Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:21 PM GMT

PDB ID	:	1F9G
Title	:	CRYSTAL STRUCTURE OF STREPTOCOCCUS PNEUMONIAE HYALURONATE LYASE COCRYSTALLIZED WITH ASCORBIC ACID
Authors	:	Li, S.; Jedrzejas, M.J.
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
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 (1)) were used in the production of this report:

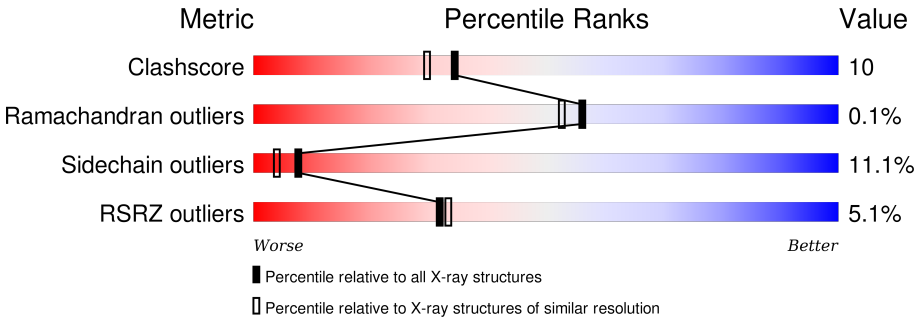
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	731	5% 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	A	950	X	-	-	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.

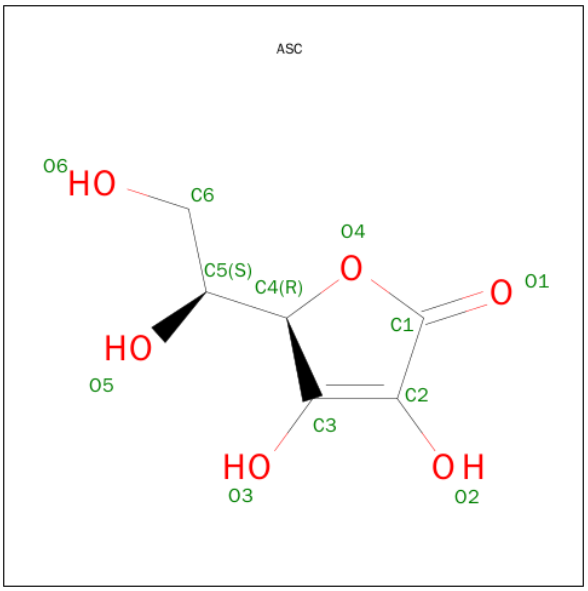
- Molecule 1 is a protein called HYALURONATE LYASE.

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

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	-	C-TERMINLA HIS-TAG	UNP Q54873
A	894	HIS	-	C-TERMINLA HIS-TAG	UNP Q54873
A	895	HIS	-	C-TERMINLA HIS-TAG	UNP Q54873
A	896	HIS	-	C-TERMINLA HIS-TAG	UNP Q54873
A	897	HIS	-	C-TERMINLA HIS-TAG	UNP Q54873
A	898	HIS	-	C-TERMINLA HIS-TAG	UNP Q54873

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



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

- Molecule 3 is water.

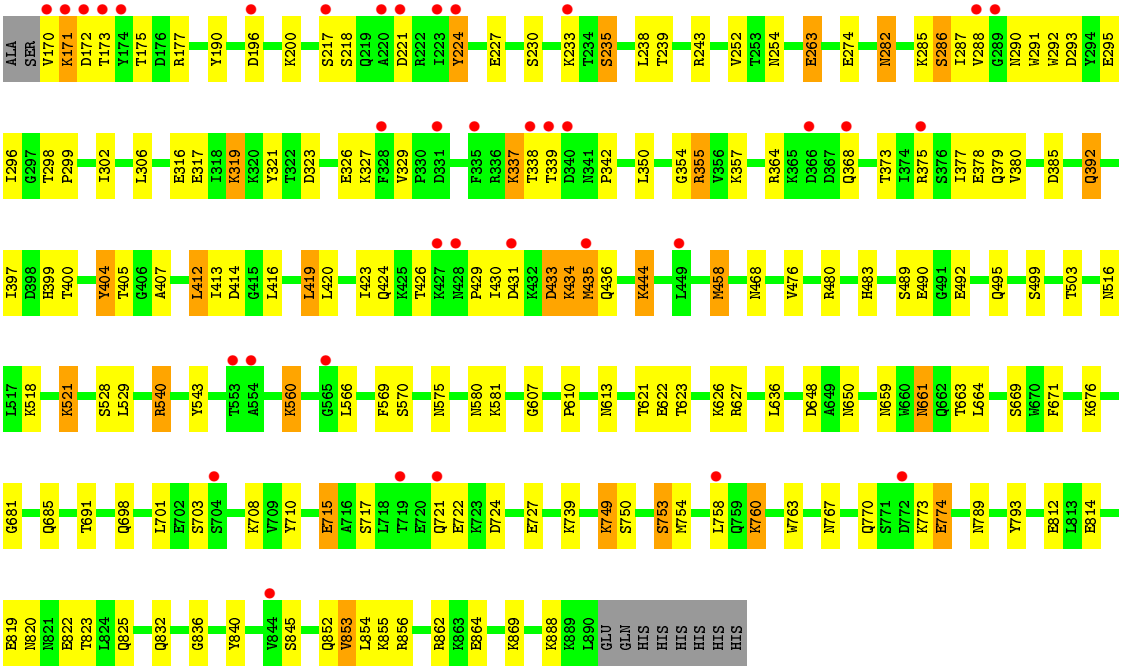
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	266	Total O 266 266	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.26Å 102.67Å 103.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.00 46.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (45.00-2.00) 88.6 (46.12-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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.	DCC
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
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 54219 reflections	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.*

[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

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	0.37	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

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	114	0
2	A	12	0	7	0	0
3	A	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HD1	1:A:224:TYR:N	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:499:SER:O	1:A:503:THR:HG22	1.98	0.63
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.80	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:OE1	1:A:326:GLU:HA	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:HD22	1:A:661:ASN:C	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:302:ILE:O	1:A:306:LEU:HG	2.09	0.53
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:O	1:A:170:VAL:HG13	2.09	0.51
1:A:476:VAL:O	1:A:480:ARG:HG2	2.11	0.50
1:A:832:GLN:HE21	1:A:862:ARG:NH2	2.08	0.50
1:A:760:LYS:HD2	1:A:774:GLU:OE1	2.12	0.50
1:A:295:GLU:HB3	1:A:329:VAL:HG22	1.93	0.50
1:A:286:SER:O	1:A:288:VAL:HG23	2.11	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:290:ASN:HD22	1:A:292:TRP:CB	2.27	0.48
1:A:287:ILE:HD12	1:A:339:THR:CG2	2.42	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:819:GLU:HG3	1:A:820:ASN:N	2.30	0.46
1:A:380:VAL:CG2	1:A:412:LEU:HD21	2.45	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:669:SER:OG	1:A:825:GLN:NE2	2.49	0.46
1:A:282:ASN:HD21	1:A:285:LYS:HG2	1.81	0.46
1:A:671:PHE:HD2	1:A:836:GLY:HA3	1.81	0.45
1:A:569:PHE:CE2	1:A:575:ASN:HB3	2.51	0.45
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.50	0.45
1:A:177:ARG:HG2	1:A:177:ARG:HH11	1.81	0.45
1:A:749:LYS:CE	1:A:749:LYS:H	2.19	0.45
1:A:543:TYR:HA	1:A:648:ASP:HB2	1.98	0.45
1:A:444:LYS:HE2	3:A:1001:HOH:O	2.16	0.45
1:A:392:GLN:O	1:A:392:GLN:HG2	2.16	0.45
1:A:820:ASN:ND2	1:A:825:GLN:HG2	2.23	0.45
1:A:431:ASP:HB2	1:A:434:LYS:HZ2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:HB3	1:A:329:VAL:CG2	2.48	0.43
1:A:235:SER:HB2	1:A:290:ASN:H	1.81	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:239:THR:HG22	1:A:298:THR:N	2.35	0.42
1:A:177:ARG:HG2	1:A:177:ARG:NH1	2.34	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:659:ASN:HD21	1:A:661:ASN:HD21	1.68	0.42
1:A:580:ASN:O	1:A:581:LYS:HB2	2.20	0.42
1:A:399:HIS:O	1:A:400:THR:HB	2.20	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:H	1:A:661:ASN:ND2	2.18	0.41
1:A:661:ASN:ND2	1:A:661:ASN:C	2.72	0.41
1:A:754:MET:HE2	1:A:754:MET:HB3	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	A	719/731 (98%)	675 (94%)	43 (6%)	1 (0%)	56 53

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%)	567 (89%)	71 (11%)	8 4

All (71) 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	243	ARG
1	A	252	VAL
1	A	254	ASN
1	A	263	GLU
1	A	282	ASN
1	A	286	SER
1	A	316	GLU
1	A	319	LYS
1	A	327	LYS

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Mol	Chain	Res	Type
1	A	337	LYS
1	A	338	THR
1	A	355	ARG
1	A	368	GLN
1	A	375	ARG
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
1	A	435	MET
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	661	ASN
1	A	676	LYS
1	A	701	LEU
1	A	703	SER
1	A	715	GLU
1	A	717	SER
1	A	721	GLN
1	A	724	ASP
1	A	727	GLU
1	A	739	LYS
1	A	749	LYS
1	A	750	SER
1	A	753	SER

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Mol	Chain	Res	Type
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	853	VAL
1	A	854	LEU
1	A	855	LYS
1	A	864	GLU
1	A	869	LYS

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	189	GLN
1	A	202	ASN
1	A	237	ASN
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	386	GLN
1	A	424	GLN
1	A	428	ASN
1	A	436	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 (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)

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	1.71	3 (25%)	17,17,17	2.92	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	0/6/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	950	ASC	O3-C3	-2.48	1.25	1.33
2	A	950	ASC	O4-C1	2.13	1.39	1.35
2	A	950	ASC	C2-C1	3.16	1.53	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	ASC	O6-C6-C5	-4.26	101.82	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	950	ASC	O4-C1-C2	-3.15	107.25	109.90
2	A	950	ASC	O2-C2-C1	2.01	127.20	121.86
2	A	950	ASC	O4-C4-C3	3.65	106.98	104.06
2	A	950	ASC	O4-C4-C5	5.04	118.20	109.71
2	A	950	ASC	C6-C5-C4	8.00	125.47	111.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	950	ASC	C5

There are no torsion outliers.

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, 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	A	721/731 (98%)	0.37	37 (5%) 32 33	15, 31, 64, 90	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	LYS	6.2
1	A	170	VAL	5.8
1	A	171	LYS	4.6
1	A	338	THR	4.1
1	A	704	SER	3.8
1	A	174	TYR	3.5
1	A	721	GLN	3.4
1	A	223	ILE	3.2
1	A	172	ASP	3.1
1	A	366	ASP	3.0
1	A	758	LEU	2.9
1	A	435	MET	2.9
1	A	173	THR	2.8
1	A	340	ASP	2.8
1	A	553	THR	2.7
1	A	368	GLN	2.7
1	A	289	GLY	2.4
1	A	288	VAL	2.4
1	A	335	PHE	2.4
1	A	220	ALA	2.3
1	A	431	ASP	2.3
1	A	328	PHE	2.3
1	A	375	ARG	2.3
1	A	196	ASP	2.3
1	A	428	ASN	2.3
1	A	221	ASP	2.3
1	A	554	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	233	LYS	2.2
1	A	719	THR	2.2
1	A	772	ASP	2.2
1	A	339	THR	2.1
1	A	844	VAL	2.1
1	A	217	SER	2.1
1	A	565	GLY	2.0
1	A	224	TYR	2.0
1	A	449	LEU	2.0
1	A	331	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 carbohydrates 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. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	ASC	A	950	12/12	0.64	0.26	3.14	58,62,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.