Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:48 AM GMT

PDB ID	:	2BRV
Title	:	Crystal structure of Streptococcus Pneumoniae Hyaluronate Lyase from 70per-cent saturated malonate.
Authors	:	Rigden, D.J.; Jedrzejas, M.J.
Deposited on	:	2005-05-11
Resolution	:	3.30 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:

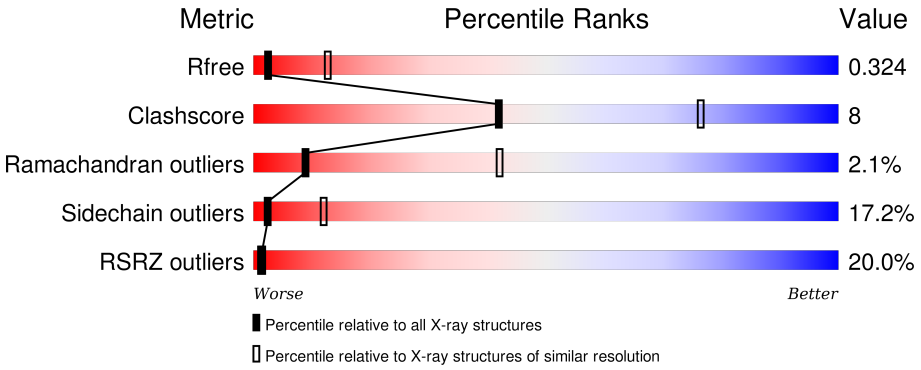
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	X	731	20% 66% 26% 5%

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	MLA	X	1892	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5776 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.

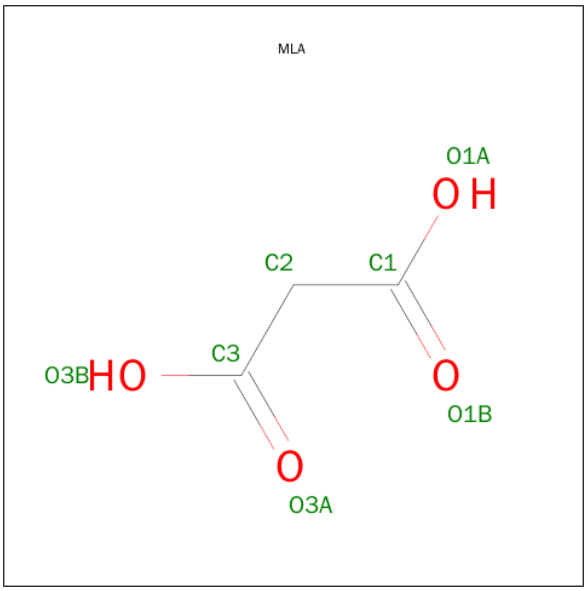
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	714	Total	C	N	O	S	0	0	0
			5734	3609	957	1146	22			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	173	THR	ALA	SEE REMARK 999	UNP Q54873
X	196	ASP	GLU	SEE REMARK 999	UNP Q54873
X	496	ARG	CYS	SEE REMARK 999	UNP Q54873
X	541	THR	PRO	SEE REMARK 999	UNP Q54873
X	704	SER	GLY	SEE REMARK 999	UNP Q54873
X	736	SER	PHE	SEE REMARK 999	UNP Q54873
X	790	GLY	ARG	SEE REMARK 999	UNP Q54873

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



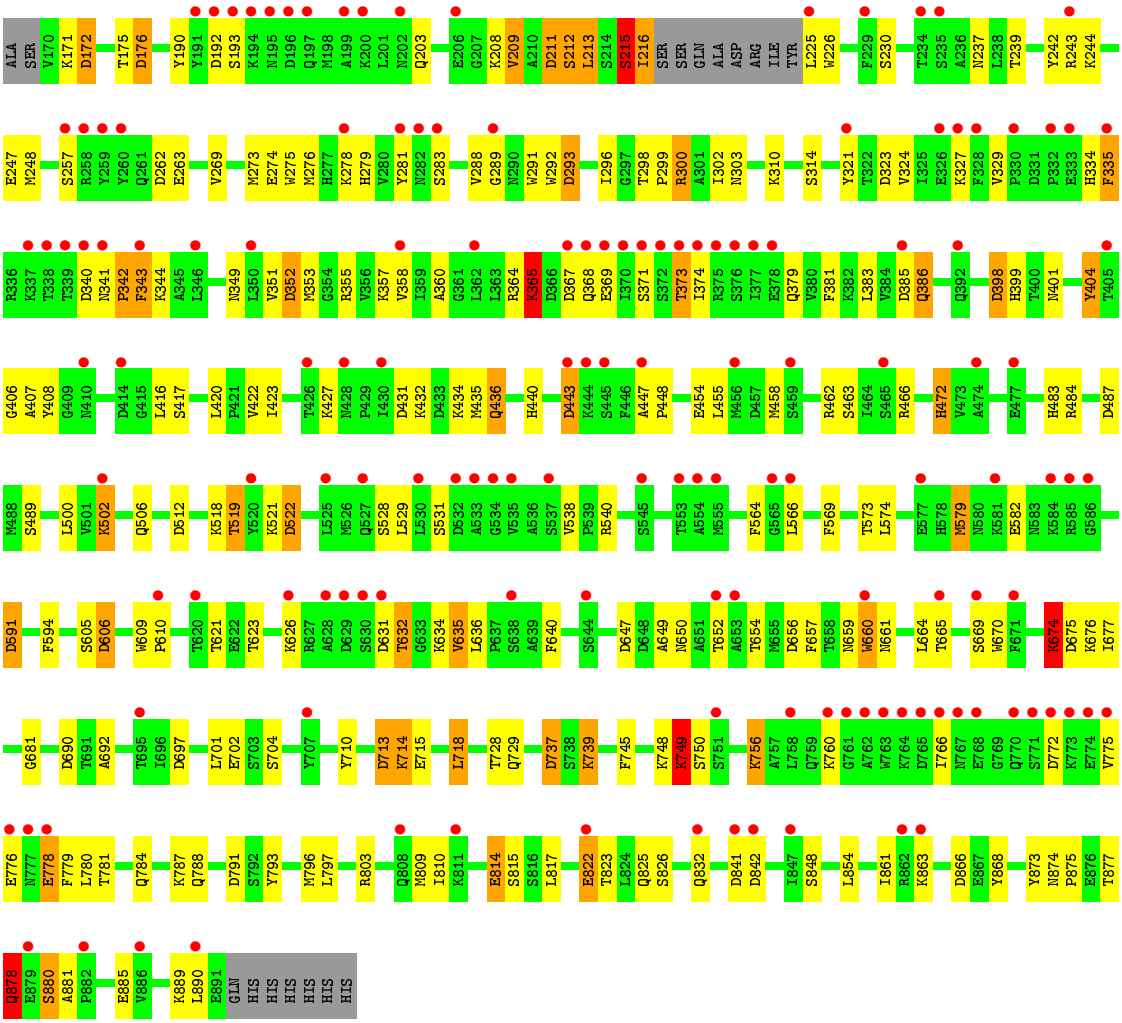
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X	1	Total	C	O	0	0
			7	3	4		
2	X	1	Total	C	O	0	0
			7	3	4		
2	X	1	Total	C	O	0	0
			7	3	4		
2	X	1	Total	C	O	0	0
			7	3	4		
2	X	1	Total	C	O	0	0
			7	3	4		
2	X	1	Total	C	O	0	0
			7	3	4		

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 X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.72Å 101.05Å 85.21Å 90.00° 125.12° 90.00°	Depositor
Resolution (Å)	69.01 – 3.30 40.91 – 3.09	Depositor EDS
% Data completeness (in resolution range)	93.8 (69.01-3.30) 94.2 (40.91-3.09)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.301 , 0.327 0.294 , 0.324	Depositor DCC
R_{free} test set	579 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	88.1	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 14155 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5776	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: MLA

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	X	0.34	0/5851	0.75	31/7901 (0.4%)

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	X	1	0

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	632	THR	CA-CB-CG2	6.54	121.56	112.40
1	X	172	ASP	CB-CG-OD2	5.80	123.53	118.30
1	X	323	ASP	CB-CG-OD2	5.80	123.52	118.30
1	X	176	ASP	CB-CG-OD2	5.76	123.48	118.30
1	X	713	ASP	CB-CG-OD2	5.70	123.43	118.30
1	X	385	ASP	CB-CG-OD2	5.68	123.42	118.30
1	X	340	ASP	CB-CG-OD2	5.60	123.34	118.30
1	X	522	ASP	CB-CG-OD2	5.51	123.26	118.30
1	X	842	ASP	CB-CG-OD2	5.51	123.26	118.30
1	X	431	ASP	CB-CG-OD2	5.46	123.22	118.30
1	X	352	ASP	CB-CG-OD2	5.42	123.18	118.30
1	X	656	ASP	CB-CG-OD2	5.41	123.17	118.30
1	X	262	ASP	CB-CG-OD2	5.40	123.16	118.30
1	X	866	ASP	CB-CG-OD2	5.34	123.11	118.30
1	X	631	ASP	CB-CG-OD2	5.26	123.03	118.30
1	X	591	ASP	CB-CG-OD2	5.24	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	606	ASP	CB-CG-OD2	5.23	123.00	118.30
1	X	443	ASP	CB-CG-OD2	5.22	123.00	118.30
1	X	192	ASP	CB-CG-OD2	5.20	122.98	118.30
1	X	367	ASP	CB-CG-OD2	5.19	122.97	118.30
1	X	211	ASP	CB-CG-OD2	5.19	122.97	118.30
1	X	737	ASP	CB-CG-OD2	5.18	122.96	118.30
1	X	697	ASP	CB-CG-OD2	5.17	122.96	118.30
1	X	293	ASP	CB-CG-OD2	5.12	122.91	118.30
1	X	690	ASP	CB-CG-OD2	5.11	122.90	118.30
1	X	841	ASP	CB-CG-OD2	5.10	122.89	118.30
1	X	675	ASP	CB-CG-OD2	5.07	122.87	118.30
1	X	512	ASP	CB-CG-OD2	5.05	122.85	118.30
1	X	647	ASP	CB-CG-OD2	5.05	122.85	118.30
1	X	487	ASP	CB-CG-OD2	5.03	122.83	118.30
1	X	398	ASP	CB-CG-OD2	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	632	THR	CB

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	X	5734	0	5556	95	0
2	X	42	0	12	0	0
All	All	5776	0	5568	95	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 8.

All (95) 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:X:873:TYR:O	1:X:875:PRO:HD3	1.95	0.67
1:X:432:LYS:O	1:X:436:GLN:NE2	2.31	0.64
1:X:342:PRO:O	1:X:343:PHE:HB3	1.98	0.64
1:X:383:LEU:HD11	1:X:440:HIS:CE1	2.33	0.63
1:X:216:ILE:HB	1:X:226:TRP:CZ2	2.36	0.61
1:X:502:LYS:HE2	1:X:506:GLN:HE22	1.65	0.61
1:X:216:ILE:HB	1:X:226:TRP:CE2	2.36	0.61
1:X:714:LYS:N	1:X:714:LYS:CD	2.65	0.59
1:X:298:THR:HB	1:X:299:PRO:HD3	1.85	0.59
1:X:216:ILE:HG12	1:X:225:LEU:HB3	1.86	0.58
1:X:650:ASN:HD21	1:X:832:GLN:HE22	1.53	0.57
1:X:714:LYS:N	1:X:714:LYS:HD3	2.20	0.57
1:X:373:THR:HG22	1:X:374:ILE:N	2.20	0.56
1:X:211:ASP:O	1:X:215:SER:OG	2.24	0.56
1:X:621:THR:HG22	1:X:664:LEU:HD21	1.88	0.56
1:X:175:THR:HG23	1:X:365:LYS:HZ1	1.70	0.56
1:X:417:SER:HB2	1:X:484:ARG:HB2	1.87	0.56
1:X:718:LEU:HD23	1:X:718:LEU:N	2.20	0.56
1:X:239:THR:HG22	1:X:243:ARG:HG3	1.89	0.55
1:X:676:LYS:C	1:X:677:ILE:HG13	2.26	0.55
1:X:649:ALA:HB1	1:X:674:LYS:HG2	1.89	0.55
1:X:341:ASN:O	1:X:342:PRO:O	2.26	0.54
1:X:296:ILE:O	1:X:300:ARG:HG3	2.08	0.54
1:X:650:ASN:ND2	1:X:832:GLN:HE22	2.07	0.52
1:X:701:LEU:HD12	1:X:778:GLU:HG2	1.90	0.52
1:X:669:SER:OG	1:X:825:GLN:NE2	2.43	0.52
1:X:566:LEU:HD21	1:X:670:TRP:CG	2.45	0.51
1:X:880:SER:OG	1:X:881:ALA:N	2.43	0.51
1:X:519:THR:HG23	1:X:522:ASP:OD2	2.09	0.51
1:X:737:ASP:OD1	1:X:739:LYS:N	2.43	0.51
1:X:574:LEU:HD12	1:X:635:VAL:HG12	1.93	0.50
1:X:483:HIS:CE1	1:X:529:LEU:HD11	2.46	0.50
1:X:728:THR:HG22	1:X:728:THR:O	2.11	0.50
1:X:175:THR:CG2	1:X:365:LYS:HZ1	2.24	0.49
1:X:321:TYR:O	1:X:324:VAL:HG12	2.12	0.49
1:X:208:LYS:O	1:X:209:VAL:C	2.51	0.49
1:X:483:HIS:HE1	1:X:529:LEU:HG	1.78	0.48
1:X:447:ALA:N	1:X:448:PRO:CD	2.76	0.48
1:X:623:THR:HA	1:X:692:ALA:HA	1.96	0.48
1:X:399:HIS:CE1	1:X:408:TYR:OH	2.67	0.48
1:X:244:LYS:HA	1:X:247:GLU:HG3	1.95	0.48
1:X:373:THR:CG2	1:X:374:ILE:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:609:TRP:N	1:X:610:PRO:HD2	2.29	0.47
1:X:274:GLU:HG3	1:X:275:TRP:N	2.29	0.47
1:X:369:GLU:O	1:X:373:THR:HB	2.15	0.47
1:X:401:ASN:HB2	1:X:573:THR:HA	1.96	0.47
1:X:502:LYS:CE	1:X:506:GLN:HE22	2.27	0.46
1:X:398:ASP:O	1:X:399:HIS:HB2	2.16	0.46
1:X:373:THR:HG22	1:X:374:ILE:HG13	1.97	0.46
1:X:358:VAL:HG23	1:X:373:THR:HG21	1.97	0.45
1:X:564:PHE:CD1	1:X:677:ILE:HD13	2.51	0.45
1:X:404:TYR:CD1	1:X:407:ALA:HB3	2.50	0.45
1:X:635:VAL:HG23	1:X:636:LEU:O	2.16	0.45
1:X:293:ASP:O	1:X:298:THR:HB	2.17	0.45
1:X:406:GLY:CA	1:X:455:LEU:HD21	2.47	0.45
1:X:566:LEU:HD21	1:X:670:TRP:CD2	2.51	0.45
1:X:518:LYS:C	1:X:519:THR:HG22	2.37	0.45
1:X:454:GLU:HB2	1:X:472:HIS:ND1	2.32	0.45
1:X:745:PHE:HB2	1:X:810:ILE:HG22	1.98	0.44
1:X:701:LEU:HD11	1:X:780:LEU:HB2	2.00	0.44
1:X:634:LYS:HA	1:X:634:LYS:HE2	1.99	0.44
1:X:175:THR:HG23	1:X:365:LYS:NZ	2.32	0.44
1:X:780:LEU:HD23	1:X:781:THR:N	2.32	0.44
1:X:406:GLY:HA3	1:X:455:LEU:HD21	1.99	0.44
1:X:640:PHE:CE2	1:X:654:THR:HG21	2.53	0.44
1:X:358:VAL:CG2	1:X:373:THR:HG21	2.48	0.43
1:X:780:LEU:C	1:X:780:LEU:HD23	2.37	0.43
1:X:242:TYR:CZ	1:X:276:MET:HE2	2.52	0.43
1:X:822:GLU:HG2	1:X:823:THR:HG23	2.01	0.43
1:X:579:MET:O	1:X:582:GLU:N	2.51	0.43
1:X:360:ALA:O	1:X:364:ARG:HG3	2.19	0.43
1:X:243:ARG:O	1:X:247:GLU:HG3	2.19	0.42
1:X:756:LYS:CG	1:X:756:LYS:O	2.67	0.42
1:X:381:PHE:CZ	1:X:416:LEU:HD21	2.54	0.42
1:X:748:LYS:O	1:X:749:LYS:C	2.58	0.42
1:X:756:LYS:HA	1:X:779:PHE:O	2.19	0.42
1:X:569:PHE:CZ	1:X:636:LEU:HD13	2.55	0.42
1:X:335:PHE:CE2	1:X:353:MET:HE2	2.54	0.42
1:X:273:MET:CE	1:X:302:ILE:HG23	2.50	0.42
1:X:564:PHE:CG	1:X:677:ILE:HD13	2.55	0.41
1:X:713:ASP:C	1:X:714:LYS:HD2	2.40	0.41
1:X:718:LEU:CD2	1:X:718:LEU:N	2.82	0.41
1:X:483:HIS:HE1	1:X:529:LEU:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:814:GLU:HG2	1:X:815:SER:N	2.35	0.41
1:X:303:ASN:HD21	1:X:360:ALA:HB2	1.84	0.41
1:X:269:VAL:O	1:X:273:MET:N	2.54	0.41
1:X:341:ASN:N	1:X:342:PRO:CD	2.84	0.41
1:X:383:LEU:CD1	1:X:440:HIS:CE1	3.03	0.41
1:X:868:TYR:CE2	1:X:889:LYS:HG3	2.55	0.41
1:X:710:TYR:CE2	1:X:803:ARG:CZ	3.03	0.41
1:X:291:TRP:CG	1:X:292:TRP:N	2.89	0.41
1:X:877:THR:O	1:X:878:GLN:C	2.58	0.41
1:X:569:PHE:HE1	1:X:591:ASP:OD1	2.05	0.40
1:X:681:GLY:HA3	1:X:793:TYR:CE2	2.57	0.40
1:X:281:TYR:CE1	1:X:324:VAL:HG21	2.56	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	X	710/731 (97%)	599 (84%)	96 (14%)	15 (2%)	9 42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	213	LEU
1	X	342	PRO
1	X	660	TRP
1	X	215	SER
1	X	343	PHE
1	X	365	LYS
1	X	423	ILE
1	X	878	GLN
1	X	212	SER

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Mol	Chain	Res	Type
1	X	386	GLN
1	X	674	LYS
1	X	209	VAL
1	X	749	LYS
1	X	422	VAL
1	X	289	GLY

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	X	634/649 (98%)	525 (83%)	109 (17%)	2 12

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	171	LYS
1	X	172	ASP
1	X	176	ASP
1	X	190	TYR
1	X	193	SER
1	X	203	GLN
1	X	212	SER
1	X	213	LEU
1	X	215	SER
1	X	216	ILE
1	X	230	SER
1	X	237	ASN
1	X	248	MET
1	X	257	SER
1	X	263	GLU
1	X	278	LYS
1	X	279	HIS
1	X	283	SER
1	X	288	VAL
1	X	300	ARG

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Mol	Chain	Res	Type
1	X	310	LYS
1	X	314	SER
1	X	327	LYS
1	X	329	VAL
1	X	334	HIS
1	X	335	PHE
1	X	344	LYS
1	X	349	ASN
1	X	351	VAL
1	X	352	ASP
1	X	355	ARG
1	X	357	LYS
1	X	365	LYS
1	X	368	GLN
1	X	371	SER
1	X	373	THR
1	X	379	GLN
1	X	386	GLN
1	X	404	TYR
1	X	420	LEU
1	X	427	LYS
1	X	434	LYS
1	X	435	MET
1	X	436	GLN
1	X	443	ASP
1	X	458	MET
1	X	462	ARG
1	X	463	SER
1	X	466	ARG
1	X	472	HIS
1	X	489	SER
1	X	500	LEU
1	X	502	LYS
1	X	519	THR
1	X	521	LYS
1	X	528	SER
1	X	531	SER
1	X	538	VAL
1	X	540	ARG
1	X	579	MET
1	X	594	PHE
1	X	605	SER

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Mol	Chain	Res	Type
1	X	606	ASP
1	X	626	LYS
1	X	632	THR
1	X	635	VAL
1	X	652	THR
1	X	657	PHE
1	X	659	ASN
1	X	660	TRP
1	X	661	ASN
1	X	665	THR
1	X	674	LYS
1	X	702	GLU
1	X	704	SER
1	X	714	LYS
1	X	715	GLU
1	X	718	LEU
1	X	729	GLN
1	X	739	LYS
1	X	749	LYS
1	X	750	SER
1	X	756	LYS
1	X	760	LYS
1	X	766	ILE
1	X	772	ASP
1	X	775	VAL
1	X	776	GLU
1	X	778	GLU
1	X	784	GLN
1	X	787	LYS
1	X	788	GLN
1	X	791	ASP
1	X	796	MET
1	X	797	LEU
1	X	809	MET
1	X	814	GLU
1	X	817	LEU
1	X	822	GLU
1	X	826	SER
1	X	848	SER
1	X	854	LEU
1	X	861	ILE
1	X	863	LYS

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Mol	Chain	Res	Type
1	X	874	ASN
1	X	878	GLN
1	X	880	SER
1	X	885	GLU
1	X	890	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	202	ASN
1	X	231	ASN
1	X	237	ASN
1	X	254	ASN
1	X	399	HIS
1	X	440	HIS
1	X	483	HIS
1	X	661	ASN
1	X	683	ASN
1	X	729	GLN
1	X	820	ASN
1	X	825	GLN
1	X	832	GLN
1	X	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)

6 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	$\#\|Z\| > 2$
2	MLA	X	1892	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	X	1893	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	X	1894	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	X	1895	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	X	1896	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	X	1897	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLA	X	1892	-	-	0/0/4/4	0/0/0/0
2	MLA	X	1893	-	-	0/0/4/4	0/0/0/0
2	MLA	X	1894	-	-	0/0/4/4	0/0/0/0
2	MLA	X	1895	-	-	0/0/4/4	0/0/0/0
2	MLA	X	1896	-	-	0/0/4/4	0/0/0/0
2	MLA	X	1897	-	-	0/0/4/4	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.

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

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	X	714/731 (97%)	1.11	143 (20%) 1 1	27, 54, 74, 76	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	330	PRO	9.7
1	X	774	GLU	7.6
1	X	338	THR	7.3
1	X	192	ASP	6.9
1	X	193	SER	6.2
1	X	343	PHE	5.9
1	X	585	ARG	5.6
1	X	768	GLU	5.5
1	X	581	LYS	5.3
1	X	445	SER	5.2
1	X	283	SER	5.2
1	X	443	ASP	4.9
1	X	197	GLN	4.9
1	X	367	ASP	4.7
1	X	761	GLY	4.6
1	X	376	SER	4.6
1	X	335	PHE	4.5
1	X	776	GLU	4.5
1	X	194	LYS	4.4
1	X	545	SER	4.3
1	X	533	ALA	4.3
1	X	378	GLU	4.3
1	X	584	LYS	4.2
1	X	229	PHE	4.1
1	X	765	ASP	4.1
1	X	760	LYS	4.1
1	X	764	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	X	206	GLU	4.0
1	X	771	SER	3.9
1	X	339	THR	3.9
1	X	430	ILE	3.9
1	X	629	ASP	3.8
1	X	863	LYS	3.8
1	X	841	ASP	3.7
1	X	762	ALA	3.7
1	X	259	TYR	3.7
1	X	195	ASN	3.7
1	X	371	SER	3.7
1	X	773	LYS	3.7
1	X	626	LYS	3.6
1	X	278	LYS	3.6
1	X	340	ASP	3.6
1	X	775	VAL	3.6
1	X	532	ASP	3.5
1	X	225	LEU	3.5
1	X	882	PRO	3.4
1	X	234	THR	3.4
1	X	459	SER	3.4
1	X	337	LYS	3.4
1	X	886	VAL	3.4
1	X	369	GLU	3.3
1	X	332	PRO	3.3
1	X	350	LEU	3.3
1	X	465	SER	3.3
1	X	630	SER	3.2
1	X	326	GLU	3.2
1	X	660	TRP	3.2
1	X	202	ASN	3.2
1	X	282	ASN	3.2
1	X	763	TRP	3.2
1	X	258	ARG	3.2
1	X	477	GLU	3.1
1	X	766	ILE	3.1
1	X	191	TYR	3.0
1	X	767	ASN	3.0
1	X	373	THR	3.0
1	X	426	THR	3.0
1	X	235	SER	2.9
1	X	772	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	527	GLN	2.9
1	X	890	LEU	2.9
1	X	758	LEU	2.9
1	X	553	THR	2.9
1	X	328	PHE	2.8
1	X	447	ALA	2.8
1	X	565	GLY	2.8
1	X	554	ALA	2.8
1	X	281	TYR	2.8
1	X	199	ALA	2.8
1	X	257	SER	2.7
1	X	260	TYR	2.7
1	X	374	ILE	2.7
1	X	638	SER	2.7
1	X	196	ASP	2.6
1	X	414	ASP	2.6
1	X	610	PRO	2.6
1	X	534	GLY	2.6
1	X	375	ARG	2.6
1	X	525	LEU	2.6
1	X	811	LYS	2.6
1	X	333	GLU	2.6
1	X	346	LEU	2.6
1	X	362	LEU	2.6
1	X	341	ASN	2.5
1	X	586	GLY	2.5
1	X	377	ILE	2.5
1	X	372	SER	2.5
1	X	832	GLN	2.5
1	X	842	ASP	2.4
1	X	243	ARG	2.4
1	X	456	MET	2.4
1	X	751	SER	2.4
1	X	321	TYR	2.4
1	X	777	ASN	2.4
1	X	770	GLN	2.4
1	X	392	GLN	2.4
1	X	520	TYR	2.4
1	X	577	GLU	2.3
1	X	428	ASN	2.3
1	X	653	ALA	2.3
1	X	695	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	862	ARG	2.3
1	X	358	VAL	2.3
1	X	200	LYS	2.3
1	X	327	LYS	2.3
1	X	671	PHE	2.3
1	X	808	GLN	2.3
1	X	628	ALA	2.2
1	X	652	THR	2.3
1	X	370	ILE	2.2
1	X	847	ILE	2.2
1	X	444	LYS	2.2
1	X	778	GLU	2.2
1	X	644	SER	2.2
1	X	879	GLU	2.2
1	X	410	ASN	2.2
1	X	385	ASP	2.2
1	X	631	ASP	2.2
1	X	502	LYS	2.2
1	X	474	ALA	2.1
1	X	620	THR	2.1
1	X	665	THR	2.1
1	X	555	MET	2.1
1	X	368	GLN	2.1
1	X	537	SER	2.1
1	X	535	VAL	2.1
1	X	405	THR	2.1
1	X	707	TYR	2.1
1	X	289	GLY	2.0
1	X	566	LEU	2.0
1	X	822	GLU	2.0
1	X	669	SER	2.0
1	X	530	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)

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	MLA	X	1892	7/7	0.75	1.40	18.10	108,108,108,108	0
2	MLA	X	1894	7/7	0.42	0.28	-	107,108,108,108	0
2	MLA	X	1893	7/7	0.78	0.19	-	107,108,108,108	0
2	MLA	X	1895	7/7	0.59	0.16	-	108,108,108,108	0
2	MLA	X	1896	7/7	0.74	0.72	-	109,109,109,109	0
2	MLA	X	1897	7/7	0.79	0.19	-	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.