



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:41 PM GMT

PDB ID : 1LK9  
Title : The Three-dimensional Structure of Alliinase from Garlic  
Authors : Kuettner, E.B.; Hilgenfeld, R.; Weiss, M.S.  
Deposited on : 2002-04-24  
Resolution : 1.53 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

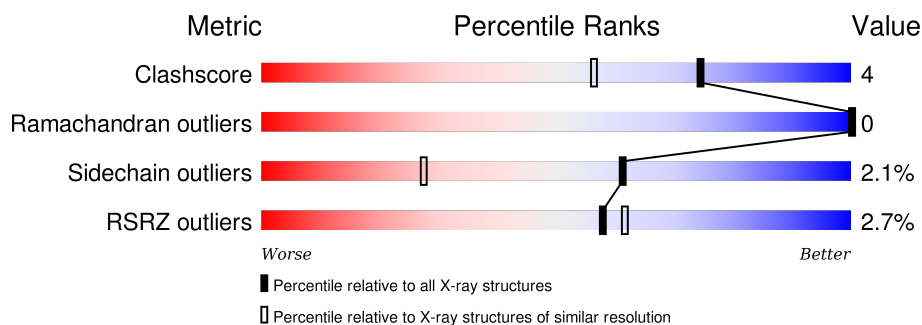
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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	1627 (1.56-1.52)
Ramachandran outliers	100387	1594 (1.56-1.52)
Sidechain outliers	100360	1592 (1.56-1.52)
RSRZ outliers	91569	1555 (1.56-1.52)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	448	
1	B	448	

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
4	NAG	B	500	-	-	-	X
5	SO4	A	907	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	910	-	-	-	X
5	SO4	B	903	-	-	-	X
8	EPE	A	851[B]	-	-	-	X
8	EPE	A	852[B]	-	-	-	X
9	DHA	B	850[A]	-	-	X	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7996 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 ALLIIN LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	11	0
			3453	2200	579	650	24			
1	B	427	Total	C	N	O	S	0	6	0
			3461	2208	580	649	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ASP	ASN	SEE REMARK 999	UNP Q01594
B	176	ASP	ASN	SEE REMARK 999	UNP Q01594

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

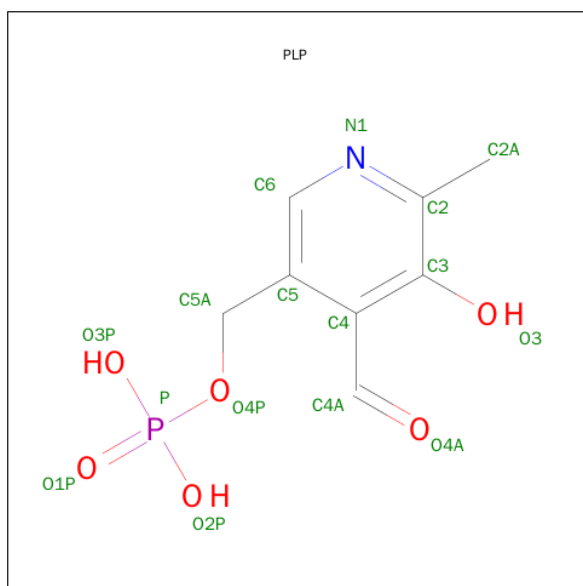
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



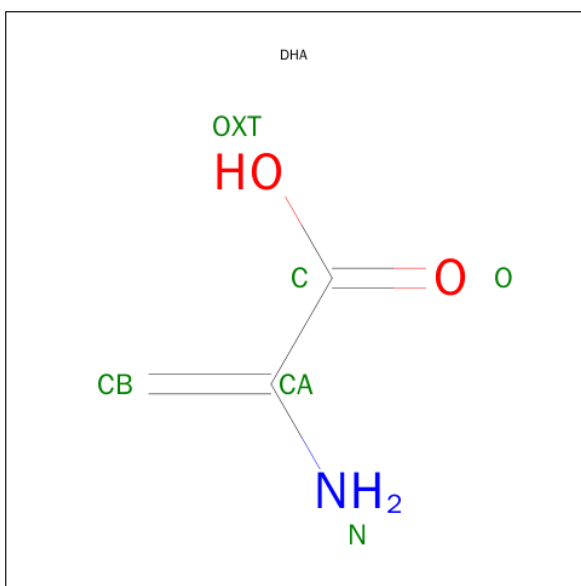
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
7	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	1
			15	8	2	4	1		
8	A	1	Total	C	N	O	S	0	1
			15	8	2	4	1		

- Molecule 9 is 2-AMINO-ACRYLIC ACID (three-letter code: DHA) (formula:  $C_3H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	1
			6	3	1	2		

- Molecule 10 is water.

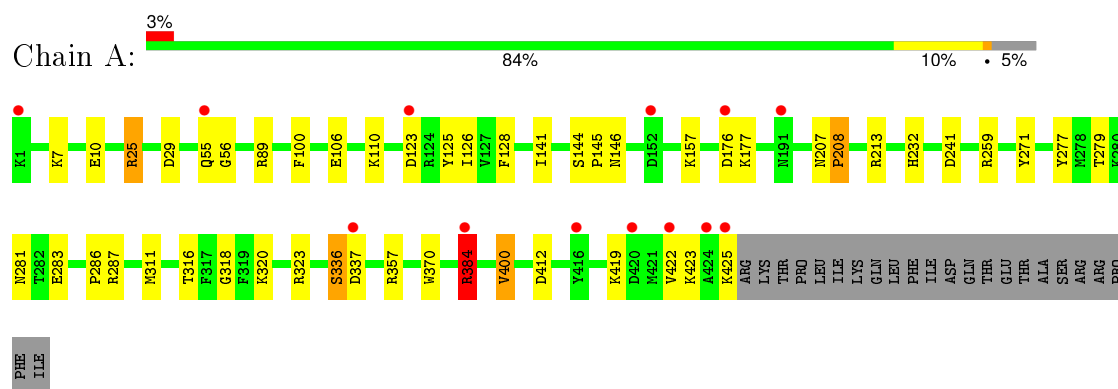
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	394	Total 394	O 394	0	0
10	B	436	Total 436	O 436	0	0



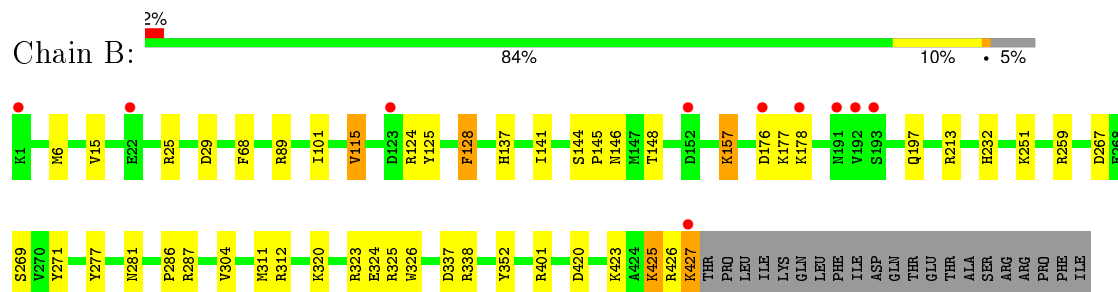
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: ALLIIN LYASE



#### • Molecule 1: ALLIIN LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.45Å 101.07Å 155.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.53 11.97 – 1.53	Depositor EDS
% Data completeness (in resolution range)	98.7 (12.00-1.53) 98.9 (11.97-1.53)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.53Å)	Xtriage
Refinement program	REFMAC 4.0.6	Depositor
R, $R_{free}$	0.193 , 0.221 0.184 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 160734 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: BMA, NAG, PLP, CL, DHA, FUC, EPE, SO4

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	0.55	0/3601	1.21	22/4874 (0.5%)
1	B	0.58	0/3579	1.22	20/4846 (0.4%)
All	All	0.57	0/7180	1.22	42/9720 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	25	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	89	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	B	128	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	A	25	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	89	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	323	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	312	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	128	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	B	128	PHE	CB-CG-CD1	7.07	125.75	120.80
1	A	128	PHE	CB-CG-CD1	6.99	125.69	120.80
1	A	287	ARG	NE-CZ-NH2	-6.98	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	287	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	357	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	208	PRO	N-CA-C	6.54	129.09	112.10
1	B	312	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	B	213	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	A	123[A]	ASP	N-CA-CB	-6.37	99.14	110.60
1	A	123[B]	ASP	N-CA-CB	-6.37	99.14	110.60
1	A	259	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	401	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	323	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	259	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	337	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	352	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	B	89	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	100	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	100	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	B	338	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	357	ARG	NH1-CZ-NH2	5.58	125.53	119.40
1	A	357	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	68	PHE	CB-CG-CD1	5.54	124.68	120.80
1	A	412	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	400	VAL	CG1-CB-CG2	5.51	119.72	110.90
1	A	29	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	213	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	259	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	241	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	29	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	384	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	124	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASN	Sidechain
1	B	146	ASN	Sidechain

## 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	3453	0	3329	28	0
1	B	3461	0	3351	28	0
2	A	49	0	43	0	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	B	24	0	22	4	0
5	A	30	0	0	0	0
5	B	25	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	15	0	7	0	0
7	B	15	0	7	1	0
8	A	30	0	36	3	0
9	B	6	0	3	4	0
10	A	394	0	0	1	0
10	B	436	0	0	3	0
All	All	7996	0	6848	56	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 4.

All (56) 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)
4:B:501:FUC:H2	4:B:501:FUC:H63	1.47	0.97
1:B:425:LYS:HD2	1:B:426:ARG:H	1.30	0.94
1:A:106:GLU:HG3	1:A:126:ILE:HD12	1.74	0.69
1:B:251:LYS:CE	9:B:850[A]:DHA:HB1	2.22	0.69
1:B:251:LYS:HE2	9:B:850[A]:DHA:HB1	1.74	0.68
1:A:286:PRO:HG2	1:B:286:PRO:HG2	1.76	0.68
1:A:177:LYS:HA	1:B:177:LYS:HG2	1.78	0.64
4:B:501:FUC:C2	4:B:501:FUC:H63	2.23	0.64
1:A:177:LYS:HB2	1:B:177:LYS:HE2	1.81	0.63
1:B:141:ILE:HD12	1:B:277[B]:TYR:CE1	2.35	0.60
1:B:144[B]:SER:HB3	1:B:145:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HD2	1:B:426:ARG:N	2.10	0.58
1:B:115[A]:VAL:HG13	1:B:304:VAL:HG11	1.84	0.58
1:B:420:ASP:HA	1:B:423:LYS:HE2	1.86	0.57
1:A:177:LYS:HB2	1:B:177:LYS:CE	2.35	0.57
1:B:267[A]:ASP:OD2	1:B:269:SER:OG	2.15	0.56
1:A:311:MET:CE	1:A:316:THR:HG22	2.37	0.55
1:A:336:SER:HB3	1:A:422:VAL:HG13	1.88	0.55
1:A:279:THR:CG2	8:A:851[B]:EPE:H72	2.37	0.54
1:A:311:MET:HE2	1:A:311:MET:HA	1.90	0.54
1:A:141:ILE:HD12	1:A:277[B]:TYR:CE1	2.42	0.54
1:A:311:MET:CE	1:A:320:LYS:HD2	2.38	0.53
1:B:144[A]:SER:HB2	1:B:145:PRO:HD2	1.91	0.51
1:A:7:LYS:HD3	1:A:10:GLU:OE1	2.10	0.51
1:B:251:LYS:HE2	9:B:850[A]:DHA:CB	2.42	0.50
4:B:501:FUC:C2	4:B:501:FUC:C6	2.84	0.49
1:B:320:LYS:O	1:B:324:GLU:HG3	2.13	0.48
1:A:144[A]:SER:HB3	1:A:145:PRO:HD2	1.96	0.48
1:B:326:TRP:HB2	10:B:1112:HOH:O	2.13	0.48
1:B:311:MET:SD	1:B:320:LYS:HD3	2.53	0.48
1:A:144[B]:SER:HB2	1:A:145:PRO:HD2	1.96	0.47
1:B:125:TYR:HB3	1:B:271:TYR:CD1	2.49	0.47
1:A:110:LYS:HE3	1:A:126:ILE:HD11	1.97	0.47
1:A:283:GLU:OE2	8:A:851[B]:EPE:N4	2.47	0.47
1:A:311:MET:HE3	1:A:320:LYS:HD2	1.97	0.46
1:A:207:ASN:HA	1:A:208:PRO:HA	1.69	0.46
1:A:232:HIS:ND1	1:A:318:GLY:HA3	2.31	0.46
1:A:125:TYR:HB3	1:A:271:TYR:CD1	2.52	0.45
7:B:600:PLP:O3	9:B:850[A]:DHA:N	2.50	0.44
1:B:427:LYS:HG2	10:B:1232:HOH:O	2.18	0.44
1:A:176:ASP:HB3	1:B:178:LYS:CE	2.48	0.43
1:B:148:THR:HG23	1:B:178:LYS:HZ1	1.82	0.43
1:A:110:LYS:HE3	1:A:126:ILE:CD1	2.48	0.43
1:A:7:LYS:HD2	10:A:1160:HOH:O	2.18	0.43
1:B:101:ILE:HG23	1:B:128:PHE:CE2	2.54	0.43
1:A:419:LYS:O	1:A:423:LYS:HG2	2.18	0.43
1:B:148:THR:HG23	1:B:178:LYS:NZ	2.35	0.42
4:B:501:FUC:H2	4:B:501:FUC:C6	2.28	0.42
1:B:137:HIS:CE1	1:B:141:ILE:HD11	2.54	0.42
1:B:157:LYS:HE3	1:B:197:GLN:HB3	2.02	0.42
1:A:56:GLY:O	1:A:384:ARG:NH2	2.53	0.42
1:A:177:LYS:HG3	1:B:176:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:MET:HE1	1:A:316:THR:HG22	2.01	0.41
8:A:852[B]:EPE:H61	8:A:852[B]:EPE:H102	1.65	0.41
1:A:370:TRP:CH2	1:A:425:LYS:HG2	2.55	0.41
1:B:15[A]:VAL:HG23	10:B:1139:HOH:O	2.21	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	434/448 (97%)	417 (96%)	17 (4%)	0	100	100
1	B	431/448 (96%)	419 (97%)	12 (3%)	0	100	100
All	All	865/896 (96%)	836 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	383/395 (97%)	375 (98%)	8 (2%)	61	27
1	B	380/395 (96%)	371 (98%)	9 (2%)	57	22
All	All	763/790 (97%)	746 (98%)	17 (2%)	61	26

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	55	GLN
1	A	157	LYS
1	A	281	ASN
1	A	336	SER
1	A	337	ASP
1	A	384	ARG
1	A	400	VAL
1	B	6	MET
1	B	25	ARG
1	B	115[A]	VAL
1	B	115[B]	VAL
1	B	157	LYS
1	B	232	HIS
1	B	281	ASN
1	B	425	LYS
1	B	427	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	A	386	ASN
1	B	408	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](#)

10 carbohydrates 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	NAG	A	500	1,2	14,14,15	1.03	1 (7%)	15,19,21	1.10	1 (6%)
2	FUC	A	501	2	10,10,11	1.09	1 (10%)	14,14,16	0.98	0
2	NAG	A	502	2	14,14,15	0.99	1 (7%)	15,19,21	1.49	3 (20%)
2	BMA	A	503	2	11,11,12	0.99	1 (9%)	14,15,17	0.57	0
3	NAG	A	504	1,3	14,14,15	1.03	1 (7%)	15,19,21	1.08	1 (6%)
3	NAG	A	505	3	14,14,15	0.79	0	15,19,21	0.92	0
4	NAG	B	500	1,4	14,14,15	1.00	1 (7%)	15,19,21	1.77	4 (26%)
4	FUC	B	501	4	10,10,11	1.17	1 (10%)	14,14,16	1.24	1 (7%)
3	NAG	B	502	1,3	14,14,15	0.98	0	15,19,21	1.25	2 (13%)
3	NAG	B	503	3	14,14,15	0.96	0	15,19,21	1.59	2 (13%)

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	NAG	A	500	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	501	2	-	0/0/17/20	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	BMA	A	503	2	-	0/2/19/22	0/1/1/1
3	NAG	A	504	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	505	3	-	0/6/23/26	0/1/1/1
4	NAG	B	500	1,4	-	0/6/23/26	0/1/1/1
4	FUC	B	501	4	-	0/0/17/20	0/1/1/1
3	NAG	B	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	503	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	BMA	C2-C3	2.06	1.55	1.52
4	B	501	FUC	C2-C3	2.22	1.55	1.52
2	A	502	NAG	C1-C2	2.24	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAG	C1-C2	2.24	1.55	1.52
2	A	501	FUC	C2-C3	2.25	1.55	1.52
3	A	504	NAG	C1-C2	2.27	1.55	1.52
4	B	500	NAG	C1-C2	2.31	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	NAG	C4-C3-C2	-3.69	105.50	111.23
4	B	500	NAG	C2-N2-C7	-3.52	118.52	123.04
3	B	502	NAG	C4-C3-C2	-3.29	106.12	111.23
2	A	500	NAG	O7-C7-C8	-3.21	116.18	122.06
3	A	504	NAG	O7-C7-C8	-3.11	116.36	122.06
2	A	502	NAG	C1-O5-C5	-2.53	109.04	112.25
2	A	502	NAG	C4-C3-C2	-2.22	107.78	111.23
3	B	503	NAG	O7-C7-C8	-2.21	118.00	122.06
4	B	500	NAG	O7-C7-C8	-2.15	118.12	122.06
3	B	502	NAG	O7-C7-C8	-2.01	118.37	122.06
4	B	500	NAG	C1-O5-C5	2.75	115.73	112.25
2	A	502	NAG	C3-C2-N2	3.21	118.25	110.56
4	B	501	FUC	O5-C5-C6	3.59	112.07	106.13
3	B	503	NAG	C2-N2-C7	4.63	128.98	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	FUC	4	0

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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
7	PLP	A	600	1	15,15,16	1.26	0	21,22,23	1.77	4 (19%)
8	EPE	A	851[B]	-	14,15,15	2.13	1 (7%)	18,20,20	2.71	7 (38%)
8	EPE	A	852[B]	-	14,15,15	2.09	1 (7%)	18,20,20	2.33	5 (27%)
5	SO4	A	904	-	4,4,4	0.89	0	6,6,6	0.10	0
5	SO4	A	905	-	4,4,4	0.93	0	6,6,6	0.15	0
5	SO4	A	906	-	4,4,4	0.91	0	6,6,6	0.16	0
5	SO4	A	907	-	4,4,4	0.87	0	6,6,6	0.12	0
5	SO4	A	910	-	4,4,4	0.94	0	6,6,6	0.33	0
5	SO4	A	911	-	4,4,4	0.91	0	6,6,6	0.17	0
7	PLP	B	600	1,9	15,15,16	1.34	3 (20%)	21,22,23	1.91	6 (28%)
9	DHA	B	850[A]	7	3,5,5	0.57	0	1,6,6	2.41	1 (100%)
5	SO4	B	901	-	4,4,4	1.06	0	6,6,6	0.58	0
5	SO4	B	902	-	4,4,4	0.97	0	6,6,6	0.35	0
5	SO4	B	903	-	4,4,4	0.92	0	6,6,6	0.28	0
5	SO4	B	908	-	4,4,4	0.83	0	6,6,6	0.22	0
5	SO4	B	909	-	4,4,4	0.91	0	6,6,6	0.25	0

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
7	PLP	A	600	1	-	0/6/6/8	0/1/1/1
8	EPE	A	851[B]	-	-	0/9/19/19	0/1/1/1
8	EPE	A	852[B]	-	-	0/9/19/19	0/1/1/1
5	SO4	A	904	-	-	0/0/0/0	0/0/0/0
5	SO4	A	905	-	-	0/0/0/0	0/0/0/0
5	SO4	A	906	-	-	0/0/0/0	0/0/0/0
5	SO4	A	907	-	-	0/0/0/0	0/0/0/0
5	SO4	A	910	-	-	0/0/0/0	0/0/0/0
5	SO4	A	911	-	-	0/0/0/0	0/0/0/0
7	PLP	B	600	1,9	-	0/6/6/8	0/1/1/1
9	DHA	B	850[A]	7	-	0/0/4/4	0/0/0/0
5	SO4	B	901	-	-	0/0/0/0	0/0/0/0
5	SO4	B	902	-	-	0/0/0/0	0/0/0/0
5	SO4	B	903	-	-	0/0/0/0	0/0/0/0
5	SO4	B	908	-	-	0/0/0/0	0/0/0/0
5	SO4	B	909	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	PLP	P-O1P	2.14	1.58	1.51
7	B	600	PLP	C4A-C4	2.35	1.56	1.51
7	B	600	PLP	C2A-C2	2.42	1.55	1.50
8	A	852[B]	EPE	O3S-S	7.25	1.65	1.46
8	A	851[B]	EPE	O3S-S	7.26	1.65	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	851[B]	EPE	O1S-S-C10	-5.48	102.23	106.91
8	A	852[B]	EPE	O1S-S-C10	-4.04	103.45	106.91
7	A	600	PLP	C3-C4-C5	-3.69	114.75	118.78
8	A	852[B]	EPE	O3S-S-O1S	-3.59	103.25	111.61
7	B	600	PLP	C5A-C5-C6	-3.08	113.46	119.28
8	A	851[B]	EPE	C6-C5-N4	-2.68	105.84	110.63
7	B	600	PLP	O4P-C5A-C5	-2.56	104.76	108.99
8	A	851[B]	EPE	O3S-S-O1S	-2.50	105.78	111.61
9	B	850[A]	DHA	CB-CA-N	-2.41	120.92	126.27
7	B	600	PLP	O4P-P-O1P	-2.29	101.31	107.14
7	B	600	PLP	C4A-C4-C3	-2.29	116.22	120.36
7	A	600	PLP	C5A-C5-C6	-2.08	115.34	119.28
8	A	852[B]	EPE	O2S-S-O1S	2.18	121.42	113.48
8	A	851[B]	EPE	C6-N1-C2	2.32	113.92	108.90
8	A	852[B]	EPE	C2-C3-N4	2.37	114.87	110.63
8	A	851[B]	EPE	C3-C2-N1	2.52	115.15	110.63
8	A	851[B]	EPE	C7-N4-C3	2.73	118.26	111.27
7	A	600	PLP	C5A-C5-C4	3.14	125.81	121.65
7	B	600	PLP	C4A-C4-C5	3.99	125.04	120.88
7	B	600	PLP	C5A-C5-C4	4.13	127.12	121.65
7	A	600	PLP	C4A-C4-C5	4.83	125.91	120.88
8	A	852[B]	EPE	O2S-S-C10	6.70	112.62	106.91
8	A	851[B]	EPE	O2S-S-C10	7.48	113.28	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	851[B]	EPE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	852[B]	EPE	1	0
7	B	600	PLP	1	0
9	B	850[A]	DHA	4	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/448 (94%)	-0.10	13 (3%) 52 56	15, 24, 38, 53	0
1	B	427/448 (95%)	-0.33	10 (2%) 64 66	15, 20, 37, 55	0
All	All	852/896 (95%)	-0.21	23 (2%) 58 61	15, 23, 38, 55	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LYS	4.9
1	B	427	LYS	4.3
1	A	55	GLN	4.2
1	B	193	SER	4.1
1	B	191	ASN	4.0
1	A	337	ASP	3.5
1	A	416	TYR	3.3
1	B	178	LYS	3.1
1	A	422	VAL	2.8
1	B	1	LYS	2.7
1	A	420	ASP	2.6
1	A	424	ALA	2.5
1	A	425	LYS	2.5
1	A	123[A]	ASP	2.5
1	B	192	VAL	2.3
1	A	152	ASP	2.3
1	B	123	ASP	2.2
1	A	384	ARG	2.1
1	B	176	ASP	2.1
1	B	22	GLU	2.1
1	A	176	ASP	2.1
1	B	152	ASP	2.1
1	A	191	ASN	2.1

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

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

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	B	500	14/15	0.53	0.30	2.75	49,56,60,61	0
3	NAG	A	504	14/15	0.84	0.17	1.47	31,34,42,49	0
3	NAG	B	502	14/15	0.89	0.10	0.67	25,28,40,43	0
4	FUC	B	501	10/11	0.52	0.30	-	41,48,50,50	0
2	FUC	A	501	10/11	0.87	0.16	-	39,41,44,48	0
2	NAG	A	502	14/15	0.80	0.19	-	38,44,50,56	0
2	NAG	A	500	14/15	0.89	0.12	-	28,31,38,39	0
2	BMA	A	503	11/12	0.69	0.40	-	55,57,59,61	0
3	NAG	B	503	14/15	0.79	0.36	-	45,55,59,62	0
3	NAG	A	505	14/15	0.79	0.38	-	56,62,66,70	0

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	DHA	B	850[A]	6/6	0.90	0.18	8.41	20,22,25,26	6
5	SO4	B	903	5/5	0.94	0.18	4.21	35,35,36,36	0
8	EPE	A	851[B]	15/15	0.89	0.15	3.69	24,26,30,31	15
5	SO4	A	907	5/5	0.97	0.16	3.63	50,50,50,50	0
8	EPE	A	852[B]	15/15	0.83	0.17	2.96	22,24,28,30	15
5	SO4	A	910	5/5	0.89	0.14	2.84	26,27,28,28	5
5	SO4	B	908	5/5	0.92	0.20	1.46	36,36,36,37	5
5	SO4	B	901	5/5	0.98	0.14	1.30	25,26,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PLP	A	600	15/16	0.97	0.07	0.46	19,23,29,37	0
5	SO4	A	906	5/5	0.85	0.16	0.24	31,32,32,32	5
7	PLP	B	600	15/16	0.98	0.05	-0.88	16,18,25,28	0
6	CL	A	1001	1/1	0.99	0.03	-2.90	18,18,18,18	0
6	CL	B	1002	1/1	0.99	0.03	-3.40	19,19,19,19	0
5	SO4	B	902	5/5	0.95	0.11	-	40,40,41,41	0
5	SO4	A	911	5/5	0.95	0.20	-	58,58,58,58	0
5	SO4	B	909	5/5	0.90	0.17	-	29,30,31,31	5
5	SO4	A	905	5/5	0.96	0.20	-	48,48,48,48	0
5	SO4	A	904	5/5	0.96	0.17	-	60,60,60,60	0

## 6.5 Other polymers

There are no such residues in this entry.