



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:22 am GMT

PDB ID : 3KU9  
Title : X-ray structure of the mutant lys300met of polyamine oxidase from zea mays  
in complex with spermine  
Authors : Fiorillo, A.; Ilari, A.; Tavladoraki, P.  
Deposited on : 2009-11-27  
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

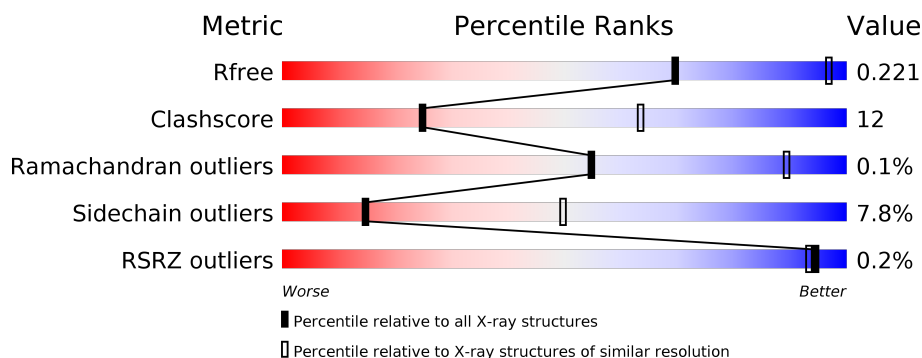
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	478	
1	B	478	

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	SPM	A	700	-	-	-	X
4	SPM	B	700	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7758 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 Polyamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	21	7	0
			3786	2419	633	718	16			
1	B	465	Total	C	N	O	S	28	1	0
			3737	2388	629	705	15			

There are 14 discrepancies between the modelled and reference sequences:

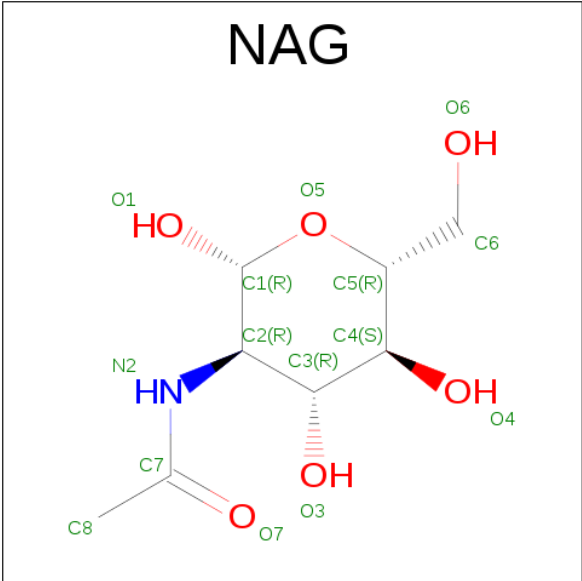
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	LYS	ENGINEERED	UNP O64411
A	473	HIS	-	EXPRESSION TAG	UNP O64411
A	474	HIS	-	EXPRESSION TAG	UNP O64411
A	475	HIS	-	EXPRESSION TAG	UNP O64411
A	476	HIS	-	EXPRESSION TAG	UNP O64411
A	477	HIS	-	EXPRESSION TAG	UNP O64411
A	478	HIS	-	EXPRESSION TAG	UNP O64411
B	300	MET	LYS	ENGINEERED	UNP O64411
B	473	HIS	-	EXPRESSION TAG	UNP O64411
B	474	HIS	-	EXPRESSION TAG	UNP O64411
B	475	HIS	-	EXPRESSION TAG	UNP O64411
B	476	HIS	-	EXPRESSION TAG	UNP O64411
B	477	HIS	-	EXPRESSION TAG	UNP O64411
B	478	HIS	-	EXPRESSION TAG	UNP O64411

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



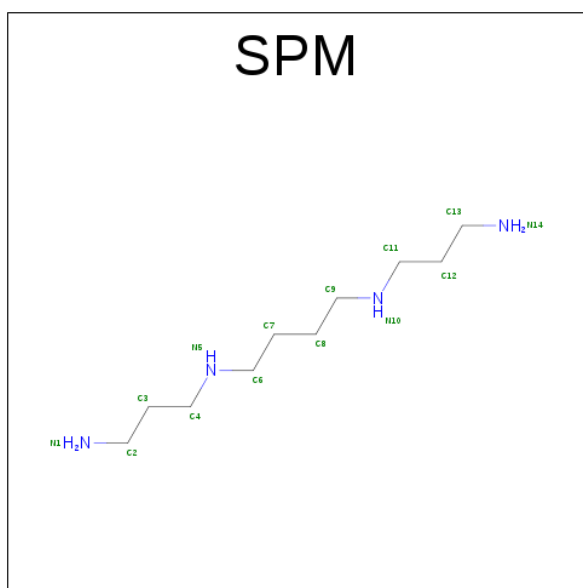
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	10	4		
4	B	1	Total	C	N	0	0
			14	10	4		

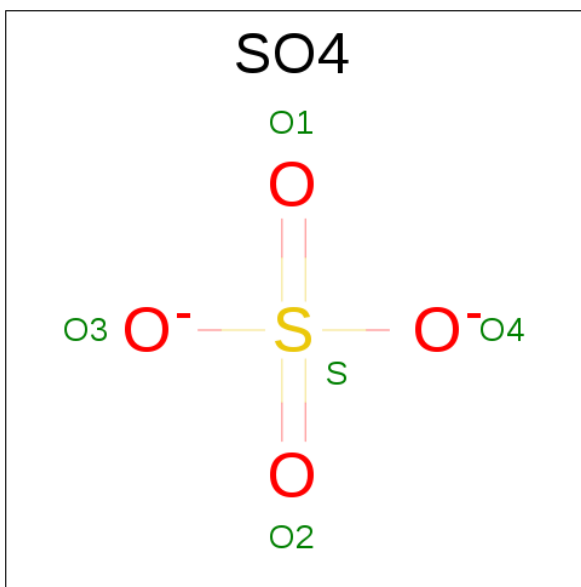
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- 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		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

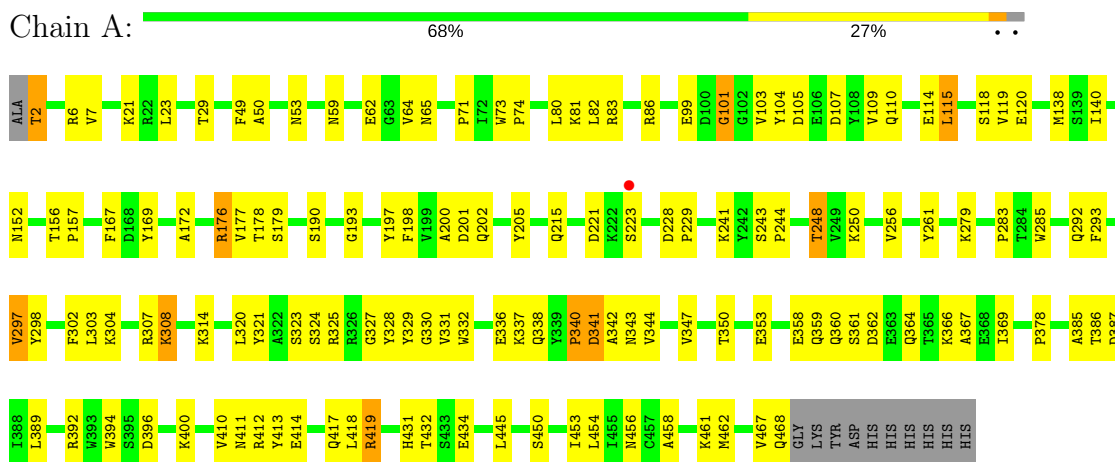
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	0
			24	24		
8	B	29	Total	O	0	0
			29	29		

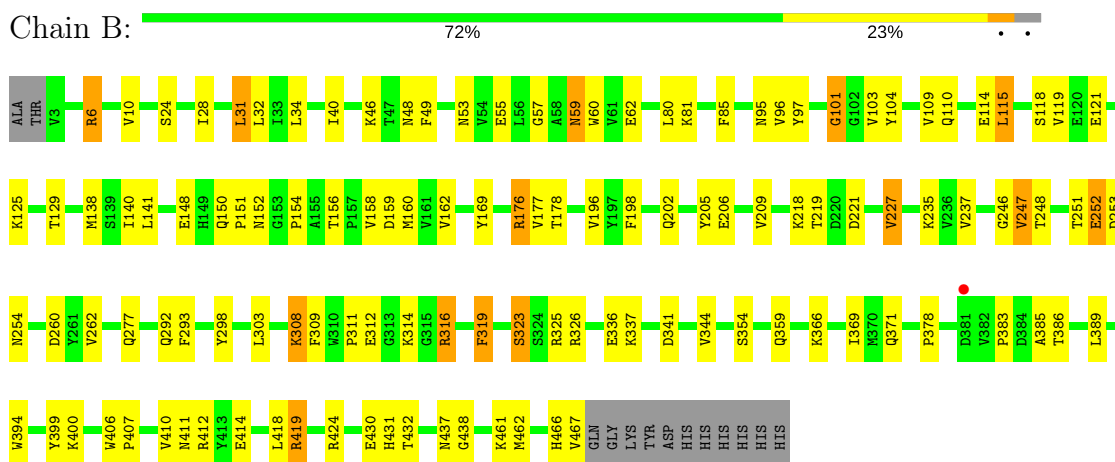
### 3 Residue-property plots

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

#### • Molecule 1: Polyamine oxidase



#### • Molecule 1: Polyamine oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.96Å 138.96Å 189.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 46.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.20) 99.9 (46.78-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0043	Depositor
R, $R_{free}$	0.183 , 0.219 0.188 , 0.221	Depositor DCC
$R_{free}$ test set	1770 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SPM, NAG, FAD, CL

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	0.53	0/3900	0.60	0/5286
1	B	0.54	0/3833	0.62	1/5196 (0.0%)
All	All	0.54	0/7733	0.61	1/10482 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ASP	CB-CG-OD2	5.15	122.93	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLY	Peptide
1	B	60	TRP	Peptide

## 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	3786	0	3686	102	0
1	B	3737	0	3636	96	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	14	0	13	0	0
4	A	14	0	26	2	0
4	B	14	0	26	7	0
5	B	28	0	25	0	0
6	B	1	0	0	0	0
7	B	5	0	0	0	0
8	A	24	0	0	0	0
8	B	29	0	0	6	0
All	All	7758	0	7474	183	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 (183) 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:B:6:ARG:HH11	1:B:6:ARG:HG2	1.08	1.08
1:A:336:GLU:O	1:A:340:PRO:HB3	1.57	1.05
1:B:251:THR:HG22	1:B:253:ASP:H	1.28	0.96
1:A:53:ASN:H	1:A:202:GLN:HE22	1.13	0.94
1:A:2:THR:N	1:A:29:THR:HG1	1.70	0.89
1:B:6:ARG:NH1	1:B:6:ARG:HG2	1.86	0.88
1:A:320:LEU:HA	1:A:330:GLY:O	1.74	0.86
1:A:321:TYR:HB3	1:A:330:GLY:HA2	1.57	0.85
1:A:340:PRO:HG2	1:A:340:PRO:O	1.78	0.83
1:A:103:VAL:HG12	1:A:104:TYR:O	1.81	0.80
1:B:251:THR:HG22	1:B:252:GLU:N	1.97	0.79
1:B:251:THR:CG2	1:B:252:GLU:N	2.48	0.77
1:A:53:ASN:H	1:A:202:GLN:NE2	1.84	0.76
1:A:138:MET:HB3	1:B:292:GLN:NE2	2.00	0.76
1:B:308:LYS:NZ	1:B:308:LYS:HB3	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HB3	1:B:292:GLN:HE22	1.52	0.73
1:B:251:THR:HG22	1:B:253:ASP:N	2.04	0.71
1:B:62:GLU:OE2	4:B:700:SPM:H32	1.90	0.71
1:B:438:GLY:O	4:B:700:SPM:N1	2.24	0.71
1:B:103:VAL:HG12	1:B:104:TYR:O	1.91	0.70
1:A:53:ASN:N	1:A:202:GLN:HE22	1.88	0.69
1:A:62:GLU:OE2	4:A:700:SPM:H32	1.93	0.69
1:A:340:PRO:O	1:A:340:PRO:CG	2.43	0.67
1:B:235:LYS:NZ	1:B:253:ASP:OD1	2.27	0.67
1:A:329:TYR:CE1	1:A:369:ILE:HG12	2.30	0.66
1:A:358:GLU:HG2	1:A:392:ARG:HG2	1.78	0.64
1:B:312:GLU:HB3	1:B:336:GLU:OE2	1.98	0.64
1:A:417:GLN:HG2	1:A:467:VAL:HG11	1.79	0.64
1:B:246:GLY:HA2	1:B:424:ARG:CD	2.28	0.63
1:B:140:ILE:HD12	1:B:178:THR:HB	1.78	0.63
1:B:251:THR:CG2	1:B:252:GLU:H	2.11	0.63
1:B:57:GLY:N	8:B:509:HOH:O	2.29	0.62
1:A:329:TYR:CE1	1:A:369:ILE:CG1	2.83	0.62
1:A:99:GLU:HG3	1:A:323:SER:HA	1.82	0.62
1:B:57:GLY:CA	8:B:509:HOH:O	2.48	0.61
1:A:331:VAL:O	1:A:347:VAL:HG23	2.01	0.61
1:A:308:LYS:HB3	1:A:308:LYS:NZ	2.16	0.60
1:A:241:LYS:HB2	1:A:248:THR:HG22	1.83	0.59
1:A:138:MET:CB	1:B:292:GLN:HE22	2.16	0.59
1:B:298:TYR:CZ	4:B:700:SPM:H61	2.38	0.58
1:A:419:ARG:HG2	1:A:419:ARG:HH11	1.67	0.58
1:B:158:VAL:HG23	8:B:482:HOH:O	2.03	0.58
1:A:337:LYS:O	1:A:340:PRO:HD3	2.04	0.58
1:A:419:ARG:HB2	1:A:432:THR:HB	1.86	0.57
1:A:302:PHE:HB2	1:A:389:LEU:HB3	1.86	0.57
1:B:253:ASP:OD2	1:B:253:ASP:C	2.42	0.57
1:A:169:TYR:CE1	1:A:331:VAL:HG11	2.40	0.56
1:B:96:VAL:O	1:B:96:VAL:HG12	2.07	0.56
1:B:298:TYR:OH	4:B:700:SPM:C6	2.53	0.55
1:B:308:LYS:HB3	1:B:308:LYS:HZ3	1.71	0.55
1:A:419:ARG:HE	1:A:453:ILE:HD11	1.71	0.55
1:A:419:ARG:NH1	1:A:434[B]:GLU:OE2	2.38	0.54
1:B:371:GLN:HG3	8:B:503:HOH:O	2.07	0.54
1:A:419:ARG:HG2	1:A:419:ARG:NH1	2.21	0.54
1:B:55:GLU:HB2	1:B:59:ASN:OD1	2.07	0.54
1:B:303:LEU:O	1:B:344:VAL:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PHE:CE1	1:B:389:LEU:HB3	2.43	0.54
1:A:411:ASN:ND2	1:A:413:TYR:H	2.05	0.54
1:A:49:PHE:O	1:A:50:ALA:HB3	2.07	0.54
1:B:158:VAL:O	1:B:162:VAL:HG23	2.08	0.53
1:A:176:ARG:HD2	1:B:177:VAL:HG11	1.89	0.53
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.89	0.53
1:A:303:LEU:O	1:A:344:VAL:HG13	2.09	0.53
1:B:246:GLY:HA2	1:B:424:ARG:HD3	1.91	0.52
1:A:2:THR:N	1:A:29:THR:OG1	2.40	0.52
1:B:53:ASN:H	1:B:202:GLN:HE22	1.58	0.52
1:B:154:PRO:HB3	1:B:159:ASP:HB3	1.92	0.52
1:A:177:VAL:HG11	1:B:176:ARG:HD2	1.92	0.51
1:B:101:GLY:HA3	1:B:378:PRO:HG3	1.91	0.51
1:B:430:GLU:O	1:B:437:ASN:HA	2.10	0.51
1:B:319:PHE:N	1:B:319:PHE:CD2	2.78	0.51
1:A:115:LEU:O	1:A:119:VAL:HG23	2.10	0.51
1:A:83:ARG:HB3	1:A:200:ALA:O	2.10	0.51
1:B:251:THR:HG23	1:B:252:GLU:H	1.74	0.51
1:A:329:TYR:HE1	1:A:369:ILE:HD11	1.75	0.51
1:B:298:TYR:CE1	4:B:700:SPM:H61	2.46	0.51
1:A:297:VAL:HG11	1:A:394:TRP:HB2	1.91	0.51
1:A:21:LYS:HE2	1:A:215:GLN:HG3	1.93	0.50
1:A:321:TYR:N	1:A:330:GLY:O	2.44	0.50
1:B:253:ASP:O	1:B:253:ASP:OD2	2.30	0.50
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.94	0.50
1:B:254:ASN:O	1:B:254:ASN:OD1	2.30	0.49
1:A:329:TYR:CD1	1:A:369:ILE:HG12	2.47	0.49
1:A:303:LEU:HD11	1:A:369:ILE:HG21	1.94	0.49
1:A:138:MET:CB	1:B:292:GLN:NE2	2.72	0.49
1:B:323:SER:HB3	8:B:493:HOH:O	2.12	0.49
1:A:394:TRP:HE1	1:B:152:ASN:ND2	2.09	0.49
1:A:325:ARG:HD2	1:B:325:ARG:NH1	2.27	0.49
1:B:40:ILE:HD12	1:B:209:VAL:HG12	1.94	0.49
1:A:321:TYR:HB3	1:A:329:TYR:O	2.13	0.49
1:B:6:ARG:NH1	1:B:260:ASP:OD2	2.46	0.49
1:A:342:ALA:O	1:A:343:ASN:HB2	2.11	0.48
1:A:327:GLY:O	1:A:353:GLU:HG3	2.13	0.48
1:B:10:VAL:HG22	1:B:237:VAL:HG21	1.94	0.48
1:A:411:ASN:HD21	1:A:413:TYR:HB3	1.78	0.48
1:B:410:VAL:HG13	1:B:414:GLU:HG3	1.95	0.48
1:A:359:GLN:HE22	1:B:156:THR:HG22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HA	1:A:201:ASP:OD2	2.14	0.48
1:B:49:PHE:HD1	1:B:389:LEU:HD22	1.79	0.48
1:B:104:TYR:CE1	1:B:158:VAL:HG22	2.49	0.47
1:A:328:TYR:CD1	1:A:328:TYR:O	2.67	0.47
1:B:85:PHE:CD2	1:B:337:LYS:HD2	2.49	0.47
1:B:316:ARG:HD2	1:B:316:ARG:HA	1.73	0.47
1:B:32:LEU:HD21	1:B:34:LEU:HD21	1.95	0.47
1:B:399:TYR:HE2	2:B:500:FAD:H3B	1.79	0.47
1:A:359:GLN:NE2	1:B:156:THR:HG22	2.29	0.47
1:A:292:GLN:NE2	1:B:138:MET:HB3	2.30	0.47
1:B:148:GLU:O	1:B:150:GLN:HG2	2.14	0.47
1:A:71:PRO:HG3	1:A:445:LEU:HD21	1.97	0.47
1:B:46:LYS:HG2	1:B:206:GLU:OE2	2.14	0.46
1:A:80:LEU:O	1:A:81:LYS:C	2.54	0.46
1:A:400:LYS:HB3	1:B:151:PRO:HG3	1.95	0.46
1:A:140:ILE:HD12	1:A:178:THR:HB	1.97	0.46
1:A:103:VAL:HG12	1:A:104:TYR:N	2.30	0.46
1:B:206:GLU:HG2	8:B:510:HOH:O	2.15	0.46
1:A:400:LYS:HD2	1:A:400:LYS:HA	1.67	0.46
1:A:396:ASP:C	1:A:396:ASP:OD1	2.54	0.45
1:A:450:SER:HA	1:A:453:ILE:HD12	1.98	0.45
1:A:103:VAL:CG1	1:A:104:TYR:N	2.79	0.45
1:B:303:LEU:HD11	1:B:369:ILE:HG21	1.99	0.45
1:B:110:GLN:HE21	1:B:114:GLU:HG3	1.81	0.45
1:B:309:PHE:CD2	1:B:383:PRO:HD2	2.51	0.45
1:A:120:GLU:HG3	1:A:167:PHE:HZ	1.82	0.45
1:A:250:LYS:HG3	1:A:256:VAL:HG22	1.99	0.44
1:B:115:LEU:O	1:B:119:VAL:HG23	2.17	0.44
1:A:156:THR:HG22	1:B:359:GLN:HE22	1.83	0.44
1:A:304:LYS:O	1:A:385:ALA:HA	2.17	0.43
1:A:456:ASN:HD22	1:A:462:MET:HB2	1.83	0.43
1:B:103:VAL:O	1:B:104:TYR:C	2.55	0.43
1:B:298:TYR:CZ	4:B:700:SPM:C6	3.00	0.43
1:B:308:LYS:HZ2	1:B:308:LYS:HB3	1.78	0.43
1:A:364[B]:GLN:HA	1:A:364[B]:GLN:NE2	2.33	0.43
1:B:366:LYS:HD2	1:B:385:ALA:HB3	2.00	0.43
1:A:101:GLY:HA2	1:A:378:PRO:HG3	2.00	0.43
1:A:320:LEU:CA	1:A:330:GLY:O	2.57	0.43
1:B:252:GLU:C	1:B:254:ASN:H	2.22	0.43
1:A:86:ARG:HG3	1:A:197:TYR:CZ	2.54	0.43
1:A:243:SER:HB2	1:A:244:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TRP:HA	1:B:407:PRO:HD3	1.79	0.43
1:B:169:TYR:O	4:B:700:SPM:H71	2.19	0.43
1:A:298:TYR:OH	4:A:700:SPM:H61	2.19	0.43
1:A:172:ALA:HA	1:A:350:THR:HG21	2.00	0.42
1:A:64:VAL:O	1:A:65:ASN:HB2	2.19	0.42
1:B:28:ILE:O	1:B:31:LEU:HD21	2.19	0.42
1:A:325:ARG:CZ	1:B:325:ARG:HD2	2.48	0.42
1:B:160:MET:HB3	1:B:326:ARG:HG3	2.00	0.42
1:A:303:LEU:O	1:A:344:VAL:HA	2.20	0.42
1:A:332:TRP:HH2	1:A:369:ILE:HG23	1.84	0.42
1:A:340:PRO:HA	1:A:341:ASP:HA	1.74	0.42
1:B:59:ASN:ND2	1:B:198:PHE:CZ	2.88	0.42
1:B:48:ASN:OD1	1:B:48:ASN:C	2.57	0.42
1:B:62:GLU:HA	1:B:196:VAL:HG12	2.02	0.42
1:A:410:VAL:HG13	1:A:414:GLU:HG3	2.02	0.42
1:A:7:VAL:HG22	1:A:261:TYR:HB2	2.02	0.42
1:B:419:ARG:HB2	1:B:432:THR:HB	2.01	0.42
1:B:400:LYS:HA	1:B:400:LYS:HD2	1.81	0.42
1:A:304:LYS:HB3	1:A:387:ASP:H	1.84	0.41
1:A:458:ALA:O	1:A:461:LYS:HE3	2.20	0.41
1:A:23:LEU:HD21	1:A:454:LEU:HD22	2.02	0.41
1:A:297:VAL:CG1	1:A:394:TRP:HB2	2.50	0.41
1:B:103:VAL:O	1:B:103:VAL:HG12	2.18	0.41
1:B:218:LYS:HG3	1:B:227:VAL:HG23	2.03	0.41
1:B:48:ASN:OD1	1:B:48:ASN:O	2.38	0.41
1:B:80:LEU:O	1:B:81:LYS:C	2.58	0.41
1:B:96:VAL:HG21	1:B:109:VAL:HG11	2.02	0.41
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.18	0.41
1:A:338:GLN:OE1	1:A:338:GLN:N	2.47	0.41
1:B:141:LEU:CD2	1:B:176:ARG:HB2	2.50	0.41
1:B:95:ASN:HB3	1:B:319:PHE:HB3	2.01	0.41
1:A:110:GLN:HE21	1:A:114:GLU:HG3	1.85	0.41
1:B:411:ASN:OD1	1:B:414:GLU:HG2	2.21	0.41
1:A:283:PRO:HB2	1:A:285:TRP:CD1	2.57	0.40
1:A:198:PHE:CE2	1:A:338:GLN:HG2	2.56	0.40
1:A:431:HIS:H	1:A:431:HIS:CD2	2.39	0.40
1:A:228:ASP:HA	1:A:229:PRO:HD2	1.86	0.40
1:A:64:VAL:O	1:A:193:GLY:HA3	2.21	0.40
1:B:247:VAL:HG21	1:B:262:VAL:HB	2.03	0.40
1:B:431:HIS:H	1:B:431:HIS:CD2	2.37	0.40
1:A:157:PRO:HG3	1:A:324:SER:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TYR:OH	1:B:311:PRO:HG2	2.22	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	472/478 (99%)	442 (94%)	30 (6%)	0	100	100
1	B	464/478 (97%)	432 (93%)	31 (7%)	1 (0%)	51	86
All	All	936/956 (98%)	874 (93%)	61 (6%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	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	A	408/410 (100%)	376 (92%)	32 (8%)	15	50
1	B	400/410 (98%)	367 (92%)	33 (8%)	13	46
All	All	808/820 (98%)	743 (92%)	65 (8%)	15	49



All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	6	ARG
1	A	59	ASN
1	A	105[A]	ASP
1	A	105[B]	ASP
1	A	107[A]	ASP
1	A	107[B]	ASP
1	A	115	LEU
1	A	118	SER
1	A	176	ARG
1	A	179	SER
1	A	190	SER
1	A	205	TYR
1	A	221[A]	ASP
1	A	221[B]	ASP
1	A	223	SER
1	A	248	THR
1	A	279	LYS
1	A	293	PHE
1	A	297	VAL
1	A	307	ARG
1	A	308	LYS
1	A	314	LYS
1	A	340	PRO
1	A	341	ASP
1	A	360	GLN
1	A	361	SER
1	A	362	ASP
1	A	386	THR
1	A	418	LEU
1	A	419	ARG
1	A	468	GLN
1	B	6	ARG
1	B	24	SER
1	B	31	LEU
1	B	59	ASN
1	B	115	LEU
1	B	118	SER
1	B	121	GLU
1	B	125	LYS
1	B	129	THR
1	B	176	ARG

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Mol	Chain	Res	Type
1	B	205	TYR
1	B	219	THR
1	B	227	VAL
1	B	247	VAL
1	B	248	THR
1	B	252	GLU
1	B	277	GLN
1	B	293	PHE
1	B	308	LYS
1	B	314	LYS
1	B	316	ARG
1	B	319	PHE
1	B	323	SER
1	B	341	ASP
1	B	354	SER
1	B	386	THR
1	B	412	ARG
1	B	418	LEU
1	B	419	ARG
1	B	461	LYS
1	B	462	MET
1	B	466	HIS
1	B	467	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	152	ASN
1	A	202	GLN
1	A	359	GLN
1	A	360	GLN
1	A	411	ASN
1	A	431	HIS
1	A	456	ASN
1	B	48	ASN
1	B	110	GLN
1	B	152	ASN
1	B	202	GLN
1	B	292	GLN
1	B	359	GLN
1	B	360	GLN

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Mol	Chain	Res	Type
1	B	431	HIS
1	B	435	HIS
1	B	437	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 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	$\# Z  > 2$
5	NAG	B	600	1,5	14,14,15	0.57	0	15,19,21	1.57	2 (13%)
5	NAG	B	601	5	14,14,15	0.63	0	15,19,21	1.27	1 (6%)

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
5	NAG	B	600	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	601	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	NAG	C4-C3-C2	3.06	115.50	111.02
5	B	600	NAG	C1-O5-C5	3.95	117.61	112.17
5	B	601	NAG	C4-C3-C2	4.22	117.21	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
2	FAD	A	500	-	51,58,58	1.38	7 (13%)	54,89,89	1.95	10 (18%)
3	NAG	A	600	1	14,14,15	0.60	0	15,19,21	1.50	3 (20%)
4	SPM	A	700	-	13,13,13	0.47	0	12,12,12	1.11	1 (8%)
7	SO4	B	480	-	4,4,4	0.19	0	6,6,6	0.30	0
2	FAD	B	500	-	51,58,58	1.38	6 (11%)	54,89,89	2.05	6 (11%)
4	SPM	B	700	-	13,13,13	1.51	4 (30%)	12,12,12	1.30	3 (25%)

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	FAD	A	500	-	-	0/28/50/50	0/6/6/6
3	NAG	A	600	1	-	0/6/23/26	0/1/1/1
4	SPM	A	700	-	-	0/11/11/11	0/0/0/0
7	SO4	B	480	-	-	0/0/0/0	0/0/0/0
2	FAD	B	500	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SPM	B	700	-	-	0/11/11/11	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	SPM	C11-N10	-2.91	1.37	1.47
4	B	700	SPM	C4-N5	-2.08	1.40	1.47
2	A	500	FAD	C1'-N10	2.13	1.50	1.48
4	B	700	SPM	C3-C4	2.20	1.60	1.51
4	B	700	SPM	C6-N5	2.33	1.54	1.47
2	B	500	FAD	C2A-N1A	2.56	1.38	1.33
2	A	500	FAD	C4-N3	2.62	1.37	1.33
2	A	500	FAD	C5X-N5	2.69	1.39	1.35
2	A	500	FAD	C2A-N1A	2.73	1.39	1.33
2	B	500	FAD	C5X-N5	2.83	1.39	1.35
2	B	500	FAD	C4-N3	3.29	1.39	1.33
2	B	500	FAD	C2A-N3A	3.61	1.38	1.32
2	A	500	FAD	C10-N1	3.88	1.38	1.33
2	A	500	FAD	C2A-N3A	4.18	1.39	1.32
2	B	500	FAD	C10-N1	4.24	1.39	1.33
2	B	500	FAD	C4X-N5	4.49	1.39	1.33
2	A	500	FAD	C4X-N5	4.54	1.39	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	N3A-C2A-N1A	-11.05	119.23	128.86
2	A	500	FAD	N3A-C2A-N1A	-10.11	120.05	128.86
3	A	600	NAG	C3-C4-C5	-3.02	104.89	110.22
2	B	500	FAD	C4X-C4-N3	-2.95	119.28	123.48
2	A	500	FAD	C1B-N9A-C4A	-2.75	121.89	126.64
2	A	500	FAD	C4A-C5A-N7A	-2.64	106.86	109.41
2	A	500	FAD	C4X-C4-N3	-2.54	119.87	123.48
4	B	700	SPM	C4-C3-C2	-2.22	105.39	114.19
2	A	500	FAD	C10-C4X-N5	-2.20	118.06	120.59
3	A	600	NAG	O7-C7-C8	-2.14	118.16	122.06
4	B	700	SPM	C11-C12-C13	-2.07	106.00	114.19
2	B	500	FAD	C10-C4X-N5	-2.06	118.22	120.59
2	A	500	FAD	C5X-C9A-N10	2.04	119.18	117.66
4	A	700	SPM	C6-N5-C4	2.25	121.51	113.33
3	A	600	NAG	C4-C3-C2	2.37	114.49	111.02
2	A	500	FAD	C4X-N5-C5X	2.39	119.28	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C1'-N10-C9A	2.49	120.63	118.35
4	B	700	SPM	C11-N10-C9	2.69	123.11	113.33
2	B	500	FAD	C4-C4X-N5	3.18	122.17	118.68
2	A	500	FAD	C4-C4X-N5	3.22	122.20	118.68
2	B	500	FAD	C4X-N5-C5X	4.22	121.22	116.76
2	A	500	FAD	C4-N3-C2	5.38	119.86	115.16
2	B	500	FAD	C4-N3-C2	6.19	120.58	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	SPM	2	0
2	B	500	FAD	1	0
4	B	700	SPM	7	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 [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, 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	467/478 (97%)	-0.45	1 (0%) 94 93	14, 24, 35, 47	16 (3%)
1	B	465/478 (97%)	-0.48	1 (0%) 94 93	15, 24, 35, 46	17 (3%)
All	All	932/956 (97%)	-0.46	2 (0%) 94 93	14, 24, 35, 47	33 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	SER	2.5
1	B	381	ASP	2.3

### 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](#)

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
5	NAG	B	600	14/15	0.93	0.28	1.47	41,45,49,54	0
5	NAG	B	601	14/15	0.72	0.52	-	59,60,60,60	0

## 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<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	SPM	B	700	14/14	0.93	0.21	6.58	36,37,45,45	0
4	SPM	A	700	14/14	0.91	0.22	3.31	33,40,46,47	0
2	FAD	B	500	53/53	0.98	0.14	-0.21	15,21,23,24	0
2	FAD	A	500	53/53	0.99	0.13	-0.26	15,17,20,21	0
7	SO4	B	480	5/5	0.97	0.12	-1.36	49,50,50,51	0
3	NAG	A	600	14/15	0.90	0.38	-	38,41,44,47	0
6	CL	B	479	1/1	0.84	0.15	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.