



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:51 AM GMT

PDB ID : 3CEM  
Title : Human glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE9423  
Authors : Wendt, K.U.; Dreyer, M.K.; Anderka, O.; Klabunde, T.; Loenze, P.; Defossa, E.; Schmoll, D.  
Deposited on : 2008-02-29  
Resolution : 2.47 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

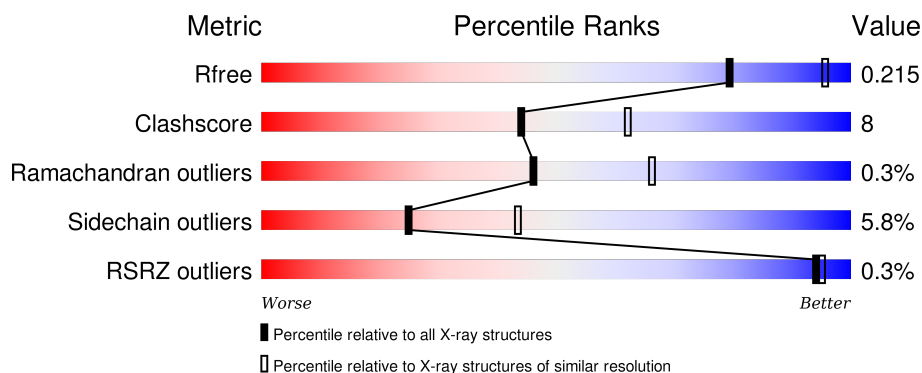
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.47 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	809	 79% 17% . .
1	B	809	 76% 19% . .

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
3	PLP	B	832	-	-	-	X

## 2 Entry composition [i](#)

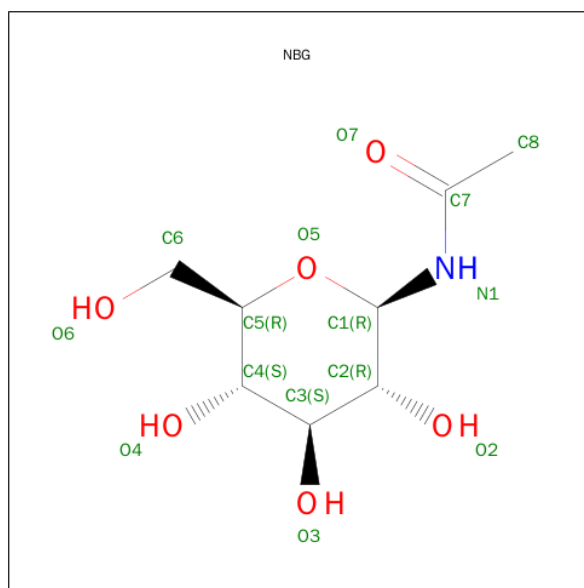
There are 5 unique types of molecules in this entry. The entry contains 13570 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	794	Total	C	N	O	S	0	1	0
			6460	4150	1097	1184	29			
1	B	794	Total	C	N	O	S	0	3	0
			6479	4161	1101	1188	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula:  $C_8H_{15}NO_6$ ).



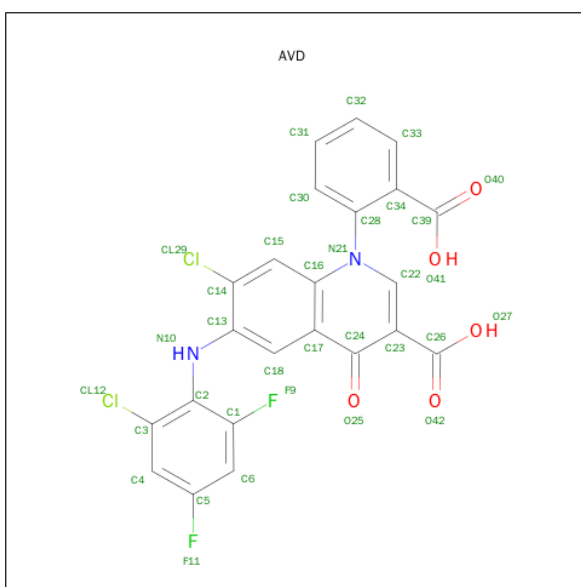
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is 1-(2-CARBOXYPHENYL)-7-CHLORO-6-[(2-CHLORO-4,6-DIFLUOROPHENYL)AMINO]-4-OXO-1,4-DIHYDROQUINOLINE-3-CARBOXYLIC ACID (three-letter code: AVD) (formula: C<sub>23</sub>H<sub>12</sub>Cl<sub>2</sub>F<sub>2</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	
			34	23	2	2	2	5	0

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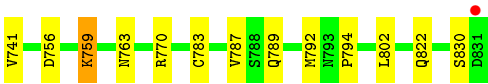
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			34	23	2	2	2	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	274	Total	O	0	0
			274	274		
5	B	227	Total	O	0	0
			227	227		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.38Å 124.38Å 123.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.39 – 2.47 49.36 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-2.47) 99.9 (49.36-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.155 , 0.215 0.156 , 0.215	Depositor DCC
$R_{free}$ test set	5343 reflections (7.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.029 for -h,-k,l 0.095 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 76582 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: AVD, NBG, PLP

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	0.97	2/6605 (0.0%)	0.92	10/8931 (0.1%)
1	B	0.94	3/6625 (0.0%)	0.92	14/8958 (0.2%)
All	All	0.95	5/13230 (0.0%)	0.92	24/17889 (0.1%)

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	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	GLU	CG-CD	5.71	1.60	1.51
1	B	182	TRP	CE3-CZ3	5.24	1.47	1.38
1	A	405	GLU	CG-CD	5.21	1.59	1.51
1	B	142	CYS	CB-SG	5.21	1.91	1.82
1	B	580	CYS	CB-SG	-5.13	1.73	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	490	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	514	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	770	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	171	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	575	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ARG	CA-CB-CG	6.36	127.38	113.40
1	B	184	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	649	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	575	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	192	SER	N-CA-CB	-6.06	101.41	110.50
1	B	714	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	474	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	277	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	661	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	160	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	714	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	514	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	377	HIS	CB-CA-C	-5.28	99.85	110.40
1	B	770	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	309	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	430	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	380	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	B	708	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	249	PRO	Peptide
1	B	250	ASN	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	6460	0	6447	106	0
1	B	6479	0	6458	108	0
2	A	15	0	15	0	0
2	B	15	0	14	0	0
3	A	16	0	7	1	0
3	B	16	0	7	2	0
4	A	34	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	34	0	10	0	0
5	A	274	0	0	17	0
5	B	227	0	0	13	0
All	All	13570	0	12968	208	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 (208) 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:547:GLN:O	1:A:551:THR:HG23	1.57	1.02
1:B:250:ASN:HA	1:B:251:ASP:OD2	1.61	1.00
1:B:96:GLN:HE21	1:B:105:GLN:HE22	0.94	0.94
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.53	0.90
1:B:361:TRP:CH2	1:B:405:GLU:HG2	2.06	0.90
1:A:66:ARG:O	1:A:70:THR:HG23	1.72	0.89
1:A:305:GLN:HG3	5:A:863:HOH:O	1.74	0.85
1:B:274:ASN:ND2	1:B:277:ARG:HH11	1.74	0.85
1:B:96:GLN:HE21	1:B:105:GLN:NE2	1.76	0.83
1:A:184:ARG:HH11	1:A:184:ARG:HG3	1.44	0.81
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.26	0.81
1:A:198:LEU:HD22	1:A:305:GLN:NE2	1.95	0.81
1:B:251:ASP:HB3	1:B:252:PHE:HA	1.62	0.81
1:B:96:GLN:NE2	1:B:105:GLN:HE22	1.79	0.79
1:B:714:ARG:HG2	1:B:714:ARG:HH11	1.48	0.78
1:B:756:ASP:HB2	5:B:1031:HOH:O	1.84	0.78
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.66	0.78
1:A:66:ARG:O	1:A:70:THR:CG2	2.32	0.77
1:A:634:PRO:HA	5:A:905:HOH:O	1.86	0.75
1:B:830:SER:HB3	5:B:1019:HOH:O	1.87	0.74
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.71	0.73
1:A:70:THR:HG21	1:A:238:VAL:H	1.52	0.73
1:A:324:THR:N	1:A:325:VAL:HB	2.04	0.72
1:A:251:ASP:OD1	1:A:251:ASP:N	2.23	0.72
1:B:274:ASN:HD22	1:B:277:ARG:HH11	1.35	0.71
1:A:386:ARG:HH11	1:A:386:ARG:HB2	1.56	0.70
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.91	0.69
1:B:251:ASP:CB	1:B:252:PHE:HA	2.22	0.68
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.74	0.68
3:B:832:PLP:H5A1	3:B:832:PLP:O4A	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.67
1:A:184:ARG:NH2	1:B:250:ASN:HB3	2.10	0.66
1:A:324:THR:HA	1:A:326:PHE:H	1.58	0.66
1:B:436:SER:O	1:B:437:LYS:HB2	1.94	0.66
1:A:615:MET:CE	1:A:761:ILE:HG12	2.25	0.66
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.78	0.65
1:B:527:ASP:OD2	1:B:529:VAL:HB	1.97	0.64
1:A:437:LYS:HD2	5:A:1057:HOH:O	1.97	0.64
1:A:184:ARG:NH1	1:A:184:ARG:HG3	2.12	0.64
1:B:547:GLN:O	1:B:551:THR:HG23	1.97	0.64
1:B:633:ASP:OD2	1:B:635:MET:HB2	1.99	0.63
1:B:181:ASP:OD2	1:B:184:ARG:HG3	1.97	0.63
1:A:181:ASP:OD2	1:A:184:ARG:NH1	2.32	0.62
1:B:250:ASN:CA	1:B:251:ASP:OD2	2.43	0.62
1:B:224:LEU:HD23	1:B:247[A]:ARG:HE	1.65	0.62
1:B:436:SER:HA	5:B:1028:HOH:O	1.99	0.62
1:B:477:ASP:HB2	5:B:901:HOH:O	2.00	0.61
1:B:324:THR:HA	1:B:327:ASP:OD1	2.01	0.61
1:B:584:ILE:HG22	1:B:741:VAL:HG22	1.82	0.61
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.84	0.61
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.83	0.61
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.49	0.60
1:B:591:LYS:NZ	1:B:635:MET:HG3	2.15	0.60
1:B:361:TRP:CZ3	1:B:405:GLU:HG2	2.36	0.60
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.84	0.60
1:B:542:LYS:NZ	1:B:661:ASP:OD2	2.26	0.60
1:B:316:PHE:C	5:B:971:HOH:O	2.40	0.60
1:A:184:ARG:HD2	1:A:185:TYR:CZ	2.38	0.59
1:B:207:GLU:HG3	5:B:859:HOH:O	2.03	0.59
1:A:597:LEU:HA	5:A:984:HOH:O	2.03	0.59
1:B:274:ASN:HD22	1:B:277:ARG:HD2	1.67	0.59
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.84	0.59
1:A:29:LYS:HE2	5:A:1046:HOH:O	2.02	0.58
1:A:592:LYS:HD2	1:A:592:LYS:O	2.04	0.58
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.39	0.58
1:B:226:TYR:OH	1:B:247[A]:ARG:NH2	2.37	0.57
1:B:23:ASN:HD22	1:B:26[A]:GLU:HG2	1.69	0.56
1:B:42:ASP:HB3	5:B:1056:HOH:O	2.04	0.56
1:A:274:ASN:HD22	1:A:277:ARG:HD2	1.71	0.56
1:B:759:LYS:O	1:B:763:ASN:HB2	2.06	0.56
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.71	0.54
1:A:785:ASP:O	1:A:789:GLN:HG3	2.06	0.54
1:B:714:ARG:CG	1:B:714:ARG:HH11	2.17	0.54
1:A:522:HIS:CD2	5:A:860:HOH:O	2.60	0.54
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.91	0.54
1:A:580:CYS:SG	1:A:622:LEU:HD13	2.48	0.53
1:A:339:ASP:OD1	1:A:340:THR:N	2.38	0.53
1:A:184:ARG:HA	1:B:247[B]:ARG:NH1	2.24	0.53
1:A:42:ASP:HB2	5:A:910:HOH:O	2.07	0.53
1:A:398:ARG:O	1:A:402:ILE:HG13	2.09	0.53
5:A:1016:HOH:O	1:B:250:ASN:HB3	2.08	0.53
1:B:579:ASN:HD22	1:B:579:ASN:C	2.12	0.53
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.90	0.52
1:A:247[B]:ARG:NH2	1:B:184:ARG:HG2	2.25	0.52
1:B:48:THR:HG22	1:B:125:ILE:HG13	1.92	0.52
1:A:275:ILE:O	1:A:295:GLN:HG2	2.09	0.52
1:B:554:LYS:HG3	1:B:555:VAL:H	1.75	0.51
1:B:591:LYS:HZ2	1:B:635:MET:HG3	1.74	0.51
1:A:455:VAL:H	1:A:459:HIS:HD2	1.59	0.51
1:B:261:ASP:HB3	5:B:1058:HOH:O	2.10	0.51
1:B:361:TRP:CH2	1:B:405:GLU:CG	2.87	0.51
1:A:420:LYS:HG2	1:A:420:LYS:O	2.11	0.51
1:A:414:ILE:HG22	1:A:425:LEU:HD23	1.93	0.51
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.46	0.50
1:A:680:LYS:NZ	3:A:832:PLP:O3	2.43	0.50
5:A:1016:HOH:O	1:B:250:ASN:CB	2.60	0.50
1:A:408:GLN:HG3	5:A:1064:HOH:O	2.12	0.49
1:A:324:THR:N	1:A:325:VAL:CB	2.73	0.49
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.95	0.49
1:B:692:MET:HG2	1:B:710:ILE:HG21	1.94	0.49
1:A:185:TYR:CD2	1:B:194:PRO:HB3	2.48	0.49
1:A:410:HIS:HD2	1:A:413:ARG:HH11	1.60	0.49
1:A:678:ASN:OD1	1:A:679:MET:N	2.45	0.49
1:A:436:SER:HB3	5:A:990:HOH:O	2.12	0.49
1:A:386:ARG:NH1	1:A:386:ARG:HB2	2.26	0.48
1:B:112:ILE:HG13	1:B:119:ILE:HD13	1.95	0.48
1:A:506:LYS:HG3	1:A:530:PHE:CE1	2.48	0.48
1:A:211:THR:O	1:A:358:LYS:NZ	2.46	0.48
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.79	0.48
1:A:53:PHE:HE1	1:A:188:PRO:HD3	1.78	0.48
1:B:593:ASP:C	1:B:595:LYS:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLY:HA3	5:B:963:HOH:O	2.13	0.48
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.96	0.48
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.49	0.47
1:B:680:LYS:NZ	3:B:832:PLP:O3	2.47	0.47
1:B:506:LYS:HB3	1:B:524:PHE:CZ	2.49	0.47
1:B:510:ASP:HB3	1:B:517:GLN:OE1	2.15	0.47
1:A:324:THR:HG21	5:A:1021:HOH:O	2.14	0.47
1:A:386:ARG:HA	1:A:439:ILE:O	2.15	0.47
1:B:381:PRO:HA	1:B:384:LEU:HD22	1.96	0.47
1:A:753:LYS:O	1:A:754:GLN:HG3	2.14	0.47
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.97	0.47
1:B:571[A]:HIS:ND1	1:B:572:GLU:N	2.62	0.47
1:B:379:VAL:CG2	1:B:673:ALA:HB2	2.45	0.47
1:B:380:LEU:HG	1:B:382:GLU:OE2	2.15	0.47
1:A:460:SER:HB2	5:A:1042:HOH:O	2.15	0.47
1:B:477:ASP:N	5:B:901:HOH:O	2.47	0.46
1:A:436:SER:HA	5:A:1018:HOH:O	2.15	0.46
1:B:539:GLN:OE1	1:B:539:GLN:HA	2.16	0.46
1:A:668:THR:OG1	1:A:771:PHE:HB3	2.15	0.46
1:A:198:LEU:HD13	1:A:305:GLN:HB3	1.96	0.46
1:A:732:TYR:O	1:A:739:LYS:HB2	2.16	0.46
1:A:410:HIS:HE1	1:A:428:MET:O	1.98	0.46
1:A:681:PHE:HB3	1:A:686:ALA:HB3	1.98	0.46
1:A:58:THR:O	1:A:62:HIS:HD2	1.98	0.46
1:A:579:ASN:C	1:A:579:ASN:HD22	2.20	0.46
1:A:184:ARG:HH21	1:B:250:ASN:HB3	1.81	0.46
1:A:494:LEU:HD23	1:A:494:LEU:C	2.37	0.45
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.56	0.45
1:A:210:ASN:C	1:A:210:ASN:HD22	2.19	0.45
1:A:57:HIS:HD2	5:A:1030:HOH:O	1.98	0.45
1:B:58:THR:O	1:B:62:HIS:HD2	1.99	0.45
1:A:378:THR:HB	5:A:1061:HOH:O	2.16	0.45
1:B:26[B]:GLU:OE1	1:B:62:HIS:HE1	2.00	0.45
1:B:593:ASP:O	1:B:595:LYS:N	2.50	0.45
1:A:547:GLN:O	1:A:551:THR:CG2	2.46	0.45
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.52	0.44
1:B:564:ASP:OD1	1:B:664:GLU:OE2	2.35	0.44
1:B:465:THR:O	1:B:469:LYS:HD3	2.16	0.44
1:B:432:GLU:O	1:B:437:LYS:HA	2.17	0.44
1:A:63:LEU:HD12	1:A:63:LEU:C	2.37	0.44
1:A:96:GLN:NE2	1:A:105:GLN:HE22	2.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HE2	1:B:114:GLN:NE2	2.32	0.44
1:A:564:ASP:OD1	1:A:664:GLU:OE2	2.35	0.43
1:B:144:LEU:HD23	1:B:147:MET:CE	2.48	0.43
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.00	0.43
1:A:649:ARG:HH11	1:A:649:ARG:HG2	1.82	0.43
1:A:410:HIS:HD2	1:A:413:ARG:NH1	2.16	0.43
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.52	0.43
1:B:635:MET:HA	5:B:992:HOH:O	2.18	0.43
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.86	0.43
1:A:756:ASP:O	1:A:759:LYS:HB2	2.18	0.43
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.54	0.43
1:B:735:LEU:HA	1:B:736:PRO:HD2	1.72	0.43
1:A:184:ARG:CG	1:A:184:ARG:HH11	2.19	0.42
1:B:577:LEU:O	1:B:580:CYS:HB3	2.18	0.42
1:B:693:ASP:O	1:B:696:ASN:HB2	2.18	0.42
1:A:205:LYS:HB3	1:A:205:LYS:HE2	1.86	0.42
1:B:596:LYS:HG2	1:B:597:LEU:N	2.34	0.42
1:B:545:PHE:CE2	1:B:549:LEU:HD11	2.53	0.42
1:A:250:ASN:ND2	1:A:269:ARG:HH22	2.18	0.42
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.55	0.42
1:B:98:THR:HG22	1:B:102:LEU:HD22	2.02	0.42
1:A:184:ARG:HH22	1:B:250:ASN:HB3	1.85	0.42
1:B:112:ILE:HG23	1:B:117:LEU:HB2	2.02	0.42
1:A:247[B]:ARG:HA	1:A:273:GLU:HG2	2.01	0.42
1:A:23:ASN:ND2	1:A:26:GLU:HG2	2.35	0.42
1:A:98:THR:HG22	1:A:102:LEU:HD22	2.02	0.41
1:B:593:ASP:N	1:B:594:PRO:HD3	2.35	0.41
1:B:270:ASN:ND2	5:B:972:HOH:O	2.52	0.41
1:B:633:ASP:HA	1:B:634:PRO:HD3	1.78	0.41
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.55	0.41
1:A:748:GLY:HA3	1:A:755:PRO:HA	2.02	0.41
1:A:80:LYS:HE3	1:A:330:PRO:O	2.21	0.41
1:B:167:ASN:HD22	1:B:647:ASN:HD21	1.68	0.41
1:A:250:ASN:OD1	1:B:184:ARG:NH2	2.53	0.41
1:B:414:ILE:HD13	1:B:428:MET:SD	2.59	0.41
1:B:363:LYS:O	1:B:363:LYS:HD3	2.20	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.84	0.41
1:A:753:LYS:HD2	1:A:753:LYS:HA	1.99	0.41
1:A:493:LEU:HD21	1:A:512:VAL:HG22	2.03	0.41
1:A:66:ARG:O	1:A:70:THR:HG22	2.18	0.41
1:B:493:LEU:HD11	1:B:512:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:MET:O	1:B:794:PRO:HD3	2.20	0.41
1:B:567:VAL:O	1:B:568:LYS:HB3	2.21	0.40
1:B:42:ASP:HB2	5:B:886:HOH:O	2.20	0.40
1:B:530:PHE:HA	1:B:533:GLU:OE2	2.20	0.40
1:B:144:LEU:HB3	1:B:230:VAL:HG11	2.04	0.40
1:A:97:ASN:ND2	5:A:891:HOH:O	2.54	0.40
1:A:433:GLU:O	1:A:434:GLU:O	2.38	0.40
1:A:52:TYR:CZ	1:A:126:GLU:HB2	2.56	0.40
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.04	0.40
1:B:308:ILE:HD13	1:B:352:ILE:HG21	2.01	0.40
1:B:53:PHE:HE1	1:B:188:PRO:HD3	1.86	0.40
1:A:329:PHE:HB3	1:A:330:PRO:HD3	2.04	0.40
1:A:663:SER:HB2	1:A:681:PHE:CG	2.56	0.40
1:B:410:HIS:HE1	1:B:428:MET:O	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	789/809 (98%)	749 (95%)	37 (5%)	3 (0%)	39	59
1	B	791/809 (98%)	750 (95%)	39 (5%)	2 (0%)	46	66
All	All	1580/1618 (98%)	1499 (95%)	76 (5%)	5 (0%)	46	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	B	555	VAL
1	B	527	ASP
1	A	593	ASP

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Mol	Chain	Res	Type
1	A	435	GLY

### 5.3.2 Protein sidechains ⓘ

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	697/706 (99%)	656 (94%)	41 (6%)	24	42
1	B	699/706 (99%)	659 (94%)	40 (6%)	25	44
All	All	1396/1412 (99%)	1315 (94%)	81 (6%)	25	43

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	70	THR
1	A	90	TYR
1	A	102	LEU
1	A	155	TYR
1	A	169	LYS
1	A	184	ARG
1	A	210	ASN
1	A	217	ASP
1	A	245	SER
1	A	251	ASP
1	A	277	ARG
1	A	300	VAL
1	A	309	ARG
1	A	325	VAL
1	A	327	ASP
1	A	363	LYS
1	A	378	THR
1	A	380	LEU
1	A	386	ARG
1	A	413	ARG
1	A	433	GLU

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Mol	Chain	Res	Type
1	A	434	GLU
1	A	436	SER
1	A	457	LYS
1	A	469	LYS
1	A	499	LEU
1	A	502	LEU
1	A	540	GLU
1	A	543	LEU
1	A	551	THR
1	A	568	LYS
1	A	579	ASN
1	A	592	LYS
1	A	622	LEU
1	A	645	LEU
1	A	652	LEU
1	A	683	LEU
1	A	724	LYS
1	A	753	LYS
1	A	822	GLN
1	B	44	ASN
1	B	72	GLN
1	B	90	TYR
1	B	102	LEU
1	B	128	ASP
1	B	150	LEU
1	B	184	ARG
1	B	191	LYS
1	B	213	THR
1	B	251	ASP
1	B	252	PHE
1	B	277	ARG
1	B	325	VAL
1	B	327	ASP
1	B	337	LEU
1	B	382	GLU
1	B	384	LEU
1	B	393	GLU
1	B	405	GLU
1	B	413	ARG
1	B	420	LYS
1	B	426	ARG
1	B	433	GLU

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Mol	Chain	Res	Type
1	B	457	LYS
1	B	462	ILE
1	B	474	LEU
1	B	475	GLU
1	B	502	LEU
1	B	573	TYR
1	B	579	ASN
1	B	593	ASP
1	B	613	TYR
1	B	621	LYS
1	B	628	ASP
1	B	645	LEU
1	B	714	ARG
1	B	723	LYS
1	B	759	LYS
1	B	789	GLN
1	B	822	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	ASN
1	A	34	HIS
1	A	57	HIS
1	A	62	HIS
1	A	96	GLN
1	A	97	ASN
1	A	114	GLN
1	A	167	ASN
1	A	208	HIS
1	A	210	ASN
1	A	239	ASN
1	A	250	ASN
1	A	270	ASN
1	A	274	ASN
1	A	305	GLN
1	A	410	HIS
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	539	GLN

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Mol	Chain	Res	Type
1	A	541	ASN
1	A	566	GLN
1	A	579	ASN
1	A	768	HIS
1	A	822	GLN
1	B	23	ASN
1	B	34	HIS
1	B	57	HIS
1	B	62	HIS
1	B	105	GLN
1	B	114	GLN
1	B	167	ASN
1	B	239	ASN
1	B	270	ASN
1	B	274	ASN
1	B	305	GLN
1	B	369	GLN
1	B	410	HIS
1	B	443	HIS
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	579	ASN
1	B	789	GLN
1	B	822	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	NBG	A	1	-	15,15,15	1.58	4 (26%)	21,21,21	1.08	2 (9%)
3	PLP	A	832	1	16,16,16	1.20	2 (12%)	21,23,23	1.10	3 (14%)
4	AVD	A	833	-	26,37,37	1.13	2 (7%)	34,55,55	2.28	6 (17%)
2	NBG	B	2	-	15,15,15	1.61	3 (20%)	21,21,21	1.84	5 (23%)
3	PLP	B	832	1	16,16,16	1.20	2 (12%)	21,23,23	1.11	3 (14%)
4	AVD	B	833	-	26,37,37	1.32	4 (15%)	34,55,55	2.34	9 (26%)

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	NBG	A	1	-	-	0/5/26/26	0/1/1/1
3	PLP	A	832	1	-	0/8/8/8	0/1/1/1
4	AVD	A	833	-	-	0/8/16/16	0/4/4/4
2	NBG	B	2	-	-	0/5/26/26	0/1/1/1
3	PLP	B	832	1	-	0/8/8/8	0/1/1/1
4	AVD	B	833	-	-	0/8/16/16	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	833	AVD	C17-C16	-3.41	1.38	1.41
4	B	833	AVD	C17-C16	-3.28	1.39	1.41
2	A	1	NBG	O5-C1	-3.04	1.39	1.43
2	B	2	NBG	O5-C1	-2.69	1.39	1.43
2	B	2	NBG	O3-C3	-2.62	1.36	1.43
2	A	1	NBG	C2-C1	-2.37	1.50	1.53
2	B	2	NBG	O5-C5	-2.24	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	833	AVD	F11-C5	-2.17	1.31	1.36
2	A	1	NBG	O5-C5	-2.07	1.39	1.44
2	A	1	NBG	C8-C7	-2.06	1.46	1.50
4	B	833	AVD	F11-C5	-2.04	1.31	1.36
3	A	832	PLP	C3-C2	-2.00	1.39	1.40
3	B	832	PLP	C3-C2	-2.00	1.39	1.40
3	A	832	PLP	C2-N1	2.06	1.38	1.34
3	B	832	PLP	C2-N1	2.09	1.38	1.34
4	B	833	AVD	C6-C5	2.16	1.41	1.37
4	B	833	AVD	C6-C1	2.27	1.41	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	833	AVD	C30-C28-C34	-8.70	118.09	122.95
4	B	833	AVD	C30-C28-C34	-8.64	118.13	122.95
4	B	833	AVD	C15-C14-CL29	-4.47	114.77	119.11
2	B	2	NBG	O2-C2-C3	-4.37	100.50	110.34
4	B	833	AVD	C18-C13-C14	-3.24	114.66	118.08
2	B	2	NBG	C2-C1-N1	-3.19	107.87	111.44
2	A	1	NBG	O2-C2-C1	-3.09	103.49	109.27
4	A	833	AVD	C15-C14-CL29	-2.98	116.21	119.11
4	B	833	AVD	C22-N21-C16	-2.90	117.44	121.22
4	B	833	AVD	C15-C16-C17	-2.79	116.50	120.69
4	A	833	AVD	C3-C4-C5	-2.58	116.28	117.81
2	B	2	NBG	C3-C4-C5	-2.54	105.77	110.20
3	B	832	PLP	O4A-C4A-C4	-2.53	119.99	125.11
3	A	832	PLP	O4A-C4A-C4	-2.51	120.03	125.11
2	B	2	NBG	O5-C1-C2	-2.43	107.02	109.91
3	A	832	PLP	C5-C6-N1	-2.18	120.08	123.86
3	B	832	PLP	C5-C6-N1	-2.17	120.10	123.86
2	A	1	NBG	C2-C1-N1	-2.06	109.13	111.44
3	A	832	PLP	C3-C4-C5	2.18	119.73	118.11
3	B	832	PLP	C3-C4-C5	2.34	119.85	118.11
4	A	833	AVD	C18-C17-C16	2.42	122.33	118.49
4	B	833	AVD	F9-C1-C2	2.66	120.03	117.74
4	B	833	AVD	C13-C14-CL29	2.70	123.00	119.45
2	B	2	NBG	C1-N1-C7	2.72	126.05	122.52
4	B	833	AVD	C17-C16-N21	2.89	121.39	118.84
4	A	833	AVD	C17-C16-N21	3.15	121.62	118.84
4	B	833	AVD	C33-C34-C28	4.27	120.08	116.45
4	A	833	AVD	C33-C34-C28	6.22	121.73	116.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	832	PLP	1	0
3	B	832	PLP	2	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	794/809 (98%)	-0.64	1 (0%) 95 96	18, 32, 56, 72	0
1	B	794/809 (98%)	-0.59	3 (0%) 93 94	16, 34, 61, 75	0
All	All	1588/1618 (98%)	-0.62	4 (0%) 94 95	16, 33, 59, 75	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	PHE	4.0
1	B	420	LYS	3.1
1	B	435	GLY	2.7
1	B	831	ASP	2.2

### 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<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( $\text{\AA}^2$ )	Q<0.9
3	PLP	B	832	16/16	0.93	0.14	2.10	19,25,32,33	0
3	PLP	A	832	16/16	0.95	0.14	1.88	18,23,33,34	0
4	AVD	A	833	34/34	0.98	0.11	0.13	22,28,37,42	0
4	AVD	B	833	34/34	0.97	0.11	-0.31	20,29,32,36	0
2	NBG	B	2	15/15	0.98	0.10	-0.47	22,27,33,35	0
2	NBG	A	1	15/15	0.98	0.10	-0.64	18,26,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.