950	ASC	C5

All (4) torsion outliers are listed below:

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

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	721/731 (98%)	0.25	40 (5%) 30 29	15, 31, 64, 90	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	5.5
1	A	435	MET	5.2
1	A	224	TYR	4.5
1	A	220	ALA	3.9
1	A	221	ASP	3.8
1	A	338	THR	3.7
1	A	289	GLY	3.6
1	A	890	LEU	3.6
1	A	704	SER	3.5
1	A	222	ARG	3.3
1	A	218	SER	3.0
1	A	339	THR	2.9
1	A	705	ASN	2.9
1	A	340	ASP	2.8
1	A	335	PHE	2.7
1	A	229	PHE	2.6
1	A	492	GLU	2.6
1	A	279	HIS	2.6
1	A	491	GLY	2.5
1	A	223	ILE	2.5
1	A	217	SER	2.4
1	A	171	LYS	2.4
1	A	235	SER	2.3
1	A	366	ASP	2.3
1	A	230	SER	2.3
1	A	385	ASP	2.3
1	A	211	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	772	ASP	2.2
1	A	174	TYR	2.2
1	A	172	ASP	2.2
1	A	495	GLN	2.2
1	A	434	LYS	2.2
1	A	382	LYS	2.2
1	A	431	ASP	2.2
1	A	233	LYS	2.1
1	A	341	ASN	2.1
1	A	375	ARG	2.1
1	A	427	LYS	2.1
1	A	232	TYR	2.0
1	A	433	ASP	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ASC	A	950	12/12	0.66	0.15	58,62,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.