



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:30 am GMT

PDB ID : 3PVB  
Title : Crystal structure of (73-244)RIa:C holoenzyme of cAMP-dependent Protein kinase  
Authors : Boettcher, A.J.; Wu, J.; Kim, C.; Yang, J.; Bruystens, J.; Cheung, N.; Penny-packer, J.K.; Blumenthal, D.A.; Kornev, A.P.; Taylor, S.S.  
Deposited on : 2010-12-06  
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](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

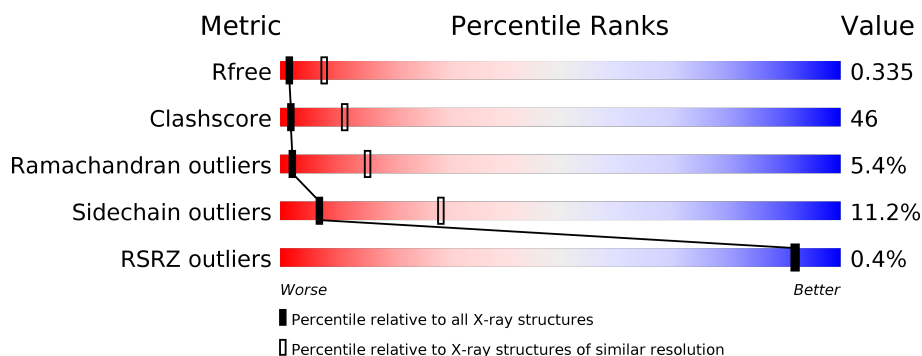
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	345	
2	B	160	

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
1	SEP	A	338	-	-	X	-
5	GOL	B	1	-	X	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4046 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.

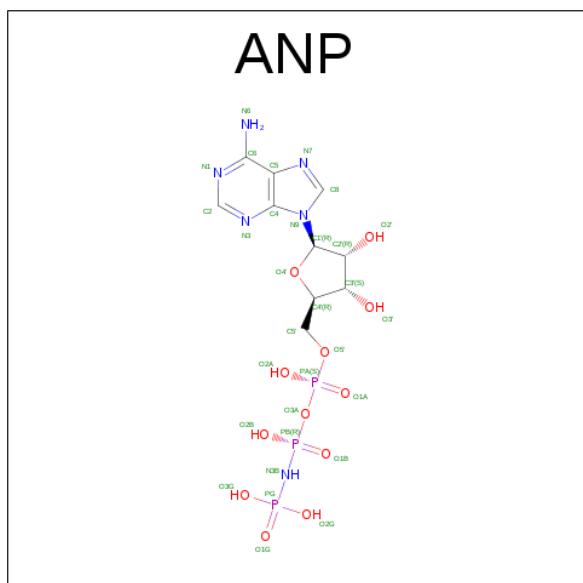
- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	P	S	0	0	0
			2774	1788	458	516	4	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1218	766	211	237	4			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	2	Total	Mn		0	0
			2	2			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

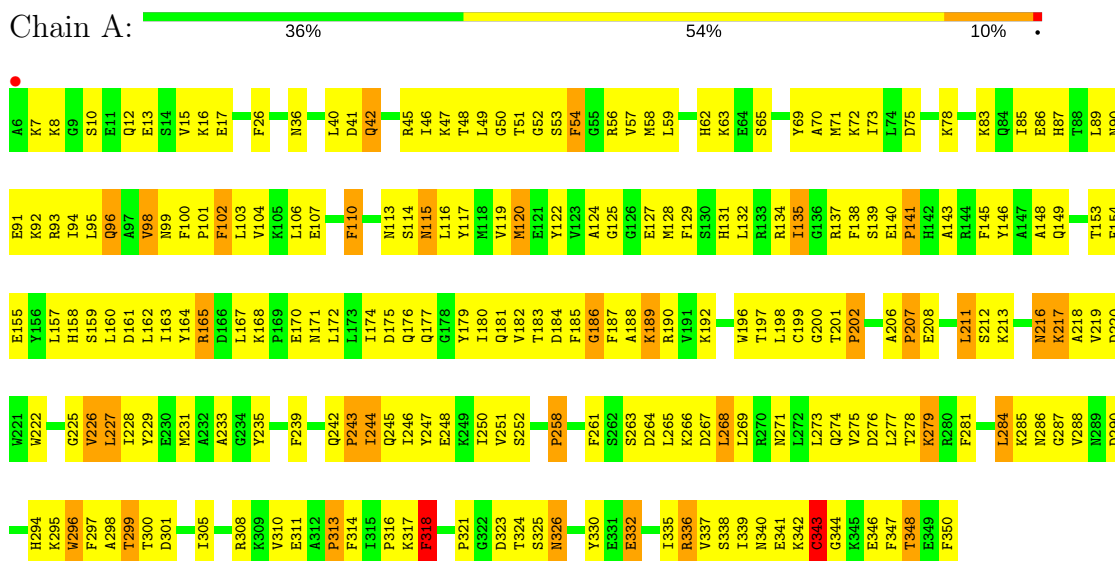
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	2	Total	O	0	0
			2	2		

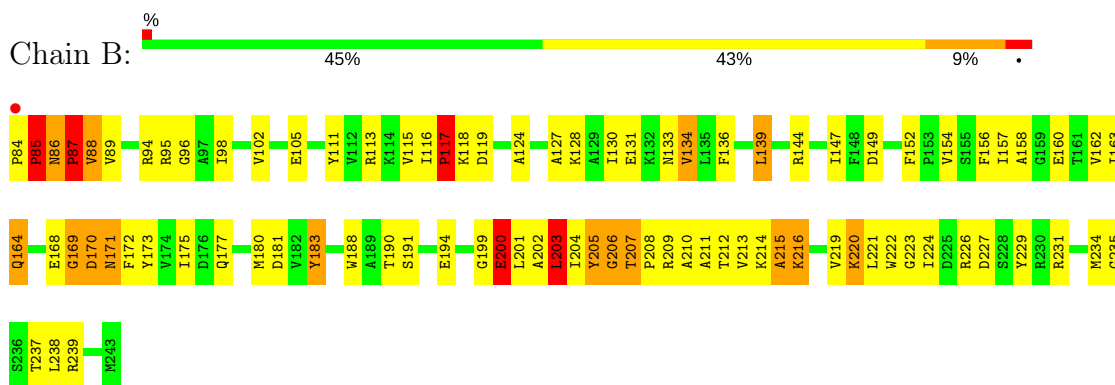
### 3 Residue-property plots

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: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.67Å 116.67Å 140.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.30 47.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-3.30) 63.1 (47.52-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.242 , 0.290 0.263 , 0.335	Depositor DCC
$R_{free}$ test set	730 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 25.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	4046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: TPO, GOL, MN, ANP, SEP

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	0.43	0/2800	0.82	11/3785 (0.3%)
2	B	0.48	0/1241	0.82	3/1683 (0.2%)
All	All	0.45	0/4041	0.82	14/5468 (0.3%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	VAL	CB-CA-C	-9.84	92.70	111.40
2	B	215	ALA	N-CA-CB	-8.56	98.11	110.10
1	A	233	ALA	CB-CA-C	7.87	121.90	110.10
1	A	317	LYS	CB-CA-C	-5.87	98.67	110.40
2	B	171	ASN	CB-CA-C	-5.86	98.67	110.40
1	A	46	ILE	CB-CA-C	-5.82	99.97	111.60
2	B	171	ASN	N-CA-CB	-5.72	100.31	110.60
1	A	120	MET	CB-CA-C	5.61	121.61	110.40
1	A	343	CYS	CB-CA-C	-5.59	99.22	110.40
1	A	318	PHE	N-CA-CB	-5.44	100.81	110.60
1	A	337	VAL	N-CA-C	-5.19	96.98	111.00
1	A	107	GLU	N-CA-C	5.16	124.92	111.00
1	A	211	LEU	CA-CB-CG	-5.08	103.60	115.30
1	A	99	ASN	N-CA-CB	-5.04	101.52	110.60

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2774	0	2650	245	0
2	B	1218	0	1154	130	0
3	A	31	0	12	4	0
4	A	2	0	0	0	0
5	B	6	0	4	1	0
6	A	13	0	0	0	0
6	B	2	0	0	0	0
All	All	4046	0	3820	358	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 46.

All (358) 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:213:LYS:HG2	2:B:237:THR:HG21	1.31	1.09
2:B:86:ASN:H	2:B:87:PRO:HD3	1.25	0.99
1:A:47:LYS:HD3	1:A:324:THR:HG21	1.49	0.93
2:B:203:LEU:H	2:B:203:LEU:HD12	1.34	0.92
1:A:185:PHE:O	1:A:187:PHE:N	2.04	0.91
1:A:62:HIS:HB3	1:A:65:SER:HB3	1.52	0.88
1:A:47:LYS:HG2	1:A:48:THR:H	1.40	0.87
2:B:169:GLY:O	2:B:170:ASP:HB2	1.73	0.87
1:A:161:ASP:HA	1:A:217:LYS:HZ1	1.42	0.84
1:A:98:VAL:HG23	1:A:98:VAL:O	1.80	0.82
1:A:135:ILE:O	1:A:135:ILE:HD13	1.79	0.82
1:A:187:PHE:CE2	1:A:199:CYS:HB2	2.14	0.82
1:A:187:PHE:HE2	1:A:200:GLY:H	1.29	0.80
2:B:86:ASN:N	2:B:87:PRO:HD3	1.93	0.80
2:B:130:ILE:HD13	2:B:136:PHE:HB3	1.63	0.80
1:A:161:ASP:HA	1:A:217:LYS:NZ	1.96	0.79
1:A:213:LYS:HG2	2:B:237:THR:CG2	2.12	0.79
1:A:91:GLU:HB2	1:A:186:GLY:HA2	1.65	0.78
1:A:187:PHE:CD2	1:A:199:CYS:HB2	2.18	0.78
1:A:187:PHE:HE2	1:A:200:GLY:N	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HE2	1:A:83:LYS:HA	1.67	0.76
1:A:93:ARG:O	1:A:96:GLN:HG3	1.85	0.76
1:A:222:TRP:CZ2	1:A:250:ILE:HG23	2.21	0.75
1:A:168:LYS:HE2	1:A:171:ASN:HD21	1.50	0.75
2:B:203:LEU:HD12	2:B:203:LEU:N	2.01	0.74
1:A:168:LYS:HE2	1:A:171:ASN:ND2	2.03	0.73
1:A:149:GLN:HE22	1:A:180:ILE:H	1.36	0.72
2:B:84:PRO:HA	2:B:87:PRO:CD	2.19	0.72
2:B:162:VAL:HG12	2:B:163:ILE:HG23	1.70	0.72
2:B:84:PRO:HA	2:B:87:PRO:CG	2.20	0.72
1:A:149:GLN:NE2	1:A:180:ILE:H	1.87	0.72
1:A:336:ARG:HH22	1:A:338:SEP:HA	1.54	0.72
2:B:85:PRO:CD	2:B:86:ASN:H	2.01	0.72
1:A:244:ILE:HD11	2:B:134:VAL:CG1	2.20	0.71
1:A:244:ILE:HD11	2:B:134:VAL:HG11	1.73	0.71
1:A:201:THR:HG23	2:B:96:GLY:O	1.91	0.70
2:B:115:VAL:HG12	2:B:117:PRO:HD3	1.72	0.70
2:B:85:PRO:HD2	2:B:86:ASN:H	1.56	0.70
2:B:163:ILE:HB	2:B:209:ARG:HE	1.56	0.69
2:B:181:ASP:HB2	2:B:183:TYR:HE1	1.57	0.69
1:A:72:LYS:HE3	3:A:400:ANP:O1A	1.92	0.69
1:A:228:ILE:CG2	1:A:269:LEU:HD11	2.23	0.69
2:B:209:ARG:HA	5:B:1:GOL:O3	1.92	0.68
2:B:219:VAL:HG12	2:B:221:LEU:CD1	2.24	0.68
1:A:50:GLY:HA2	1:A:330:TYR:CE2	2.28	0.68
2:B:130:ILE:O	2:B:130:ILE:HD12	1.94	0.68
2:B:177:GLN:HA	2:B:194:GLU:HG3	1.76	0.68
2:B:190:THR:OG1	2:B:191:SER:N	2.27	0.68
1:A:227:LEU:O	1:A:227:LEU:HD12	1.94	0.67
1:A:314:PHE:O	1:A:316:PRO:HD3	1.96	0.67
1:A:49:LEU:HD21	1:A:59:LEU:HD12	1.76	0.66
1:A:174:ILE:HD12	1:A:174:ILE:N	2.11	0.66
1:A:90:ASN:O	1:A:94:ILE:HG13	1.95	0.66
2:B:207:THR:HB	2:B:208:PRO:CD	2.25	0.66
2:B:170:ASP:H	2:B:202:ALA:HB1	1.61	0.66
2:B:220:LYS:C	2:B:221:LEU:HD12	2.16	0.66
2:B:201:LEU:O	2:B:201:LEU:HD22	1.97	0.65
1:A:122:TYR:CE2	1:A:124:ALA:HB2	2.31	0.65
2:B:111:TYR:CE2	2:B:231:ARG:HD2	2.32	0.64
1:A:216:ASN:HD21	1:A:218:ALA:HB3	1.62	0.64
2:B:180:MET:HB3	2:B:214:LYS:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:O	1:A:250:ILE:HD12	1.97	0.64
1:A:170:GLU:N	1:A:170:GLU:OE1	2.31	0.63
1:A:213:LYS:CG	2:B:237:THR:HG21	2.20	0.63
2:B:204:ILE:HG13	2:B:205:TYR:CD1	2.34	0.63
1:A:332:GLU:H	1:A:332:GLU:CD	2.02	0.63
1:A:91:GLU:HB2	1:A:186:GLY:CA	2.29	0.62
1:A:175:ASP:OD2	1:A:308:ARG:NH1	2.33	0.62
2:B:139:LEU:O	2:B:144:ARG:NH2	2.33	0.62
2:B:183:TYR:O	2:B:211:ALA:HB1	2.00	0.62
1:A:180:ILE:HG22	1:A:181:GLN:N	2.15	0.61
1:A:26:PHE:CG	1:A:160:LEU:HD13	2.36	0.61
2:B:181:ASP:HB2	2:B:183:TYR:CE1	2.36	0.61
1:A:115:ASN:O	1:A:116:LEU:HD23	2.00	0.61
1:A:187:PHE:CE2	1:A:200:GLY:N	2.66	0.61
2:B:128:LYS:HA	2:B:131:GLU:HB3	1.82	0.60
1:A:98:VAL:O	1:A:98:VAL:CG2	2.49	0.60
1:A:165:ARG:HH12	1:A:189:LYS:HB3	1.66	0.60
1:A:49:LEU:HD11	1:A:59:LEU:HG	1.82	0.60
1:A:116:LEU:HD11	1:A:347:PHE:CD2	2.37	0.60
2:B:116:ILE:O	2:B:118:LYS:HE2	2.01	0.60
1:A:85:ILE:O	1:A:89:LEU:HG	2.02	0.60
2:B:105:GLU:HG2	2:B:238:LEU:HD21	1.82	0.59
1:A:42:GLN:HB2	1:A:62:HIS:CE1	2.37	0.59
2:B:85:PRO:CD	2:B:86:ASN:N	2.61	0.59
1:A:228:ILE:HG21	1:A:269:LEU:HD11	1.84	0.59
1:A:139:SEP:O1P	1:A:141:PRO:HG2	2.03	0.59
2:B:202:ALA:O	2:B:226:ARG:HD3	2.01	0.59
2:B:84:PRO:HB3	2:B:89:VAL:CG1	2.31	0.59
1:A:100:PHE:HB3	1:A:103:LEU:HD12	1.83	0.59
1:A:336:ARG:NH2	1:A:338:SEP:HA	2.17	0.59
2:B:175:ILE:H	2:B:175:ILE:HD12	1.68	0.59
2:B:219:VAL:CG1	2:B:221:LEU:HD11	2.34	0.58
1:A:198:LEU:HD23	1:A:198:LEU:C	2.24	0.57
1:A:268:LEU:HD12	1:A:294:HIS:CG	2.39	0.57
1:A:103:LEU:HD23	1:A:182:VAL:HB	1.86	0.57
1:A:180:ILE:HG22	1:A:181:GLN:H	1.70	0.57
1:A:344:GLY:O	1:A:348:THR:HG22	2.05	0.57
1:A:201:THR:HG21	2:B:95:ARG:HB3	1.86	0.57
1:A:135:ILE:HD12	1:A:137:ARG:O	2.05	0.57
1:A:235:TYR:OH	1:A:258:PRO:HG3	2.05	0.56
1:A:332:GLU:N	1:A:332:GLU:OE1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASN:H	2:B:87:PRO:CD	2.09	0.56
1:A:48:THR:OG1	1:A:332:GLU:HB3	2.05	0.56
2:B:219:VAL:HG12	2:B:221:LEU:HD12	1.86	0.56
1:A:13:GLU:O	1:A:17:GLU:HG3	2.05	0.56
1:A:163:ILE:HG12	1:A:165:ARG:HG2	1.88	0.56
1:A:161:ASP:OD1	1:A:192:LYS:HG3	2.05	0.56
1:A:57:VAL:HA	1:A:71:MET:O	2.06	0.56
1:A:208:GLU:N	1:A:208:GLU:OE2	2.28	0.56
2:B:199:GLY:C	2:B:201:LEU:H	2.08	0.56
1:A:113:ASN:HB3	1:A:340:ASN:O	2.06	0.55
1:A:145:PHE:CE2	1:A:313:PRO:HD3	2.41	0.55
1:A:279:LYS:HA	1:A:284:LEU:HD11	1.89	0.55
2:B:118:LYS:HD3	2:B:222:TRP:CZ3	2.42	0.55
2:B:181:ASP:OD1	2:B:216:LYS:HG3	2.06	0.55
2:B:219:VAL:HG12	2:B:221:LEU:HD11	1.88	0.55
1:A:281:PHE:HA	1:A:284:LEU:CD2	2.36	0.55
1:A:47:LYS:HG2	1:A:48:THR:N	2.15	0.55
1:A:128:MET:HA	1:A:174:ILE:HD11	1.89	0.55
1:A:57:VAL:CG1	1:A:70:ALA:HB1	2.37	0.55
1:A:222:TRP:HZ2	1:A:250:ILE:HG23	1.72	0.54
1:A:338:SEP:OG	1:A:342:LYS:HE3	2.07	0.54
2:B:203:LEU:H	2:B:203:LEU:CD1	1.97	0.54
1:A:201:THR:CG2	2:B:95:ARG:HB3	2.38	0.54
1:A:216:ASN:ND2	1:A:218:ALA:HB3	2.22	0.54
2:B:172:PHE:O	2:B:223:GLY:HA2	2.07	0.54
2:B:183:TYR:CD1	2:B:183:TYR:N	2.75	0.54
1:A:216:ASN:HD22	1:A:216:ASN:C	2.10	0.54
1:A:242:GLN:HG3	1:A:243:PRO:HD2	1.90	0.54
2:B:133:ASN:ND2	2:B:136:PHE:HD2	2.06	0.54
2:B:181:ASP:CG	2:B:216:LYS:HG3	2.28	0.54
1:A:165:ARG:NH1	1:A:189:LYS:HB3	2.23	0.54
2:B:172:PHE:HB3	2:B:224:ILE:CG2	2.39	0.53
1:A:242:GLN:HB3	1:A:245:GLN:OE1	2.08	0.53
2:B:172:PHE:HB3	2:B:224:ILE:HG23	1.91	0.53
1:A:242:GLN:NE2	1:A:243:PRO:HD2	2.23	0.53
2:B:205:TYR:O	2:B:206:GLY:O	2.27	0.53
1:A:274:GLN:NE2	1:A:279:LYS:HG3	2.23	0.53
1:A:114:SER:OG	1:A:338:SEP:HB2	2.08	0.53
1:A:184:ASP:HB2	3:A:400:ANP:O1A	2.08	0.53
1:A:264:ASP:HB3	1:A:296:TRP:HB2	1.91	0.53
2:B:199:GLY:O	2:B:201:LEU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:MET:O	2:B:235:GLY:C	2.47	0.53
1:A:199:CYS:HA	2:B:98:ILE:O	2.08	0.53
1:A:226:VAL:O	1:A:227:LEU:C	2.46	0.53
1:A:45:ARG:CZ	1:A:335:ILE:HG13	2.39	0.53
1:A:318:PHE:HZ	1:A:321:PRO:HA	1.74	0.52
2:B:203:LEU:O	2:B:226:ARG:HG3	2.07	0.52
2:B:147:ILE:HD11	2:B:229:TYR:HA	1.91	0.52
1:A:268:LEU:N	1:A:294:HIS:HE2	2.08	0.52
1:A:62:HIS:HB2	1:A:69:TYR:HE1	1.74	0.52
2:B:164:GLN:HG2	2:B:212:THR:OG1	2.10	0.52
1:A:279:LYS:HA	1:A:284:LEU:CD1	2.40	0.52
2:B:154:VAL:HG12	2:B:156:PHE:HE1	1.75	0.52
1:A:242:GLN:HE21	1:A:243:PRO:HD2	1.75	0.52
2:B:84:PRO:HB3	2:B:89:VAL:HG13	1.91	0.52
2:B:152:PHE:CE2	2:B:224:ILE:HA	2.45	0.52
1:A:155:GLU:HG3	1:A:288:VAL:HG11	1.92	0.51
1:A:159:SER:O	1:A:160:LEU:HD23	2.10	0.51
1:A:149:GLN:NE2	1:A:179:TYR:HD1	2.08	0.51
1:A:190:ARG:HH12	1:A:192:LYS:NZ	2.08	0.51
2:B:130:ILE:HD13	2:B:136:PHE:CB	2.39	0.51
2:B:163:ILE:HD12	2:B:209:ARG:CD	2.40	0.51
1:A:294:HIS:ND1	1:A:295:LYS:N	2.58	0.51
1:A:48:THR:HA	1:A:58:MET:HA	1.93	0.51
1:A:87:HIS:O	1:A:90:ASN:HB2	2.10	0.51
2:B:163:ILE:CB	2:B:209:ARG:HE	2.24	0.51
1:A:104:VAL:HG22	1:A:182:VAL:O	2.10	0.51
1:A:196:TRP:CD1	1:A:196:TRP:N	2.78	0.51
2:B:157:ILE:HG13	2:B:160:GLU:HG3	1.92	0.51
1:A:72:LYS:HE3	3:A:400:ANP:PA	2.51	0.51
1:A:10:SEP:C	1:A:12:GLN:N	2.70	0.51
2:B:239:ARG:O	2:B:239:ARG:HG2	2.09	0.51
2:B:207:THR:HB	2:B:208:PRO:HD2	1.90	0.51
1:A:69:TYR:HA	1:A:122:TYR:H	1.75	0.51
2:B:158:ALA:HA	2:B:215:ALA:O	2.11	0.51
1:A:148:ALA:HB2	1:A:297:PHE:HE2	1.75	0.50
1:A:53:SER:HB2	1:A:54:PHE:CE1	2.47	0.50
1:A:94:ILE:HD12	1:A:188:ALA:HB3	1.93	0.50
1:A:116:LEU:HD13	1:A:350:PHE:CD2	2.47	0.50
2:B:85:PRO:HD2	2:B:87:PRO:HD3	1.93	0.50
1:A:170:GLU:OE2	2:B:95:ARG:HB2	2.11	0.50
1:A:246:ILE:HG22	1:A:250:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SEP:C	1:A:12:GLN:H	2.24	0.50
1:A:135:ILE:HG21	1:A:138:PHE:CE1	2.47	0.50
1:A:161:ASP:O	1:A:190:ARG:HG3	2.11	0.50
1:A:285:LYS:C	1:A:287:GLY:N	2.65	0.50
1:A:297:PHE:O	1:A:299:THR:N	2.45	0.50
1:A:52:GLY:HA3	3:A:400:ANP:O1B	2.12	0.50
1:A:86:GLU:OE1	2:B:102:VAL:HG11	2.12	0.50
2:B:133:ASN:HD22	2:B:136:PHE:HD2	1.58	0.50
1:A:227:LEU:C	1:A:227:LEU:HD12	2.31	0.50
1:A:165:ARG:NH2	1:A:197:TPO:O1P	2.45	0.49
1:A:248:GLU:O	1:A:252:SER:HB3	2.12	0.49
2:B:87:PRO:O	2:B:88:VAL:HB	2.11	0.49
1:A:127:GLU:HA	1:A:172:LEU:O	2.13	0.49
1:A:263:SER:HA	1:A:266:LYS:HE3	1.94	0.49
1:A:42:GLN:HA	1:A:63:LYS:HD2	1.93	0.49
1:A:318:PHE:CZ	1:A:321:PRO:HA	2.48	0.49
2:B:163:ILE:HD12	2:B:209:ARG:HD2	1.95	0.49
2:B:221:LEU:HD12	2:B:221:LEU:N	2.28	0.49
2:B:227:ASP:O	2:B:231:ARG:HG3	2.13	0.49
1:A:189:LYS:HG3	1:A:190:ARG:N	2.27	0.49
2:B:239:ARG:HB2	2:B:239:ARG:CZ	2.42	0.49
1:A:143:ALA:HB1	1:A:231:MET:HE3	1.94	0.49
1:A:49:LEU:HD21	1:A:59:LEU:CD1	2.42	0.49
1:A:51:THR:O	2:B:94:ARG:NH2	2.46	0.49
2:B:181:ASP:OD2	2:B:216:LYS:HG3	2.13	0.49
1:A:216:ASN:O	1:A:219:VAL:HG22	2.13	0.48
1:A:190:ARG:NH1	1:A:192:LYS:NZ	2.61	0.48
1:A:15:VAL:O	1:A:16:LYS:C	2.50	0.48
1:A:285:LYS:C	1:A:287:GLY:H	2.16	0.48
1:A:200:GLY:O	2:B:98:ILE:N	2.44	0.48
1:A:276:ASP:OD2	1:A:278:THR:HG23	2.13	0.48
2:B:113:ARG:HH12	2:B:149:ASP:HB2	1.79	0.48
1:A:56:ARG:O	1:A:72:LYS:HA	2.14	0.48
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.79	0.48
1:A:347:PHE:O	1:A:348:THR:C	2.52	0.48
1:A:62:HIS:CB	1:A:65:SER:HB3	2.34	0.48
2:B:172:PHE:CE2	2:B:200:GLU:HB3	2.49	0.48
2:B:175:ILE:HD12	2:B:175:ILE:N	2.29	0.47
2:B:239:ARG:HB2	2:B:239:ARG:NH1	2.30	0.47
1:A:301:ASP:O	1:A:305:ILE:HG12	2.15	0.47
1:A:297:PHE:HD2	1:A:300:THR:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:N	1:A:110:PHE:CD1	2.83	0.47
1:A:91:GLU:HB2	1:A:186:GLY:N	2.30	0.47
1:A:190:ARG:HH12	1:A:192:LYS:HZ2	1.61	0.47
1:A:216:ASN:HD21	1:A:218:ALA:CB	2.27	0.47
1:A:47:LYS:CD	1:A:324:THR:HG21	2.34	0.47
2:B:173:TYR:HB3	2:B:221:LEU:HD23	1.97	0.47
1:A:198:LEU:HD23	1:A:199:CYS:N	2.30	0.47
2:B:205:TYR:CE2	2:B:207:THR:HG23	2.50	0.47
1:A:122:TYR:HE2	1:A:124:ALA:HB2	1.79	0.46
1:A:45:ARG:CD	1:A:335:ILE:HG13	2.46	0.46
1:A:129:PHE:HE1	2:B:95:ARG:HH21	1.62	0.46
1:A:229:TYR:O	1:A:229:TYR:CD1	2.69	0.46
1:A:242:GLN:CG	1:A:243:PRO:HD2	2.44	0.46
1:A:338:SEP:P	1:A:339:ILE:H	2.38	0.46
2:B:130:ILE:CD1	2:B:136:PHE:HB3	2.40	0.46
1:A:170:GLU:OE2	2:B:95:ARG:NE	2.49	0.46
1:A:274:GLN:HE22	1:A:279:LYS:HD3	1.81	0.46
2:B:154:VAL:HG12	2:B:156:PHE:CE1	2.51	0.46
2:B:130:ILE:C	2:B:130:ILE:HD12	2.37	0.45
2:B:210:ALA:O	2:B:211:ALA:HB2	2.16	0.45
2:B:239:ARG:CB	2:B:239:ARG:CZ	2.94	0.45
1:A:102:PHE:HZ	1:A:305:ILE:O	1.99	0.45
1:A:73:ILE:N	1:A:73:ILE:HD12	2.32	0.45
1:A:165:ARG:HH12	1:A:189:LYS:CB	2.29	0.45
1:A:127:GLU:OE1	2:B:94:ARG:NH1	2.49	0.45
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.52	0.45
1:A:36:ASN:N	1:A:36:ASN:HD22	2.13	0.45
1:A:69:TYR:HB3	1:A:120:MET:O	2.16	0.45
2:B:220:LYS:HD3	2:B:221:LEU:N	2.31	0.45
1:A:167:LEU:HD21	1:A:227:LEU:HD23	1.98	0.45
1:A:244:ILE:CD1	2:B:134:VAL:HG11	2.44	0.45
2:B:139:LEU:N	2:B:139:LEU:HD23	2.32	0.45
1:A:149:GLN:HE22	1:A:180:ILE:N	2.11	0.45
2:B:215:ALA:O	2:B:216:LYS:C	2.55	0.44
2:B:85:PRO:HD2	2:B:87:PRO:HG3	1.99	0.44
1:A:116:LEU:HD11	1:A:347:PHE:CE2	2.52	0.44
1:A:344:GLY:C	1:A:346:GLU:H	2.18	0.44
1:A:154:PHE:CD2	1:A:220:ASP:HB3	2.52	0.44
1:A:208:GLU:CD	1:A:208:GLU:H	2.12	0.44
1:A:174:ILE:HA	1:A:179:TYR:O	2.18	0.44
1:A:207:PRO:HG2	1:A:275:VAL:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:C	1:A:325:SER:H	2.21	0.44
2:B:205:TYR:CD2	2:B:207:THR:HG23	2.52	0.44
1:A:132:LEU:CD1	1:A:137:ARG:HA	2.48	0.44
1:A:265:LEU:HD13	1:A:296:TRP:CE2	2.53	0.44
2:B:181:ASP:HB3	2:B:188:TRP:NE1	2.32	0.44
2:B:207:THR:O	2:B:208:PRO:C	2.57	0.43
1:A:113:ASN:HA	1:A:341:GLU:HA	2.01	0.43
1:A:140:GLU:N	1:A:141:PRO:HD2	2.33	0.43
1:A:174:ILE:N	1:A:174:ILE:CD1	2.79	0.43
1:A:187:PHE:HD1	1:A:187:PHE:N	2.16	0.43
1:A:243:PRO:O	1:A:245:GLN:N	2.52	0.43
1:A:323:ASP:OD1	1:A:323:ASP:N	2.51	0.43
1:A:146:TYR:CD2	1:A:180:ILE:HD11	2.54	0.43
1:A:338:SEP:OG	1:A:339:ILE:N	2.51	0.43
1:A:344:GLY:C	1:A:346:GLU:N	2.72	0.43
1:A:350:PHE:OXT	1:A:350:PHE:CD1	2.72	0.43
1:A:187:PHE:N	1:A:187:PHE:CD1	2.85	0.43
1:A:75:ASP:HB3	1:A:78:LYS:HB3	1.99	0.43
1:A:91:GLU:HB2	1:A:186:GLY:H	1.83	0.43
2:B:113:ARG:O	2:B:113:ARG:HG3	2.18	0.43
2:B:175:ILE:HG22	2:B:194:GLU:HA	2.00	0.43
1:A:140:GLU:OE1	1:A:265:LEU:HB2	2.19	0.43
1:A:185:PHE:O	1:A:186:GLY:C	2.51	0.43
1:A:206:ALA:HB3	1:A:219:VAL:HG12	2.01	0.43
1:A:158:HIS:CE1	1:A:217:LYS:HB3	2.54	0.42
1:A:146:TYR:CG	1:A:180:ILE:HD11	2.54	0.42
1:A:164:TYR:O	1:A:164:TYR:CD2	2.73	0.42
1:A:216:ASN:ND2	1:A:216:ASN:C	2.71	0.42
1:A:276:ASP:C	1:A:276:ASP:OD2	2.57	0.42
2:B:156:PHE:CE2	2:B:162:VAL:HA	2.53	0.42
2:B:175:ILE:HG13	2:B:180:MET:HE1	2.00	0.42
1:A:229:TYR:CA	1:A:269:LEU:HD21	2.49	0.42
1:A:250:ILE:HD12	1:A:250:ILE:H	1.84	0.42
1:A:45:ARG:HB3	1:A:58:MET:SD	2.59	0.42
1:A:158:HIS:CE1	1:A:220:ASP:HB2	2.54	0.42
1:A:42:GLN:O	1:A:63:LYS:HG3	2.19	0.42
2:B:212:THR:HG22	2:B:213:VAL:N	2.34	0.42
2:B:87:PRO:HD2	2:B:89:VAL:HG22	2.01	0.42
1:A:102:PHE:N	1:A:102:PHE:CD1	2.87	0.42
1:A:229:TYR:CD1	1:A:229:TYR:C	2.92	0.42
1:A:258:PRO:HD2	1:A:261:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:HB3	1:A:266:LYS:HG3	2.00	0.42
1:A:344:GLY:O	1:A:348:THR:N	2.46	0.42
1:A:149:GLN:NE2	1:A:179:TYR:CD1	2.87	0.42
2:B:113:ARG:NH2	2:B:149:ASP:OD2	2.52	0.42
1:A:190:ARG:NH1	1:A:192:LYS:HZ3	2.18	0.42
1:A:269:LEU:O	1:A:273:LEU:HB2	2.20	0.42
2:B:124:ALA:O	2:B:127:ALA:HB3	2.19	0.42
1:A:267:ASP:O	1:A:268:LEU:C	2.57	0.42
1:A:228:ILE:HG22	1:A:229:TYR:N	2.35	0.42
1:A:225:GLY:O	1:A:226:VAL:C	2.57	0.41
2:B:163:ILE:HB	2:B:209:ARG:NE	2.30	0.41
1:A:161:ASP:HA	1:A:217:LYS:HZ3	1.84	0.41
1:A:45:ARG:HD3	1:A:58:MET:SD	2.60	0.41
2:B:164:GLN:HE21	2:B:164:GLN:HB3	1.69	0.41
2:B:85:PRO:CD	2:B:87:PRO:HD3	2.50	0.41
1:A:343:CYS:HB3	1:A:346:GLU:OE1	2.21	0.41
1:A:134:ARG:HH11	1:A:134:ARG:HB2	1.86	0.41
1:A:347:PHE:O	1:A:350:PHE:N	2.43	0.41
2:B:171:ASN:HA	2:B:224:ILE:O	2.19	0.41
1:A:100:PHE:CD1	1:A:101:PRO:CD	3.04	0.41
1:A:132:LEU:HD12	1:A:137:ARG:HA	2.03	0.41
1:A:247:TYR:O	1:A:251:VAL:HG12	2.21	0.41
1:A:45:ARG:NE	1:A:335:ILE:HG13	2.35	0.41
1:A:180:ILE:CG2	1:A:181:GLN:N	2.81	0.41
1:A:242:GLN:CB	1:A:245:GLN:OE1	2.68	0.41
2:B:130:ILE:HD13	2:B:136:PHE:CD1	2.56	0.41
2:B:181:ASP:OD1	2:B:216:LYS:HE2	2.20	0.41
1:A:125:GLY:O	1:A:131:HIS:NE2	2.50	0.41
1:A:157:LEU:O	1:A:162:LEU:HB2	2.20	0.41
1:A:177:GLN:HG2	1:A:177:GLN:O	2.21	0.41
1:A:228:ILE:HA	1:A:231:MET:HE2	2.03	0.41
1:A:271:ASN:HD22	1:A:271:ASN:HA	1.63	0.41
1:A:116:LEU:HD13	1:A:350:PHE:CE2	2.56	0.41
1:A:96:GLN:HB2	1:A:96:GLN:HE21	1.60	0.41
2:B:221:LEU:N	2:B:221:LEU:CD1	2.84	0.41
1:A:168:LYS:CE	1:A:171:ASN:ND2	2.80	0.41
1:A:326:ASN:OD1	1:A:326:ASN:N	2.53	0.41
2:B:85:PRO:HD2	2:B:87:PRO:CD	2.50	0.41
1:A:100:PHE:CD1	1:A:101:PRO:HD2	2.56	0.40
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.72	0.40
2:B:219:VAL:HG11	2:B:221:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:O	1:A:311:GLU:C	2.58	0.40
1:A:41:ASP:O	1:A:63:LYS:CE	2.70	0.40
2:B:199:GLY:C	2:B:201:LEU:N	2.73	0.40
2:B:163:ILE:HD12	2:B:209:ARG:NE	2.36	0.40
1:A:100:PHE:CE2	1:A:153:THR:HA	2.56	0.40
1:A:41:ASP:O	1:A:63:LYS:HE3	2.21	0.40
1:A:228:ILE:HD13	1:A:296:TRP:HZ3	1.87	0.40
2:B:168:GLU:O	2:B:169:GLY:O	2.39	0.40
1:A:332:GLU:N	1:A:332:GLU:CD	2.72	0.40
2:B:84:PRO:HB3	2:B:89:VAL:CG2	2.52	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	339/345 (98%)	262 (77%)	62 (18%)	15 (4%)	3	20
2	B	158/160 (99%)	124 (78%)	22 (14%)	12 (8%)	1	9
All	All	497/505 (98%)	386 (78%)	84 (17%)	27 (5%)	2	15

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	8	LYS
1	A	186	GLY
1	A	298	ALA
2	B	86	ASN
2	B	87	PRO
2	B	117	PRO
2	B	170	ASP

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Mol	Chain	Res	Type
2	B	200	GLU
2	B	206	GLY
1	A	202	PRO
1	A	296	TRP
1	A	343	CYS
2	B	169	GLY
2	B	203	LEU
2	B	85	PRO
2	B	216	LYS
1	A	244	ILE
2	B	205	TYR
1	A	165	ARG
2	B	88	VAL
1	A	284	LEU
1	A	243	PRO
1	A	226	VAL
1	A	258	PRO
1	A	207	PRO
1	A	141	PRO

### 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	281/300 (94%)	248 (88%)	33 (12%)	6	27
2	B	121/132 (92%)	109 (90%)	12 (10%)	9	34
All	All	402/432 (93%)	357 (89%)	45 (11%)	7	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	42	GLN
1	A	54	PHE
1	A	92	LYS

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Mol	Chain	Res	Type
1	A	95	LEU
1	A	96	GLN
1	A	102	PHE
1	A	106	LEU
1	A	110	PHE
1	A	115	ASN
1	A	119	VAL
1	A	135	ILE
1	A	176	GLN
1	A	183	THR
1	A	189	LYS
1	A	202	PRO
1	A	212	SER
1	A	216	ASN
1	A	217	LYS
1	A	227	LEU
1	A	239	PHE
1	A	268	LEU
1	A	277	LEU
1	A	279	LYS
1	A	286	ASN
1	A	290	ASP
1	A	299	THR
1	A	313	PRO
1	A	318	PHE
1	A	326	ASN
1	A	332	GLU
1	A	336	ARG
1	A	348	THR
2	B	85	PRO
2	B	87	PRO
2	B	117	PRO
2	B	119	ASP
2	B	134	VAL
2	B	139	LEU
2	B	164	GLN
2	B	183	TYR
2	B	200	GLU
2	B	203	LEU
2	B	207	THR
2	B	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	39	GLN
1	A	67	ASN
1	A	87	HIS
1	A	90	ASN
1	A	96	GLN
1	A	149	GLN
1	A	181	GLN
1	A	216	ASN
1	A	242	GLN
1	A	271	ASN
1	A	274	GLN
1	A	307	GLN
2	B	164	GLN
2	B	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SEP	A	10	1	9,9,10	0.88	0	9,12,14	1.28	1 (11%)
1	SEP	A	139	1	9,9,10	0.84	0	9,12,14	1.13	0
1	TPO	A	197	1	9,10,11	0.86	0	10,14,16	1.16	0
1	SEP	A	338	1	9,9,10	0.95	1 (11%)	9,12,14	1.22	1 (11%)

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
1	SEP	A	10	1	-	0/5/8/10	0/0/0/0
1	SEP	A	139	1	-	0/5/8/10	0/0/0/0
1	TPO	A	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	CA-C	2.14	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SEP	OG-CB-CA	2.82	110.94	108.17
1	A	10	SEP	OG-CB-CA	2.92	111.05	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	SEP	2	0
1	A	139	SEP	1	0
1	A	197	TPO	1	0
1	A	338	SEP	6	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	ANP	A	400	4	29,33,33	1.53	3 (10%)	28,52,52	1.30	1 (3%)
5	GOL	B	1	-	5,5,5	4.83	5 (100%)	5,5,5	5.49	3 (60%)

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
3	ANP	A	400	4	-	0/13/38/38	0/3/3/3
5	GOL	B	1	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	GOL	C3-C2	-8.28	1.21	1.52
5	B	1	GOL	C1-C2	-3.07	1.40	1.52
3	A	400	ANP	PB-O2B	-2.88	1.48	1.56
5	B	1	GOL	O2-C2	-2.72	1.35	1.43
3	A	400	ANP	PB-O1B	2.98	1.49	1.46
5	B	1	GOL	O3-C3	3.27	1.56	1.42
5	B	1	GOL	O1-C1	4.51	1.61	1.42
3	A	400	ANP	PG-O1G	6.13	1.53	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ANP	PA-O3A-PB	-5.61	112.56	132.38
5	B	1	GOL	O1-C1-C2	3.26	126.51	110.07
5	B	1	GOL	O2-C2-C3	6.32	138.69	108.84
5	B	1	GOL	O3-C3-C2	9.98	160.35	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	ANP	4	0
5	B	1	GOL	1	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	341/345 (98%)	-0.67	1 (0%) 93 93	2, 29, 61, 81	0
2	B	160/160 (100%)	-0.75	1 (0%) 89 88	4, 24, 56, 74	0
All	All	501/505 (99%)	-0.69	2 (0%) 92 92	2, 27, 61, 81	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	3.7
2	B	84	PRO	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	338	10/11	0.87	0.13	-	60,63,64,65	0
1	TPO	A	197	11/12	0.96	0.16	-	20,22,23,23	0
1	SEP	A	139	10/11	0.91	0.10	-	32,37,40,41	0
1	SEP	A	10	10/11	0.84	0.15	-	66,71,77,77	0

### 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(Å <sup>2</sup> )	Q<0.9
5	GOL	B	1	6/6	0.88	0.37	7.69	54,55,56,57	0
3	ANP	A	400	31/31	0.93	0.19	0.96	17,28,33,33	0
4	MN	A	401	1/1	0.92	0.17	-	18,18,18,18	0
4	MN	A	402	1/1	0.94	0.12	-	7,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.