Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1N7O
Title	:	Streptococcus pneumoniae Hyaluronate Lyase F343V Mutant
Authors	:	Nukui, M.; Taylor, K.B.; McPherson, D.T.; Shigenaga, M.; Jedrzejas, M.J.
Deposited on	:	2002-11-16
Resolution	:	1.50 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 (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	Percentile Ranks	Value
Rfree		0.215
Clashscore		12
Ramachandran outliers		0.8%
Sidechain outliers		6.1%
RSRZ outliers		6.8%

Worse　　*Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
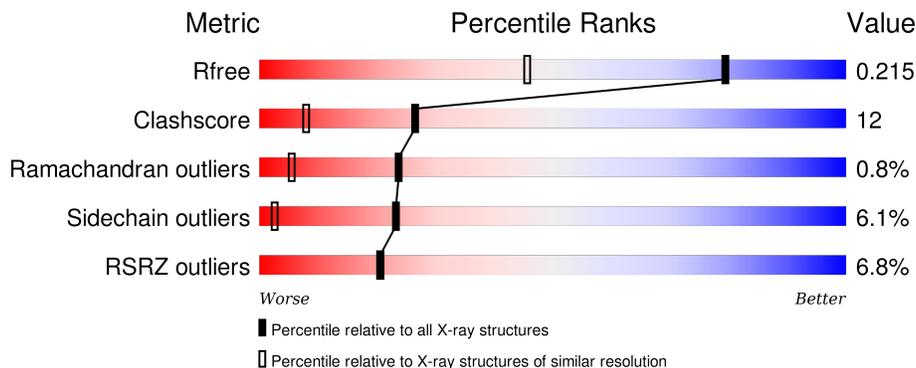
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 <=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	721	7% · · · 83% · 12% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6366 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 hyaluronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total 5780	C 3634	N 968	O 1156	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	VAL	PHE	ENGINEERED	UNP Q54873
A	731	VAL	GLY	SEE REMARK 999	UNP Q54873

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	586	Total 586	O 586	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: hyaluronidase
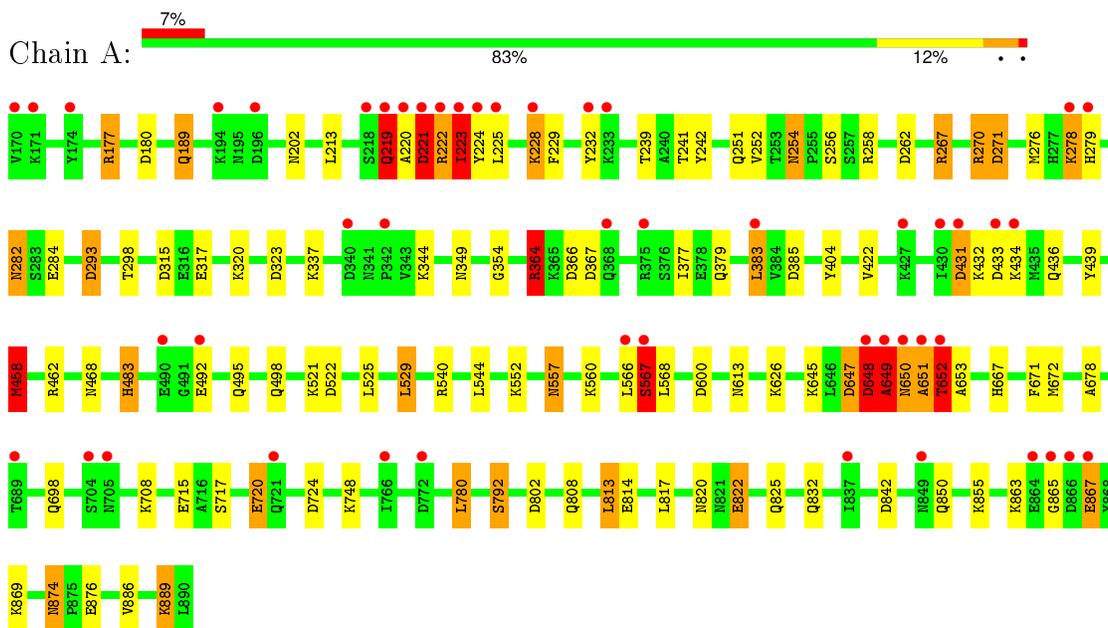
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.07Å 103.35Å 101.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 19.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.50) 87.0 (19.99-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	1.22 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.211 0.196 , 0.215	Depositor DCC
R_{free} test set	1241 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 59.4	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning [2]	$<\|L\|>\ = 0.49, <L^2>\ = 0.32$	Xtriage
Outliers	1 of 123680 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6366	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.82	6/5898 (0.1%)	0.99	42/7967 (0.5%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	652	THR	CA-C	7.69	1.73	1.52
1	A	652	THR	CA-CB	-6.64	1.36	1.53
1	A	566	LEU	CA-C	-6.13	1.37	1.52
1	A	652	THR	C-O	-5.79	1.12	1.23
1	A	267	ARG	CG-CD	5.65	1.66	1.51
1	A	652	THR	CB-OG1	5.40	1.54	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	THR	N-CA-C	10.12	138.34	111.00
1	A	567	SER	C-N-CA	8.67	143.37	121.70
1	A	262	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	724	ASP	CB-CG-OD2	7.86	125.38	118.30
1	A	648	ASP	N-CA-C	-7.85	89.80	111.00
1	A	364	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	652	THR	N-CA-CB	-7.75	95.58	110.30
1	A	842	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	652	THR	CA-CB-CG2	-7.44	101.99	112.40
1	A	323	ASP	CB-CG-OD2	7.19	124.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	566	LEU	CB-CA-C	-7.01	96.89	110.20
1	A	271	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	567	SER	N-CA-CB	-6.75	100.37	110.50
1	A	458	MET	CB-CG-SD	6.64	132.32	112.40
1	A	385	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	221	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	367	ASP	CB-CG-OD2	6.33	123.99	118.30
1	A	802	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	366	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	648	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	364	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	650	ASN	N-CA-CB	5.95	121.31	110.60
1	A	315	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	780	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	383	LEU	CB-CG-CD1	5.86	120.97	111.00
1	A	649	ALA	N-CA-C	5.84	126.76	111.00
1	A	270	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	780	LEU	CB-CG-CD1	5.80	120.86	111.00
1	A	270	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	600	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	180	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	462	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	522	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	293	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	567	SER	O-C-N	5.27	131.13	122.70
1	A	433	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	649	ALA	CA-C-N	5.12	128.47	117.20
1	A	650	ASN	N-CA-C	-5.08	97.30	111.00
1	A	813	LEU	CB-CG-CD1	5.02	119.53	111.00
1	A	258	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	431	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	652	THR	CA-C-N	5.01	128.22	117.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ALA	Peptide
1	A	223	ILE	Peptide
1	A	567	SER	Mainchain,Peptide
1	A	647	ASP	Peptide
1	A	648	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	652	THR	Peptide

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	A	5780	0	5594	139	0
2	A	586	0	0	57	0
All	All	6366	0	5594	139	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 12.

All (139) 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:458:MET:SD	1:A:458:MET:CE	2.05	1.43
1:A:458:MET:HG2	2:A:1329:HOH:O	1.30	1.31
1:A:652:THR:HG21	2:A:1339:HOH:O	1.16	1.29
1:A:239:THR:HB	2:A:1413:HOH:O	1.29	1.28
1:A:649:ALA:O	2:A:1380:HOH:O	1.59	1.18
1:A:458:MET:CE	2:A:1329:HOH:O	1.92	1.18
1:A:458:MET:CG	2:A:1329:HOH:O	1.88	1.09
1:A:649:ALA:O	2:A:1332:HOH:O	1.71	1.05
1:A:567:SER:C	2:A:1331:HOH:O	1.95	1.05
1:A:552:LYS:HD2	1:A:567:SER:OG	1.59	1.03
1:A:483:HIS:HE1	2:A:1212:HOH:O	1.46	0.99
1:A:552:LYS:CD	1:A:567:SER:HB2	1.94	0.98
1:A:645:LYS:HA	1:A:651:ALA:HA	1.43	0.97
1:A:552:LYS:HD2	1:A:567:SER:CB	1.94	0.96
1:A:613:ASN:H	1:A:698:GLN:HE22	1.11	0.96
1:A:552:LYS:HA	1:A:567:SER:HB2	1.45	0.95
1:A:567:SER:O	2:A:1331:HOH:O	1.82	0.94
1:A:650:ASN:HA	2:A:1332:HOH:O	1.71	0.91
1:A:364:ARG:HD3	2:A:1137:HOH:O	1.71	0.91
1:A:458:MET:SD	2:A:1329:HOH:O	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:O	2:A:1347:HOH:O	1.90	0.87
1:A:567:SER:O	2:A:1330:HOH:O	1.97	0.83
1:A:652:THR:CG2	2:A:1349:HOH:O	2.30	0.78
1:A:364:ARG:CD	2:A:1137:HOH:O	2.29	0.78
1:A:267:ARG:HD3	2:A:1174:HOH:O	1.83	0.78
1:A:552:LYS:HA	1:A:567:SER:CB	2.15	0.77
1:A:552:LYS:CA	1:A:567:SER:HB2	2.15	0.76
1:A:552:LYS:HD2	1:A:567:SER:HB2	1.62	0.73
1:A:645:LYS:HA	1:A:651:ALA:CA	2.17	0.72
1:A:458:MET:HE2	2:A:1329:HOH:O	1.69	0.72
1:A:189:GLN:HG3	2:A:1476:HOH:O	1.89	0.71
1:A:483:HIS:CE1	2:A:1212:HOH:O	2.29	0.70
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.38	0.69
1:A:649:ALA:HB1	2:A:1380:HOH:O	1.93	0.69
1:A:267:ARG:CD	2:A:1174:HOH:O	2.39	0.68
1:A:552:LYS:HD3	1:A:567:SER:HB2	1.76	0.68
1:A:552:LYS:CD	1:A:567:SER:CB	2.59	0.67
1:A:544:LEU:CD1	1:A:651:ALA:HB3	2.25	0.66
1:A:544:LEU:HD13	1:A:651:ALA:HB3	1.76	0.66
1:A:720:GLU:HG3	2:A:1315:HOH:O	1.96	0.65
1:A:652:THR:HA	1:A:672:MET:CE	2.27	0.65
1:A:552:LYS:CB	1:A:567:SER:HB2	2.26	0.65
1:A:863:LYS:NZ	1:A:865:GLY:O	2.25	0.64
1:A:431:ASP:OD1	1:A:434:LYS:HE2	1.97	0.63
1:A:241:THR:HG21	1:A:276:MET:HE3	1.80	0.63
1:A:647:ASP:O	1:A:650:ASN:O	2.15	0.63
1:A:557:ASN:HD22	1:A:557:ASN:C	2.02	0.63
1:A:874:ASN:C	1:A:874:ASN:HD22	2.02	0.62
1:A:720:GLU:CG	2:A:1315:HOH:O	2.49	0.61
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.66	0.61
1:A:225:LEU:HG	1:A:276:MET:HE2	1.83	0.61
1:A:222:ARG:O	1:A:223:ILE:HG23	2.01	0.60
1:A:544:LEU:HD22	1:A:651:ALA:CB	2.32	0.60
1:A:649:ALA:C	2:A:1380:HOH:O	2.21	0.59
1:A:652:THR:CG2	1:A:653:ALA:N	2.60	0.59
1:A:647:ASP:OD1	1:A:650:ASN:N	2.36	0.59
1:A:652:THR:CG2	2:A:1339:HOH:O	2.00	0.58
1:A:483:HIS:CE1	2:A:1311:HOH:O	2.56	0.58
1:A:648:ASP:HB3	2:A:1247:HOH:O	2.03	0.58
1:A:652:THR:HG21	2:A:1349:HOH:O	2.01	0.57
1:A:650:ASN:O	1:A:651:ALA:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:THR:HA	1:A:672:MET:HE1	1.86	0.57
1:A:889:LYS:HD2	1:A:889:LYS:N	2.20	0.56
1:A:254:ASN:HD22	1:A:254:ASN:C	2.09	0.56
1:A:855:LYS:HE2	1:A:886:VAL:HG12	1.87	0.56
1:A:650:ASN:CA	2:A:1332:HOH:O	2.44	0.55
1:A:557:ASN:ND2	1:A:560:LYS:H	2.05	0.55
1:A:645:LYS:HG3	1:A:651:ALA:HB2	1.88	0.55
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.89	0.55
1:A:225:LEU:HG	1:A:276:MET:CE	2.37	0.54
1:A:436:GLN:HA	2:A:1393:HOH:O	2.06	0.54
1:A:458:MET:CG	1:A:458:MET:CE	2.86	0.54
1:A:239:THR:CB	2:A:1413:HOH:O	2.12	0.54
1:A:652:THR:HG23	1:A:653:ALA:N	2.22	0.53
1:A:228:LYS:HG3	1:A:229:PHE:CE2	2.44	0.53
1:A:239:THR:HG21	1:A:293:ASP:OD2	2.08	0.53
1:A:889:LYS:H	1:A:889:LYS:CD	2.21	0.53
1:A:792:SER:HB2	2:A:1412:HOH:O	2.07	0.53
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.38	0.53
1:A:282:ASN:HD22	1:A:284:GLU:H	1.55	0.53
1:A:648:ASP:O	1:A:648:ASP:CG	2.47	0.53
1:A:521:LYS:CD	2:A:1353:HOH:O	2.57	0.53
1:A:177:ARG:HG3	1:A:422:VAL:HG13	1.90	0.53
1:A:223:ILE:HD12	1:A:224:TYR:H	1.75	0.52
1:A:649:ALA:C	2:A:1332:HOH:O	2.31	0.52
1:A:222:ARG:C	1:A:223:ILE:HG13	2.30	0.52
1:A:224:TYR:HB3	2:A:1347:HOH:O	2.09	0.52
1:A:645:LYS:HA	1:A:651:ALA:CB	2.39	0.51
1:A:874:ASN:HD22	1:A:876:GLU:H	1.59	0.51
1:A:568:LEU:N	2:A:1331:HOH:O	2.31	0.51
1:A:671:PHE:HB2	1:A:678:ALA:HB3	1.94	0.50
1:A:439:TYR:CE2	2:A:1393:HOH:O	2.64	0.50
1:A:867:GLU:HG3	2:A:1268:HOH:O	2.10	0.50
1:A:521:LYS:HD2	2:A:1353:HOH:O	2.11	0.50
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.08	0.50
1:A:652:THR:HA	1:A:672:MET:HE3	1.93	0.49
1:A:667:HIS:HE1	2:A:1225:HOH:O	1.95	0.49
1:A:867:GLU:HG2	2:A:1324:HOH:O	2.12	0.48
1:A:483:HIS:HE2	1:A:529:LEU:HB2	1.76	0.48
1:A:224:TYR:CA	2:A:1347:HOH:O	2.62	0.48
1:A:228:LYS:CD	2:A:1373:HOH:O	2.61	0.48
1:A:278:LYS:HG2	1:A:279:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LYS:CD	1:A:889:LYS:N	2.75	0.48
1:A:867:GLU:CG	2:A:1324:HOH:O	2.62	0.47
1:A:228:LYS:HD3	2:A:1373:HOH:O	2.13	0.47
1:A:652:THR:HG23	1:A:653:ALA:H	1.80	0.46
1:A:850:GLN:HE22	1:A:863:LYS:CD	2.29	0.46
1:A:648:ASP:HB2	2:A:1118:HOH:O	2.14	0.46
1:A:222:ARG:NH2	1:A:271:ASP:HB3	2.31	0.46
1:A:850:GLN:NE2	1:A:863:LYS:HD2	2.31	0.46
1:A:708:LYS:HE3	1:A:715:GLU:CD	2.36	0.46
1:A:648:ASP:O	1:A:649:ALA:CB	2.65	0.45
1:A:552:LYS:CG	1:A:567:SER:HB2	2.46	0.45
1:A:267:ARG:HD2	2:A:1174:HOH:O	2.14	0.45
1:A:874:ASN:ND2	1:A:876:GLU:H	2.14	0.45
1:A:540:ARG:HG3	2:A:997:HOH:O	2.16	0.45
1:A:817:LEU:C	1:A:817:LEU:HD13	2.37	0.45
1:A:219:GLN:O	1:A:222:ARG:HA	2.17	0.45
1:A:498:GLN:HB3	1:A:529:LEU:HD21	2.00	0.44
1:A:364:ARG:HD2	2:A:1137:HOH:O	2.07	0.44
1:A:850:GLN:HE22	1:A:863:LYS:HD2	1.82	0.44
1:A:349:ASN:ND2	2:A:1076:HOH:O	2.50	0.43
1:A:649:ALA:CB	2:A:1380:HOH:O	2.58	0.43
1:A:439:TYR:CD2	2:A:1393:HOH:O	2.57	0.43
1:A:254:ASN:ND2	1:A:256:SER:H	2.17	0.42
1:A:650:ASN:O	1:A:651:ALA:CB	2.65	0.42
1:A:889:LYS:H	1:A:889:LYS:HE2	1.84	0.42
1:A:270:ARG:NH2	1:A:317:GLU:OE1	2.53	0.42
1:A:458:MET:CE	1:A:458:MET:HG2	2.49	0.42
1:A:483:HIS:NE2	1:A:525:LEU:O	2.52	0.42
1:A:889:LYS:H	1:A:889:LYS:CE	2.33	0.41
1:A:293:ASP:O	1:A:298:THR:HB	2.21	0.41
1:A:224:TYR:HA	2:A:1347:HOH:O	2.20	0.41
1:A:242:TYR:CD2	1:A:298:THR:HG23	2.55	0.41
1:A:254:ASN:ND2	1:A:254:ASN:C	2.73	0.41
1:A:344:LYS:NZ	1:A:379:GLN:HE22	2.19	0.41
1:A:822:GLU:H	1:A:822:GLU:HG3	1.66	0.40
1:A:213:LEU:HB3	2:A:1421:HOH:O	2.20	0.40
1:A:568:LEU:CA	2:A:1331:HOH:O	2.70	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	719/721 (100%)	689 (96%)	24 (3%)	6 (1%)	24	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	649	ALA
1	A	651	ALA
1	A	652	THR
1	A	223	ILE
1	A	221	ASP
1	A	219	GLN

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	638/640 (100%)	599 (94%)	39 (6%)	23	2

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	189	GLN
1	A	219	GLN
1	A	221	ASP
1	A	222	ARG

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Mol	Chain	Res	Type
1	A	228	LYS
1	A	232	TYR
1	A	252	VAL
1	A	254	ASN
1	A	278	LYS
1	A	282	ASN
1	A	320	LYS
1	A	337	LYS
1	A	364	ARG
1	A	383	LEU
1	A	404	TYR
1	A	432	LYS
1	A	458	MET
1	A	468	ASN
1	A	483	HIS
1	A	492	GLU
1	A	495	GLN
1	A	529	LEU
1	A	557	ASN
1	A	626	LYS
1	A	648	ASP
1	A	717	SER
1	A	720	GLU
1	A	748	LYS
1	A	780	LEU
1	A	792	SER
1	A	808	GLN
1	A	813	LEU
1	A	814	GLU
1	A	822	GLU
1	A	867	GLU
1	A	869	LYS
1	A	874	ASN
1	A	889	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	254	ASN
1	A	279	HIS
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	349	ASN
1	A	379	GLN
1	A	386	GLN
1	A	468	ASN
1	A	483	HIS
1	A	557	ASN
1	A	667	HIS
1	A	685	GLN
1	A	698	GLN
1	A	759	GLN
1	A	789	ASN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	850	GLN
1	A	874	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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(Å²)	Q<0.9
1	A	721/721 (100%)	0.36	49 (6%)	20	20	13, 21, 36, 65	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ASP	10.4
1	A	567	SER	10.4
1	A	223	ILE	8.8
1	A	232	TYR	8.5
1	A	220	ALA	6.8
1	A	651	ALA	6.7
1	A	434	LYS	6.4
1	A	219	GLN	6.2
1	A	170	VAL	6.1
1	A	224	TYR	5.4
1	A	222	ARG	5.2
1	A	649	ALA	4.4
1	A	652	THR	4.3
1	A	689	THR	4.2
1	A	171	LYS	4.1
1	A	340	ASP	4.0
1	A	648	ASP	3.9
1	A	849	ASN	3.9
1	A	427	LYS	3.8
1	A	566	LEU	3.8
1	A	433	ASP	3.6
1	A	704	SER	3.5
1	A	650	ASN	3.2
1	A	865	GLY	3.2
1	A	490	GLU	3.1
1	A	218	SER	3.0
1	A	431	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	2.7
1	A	705	ASN	2.6
1	A	174	TYR	2.5
1	A	368	GLN	2.5
1	A	866	ASP	2.5
1	A	867	GLU	2.5
1	A	492	GLU	2.4
1	A	279	HIS	2.4
1	A	342	PRO	2.4
1	A	233	LYS	2.3
1	A	721	GLN	2.3
1	A	375	ARG	2.3
1	A	864	GLU	2.2
1	A	196	ASP	2.2
1	A	194	LYS	2.2
1	A	772	ASP	2.2
1	A	430	ILE	2.2
1	A	766	ILE	2.1
1	A	837	ILE	2.1
1	A	278	LYS	2.1
1	A	228	LYS	2.0
1	A	383	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.