



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:51 PM GMT

PDB ID : 2ACX  
Title : Crystal Structure of G protein coupled receptor kinase 6 bound to AMPPNP  
Authors : Lodowski, D.T.; Tesmer, V.M.; Benovic, J.L.; Tesmer, J.J.  
Deposited on : 2005-07-19  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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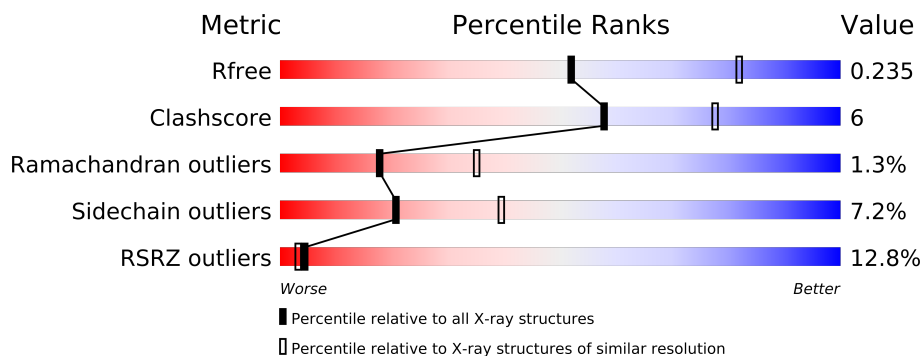
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogen and 0 are deuterium.

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 G protein-coupled receptor kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			4011	2548	714	721	28			
1	B	492	Total	C	N	O	S	0	0	0
			3984	2535	705	717	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	GLN	SEE REMARK 999	UNP P43250
A	104	ASN	GLN	SEE REMARK 999	UNP P43250
A	561	SER	CYS	ENGINEERED	UNP P43250
A	562	SER	CYS	ENGINEERED	UNP P43250
A	565	SER	CYS	ENGINEERED	UNP P43250
B	60	ASN	GLN	SEE REMARK 999	UNP P43250
B	104	ASN	GLN	SEE REMARK 999	UNP P43250
B	561	SER	CYS	ENGINEERED	UNP P43250
B	562	SER	CYS	ENGINEERED	UNP P43250
B	565	SER	CYS	ENGINEERED	UNP P43250

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

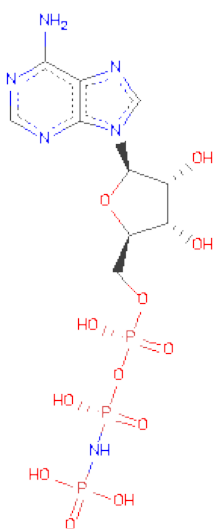
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

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

- Molecule 5 is water.

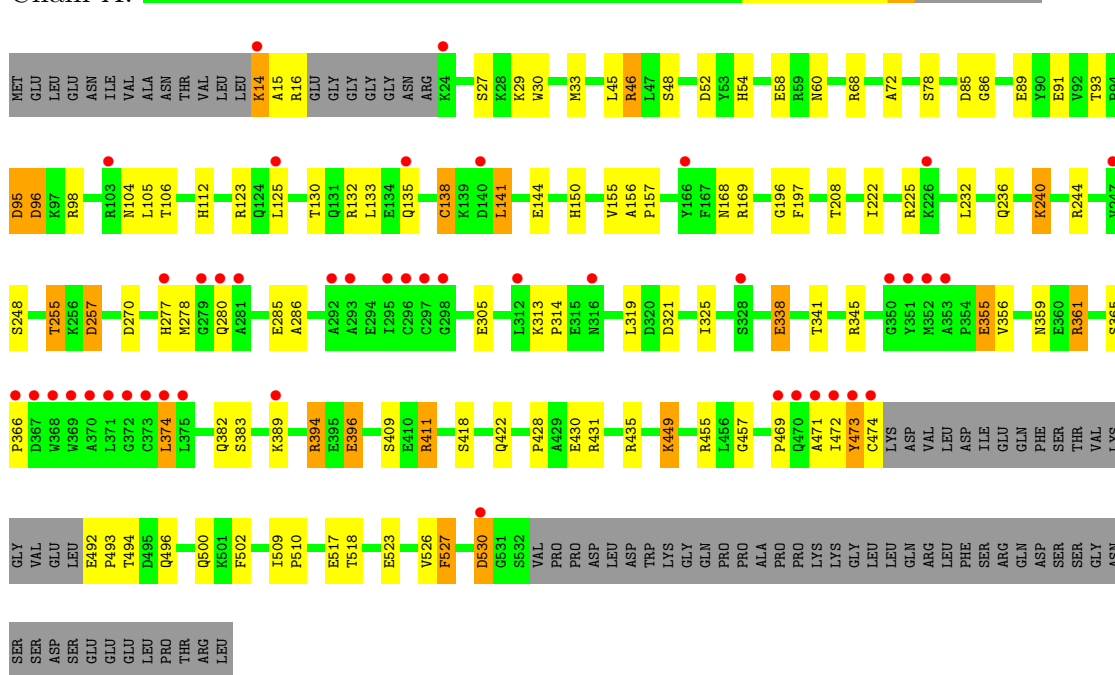
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	7	Total	O	0	0
			7	7		

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

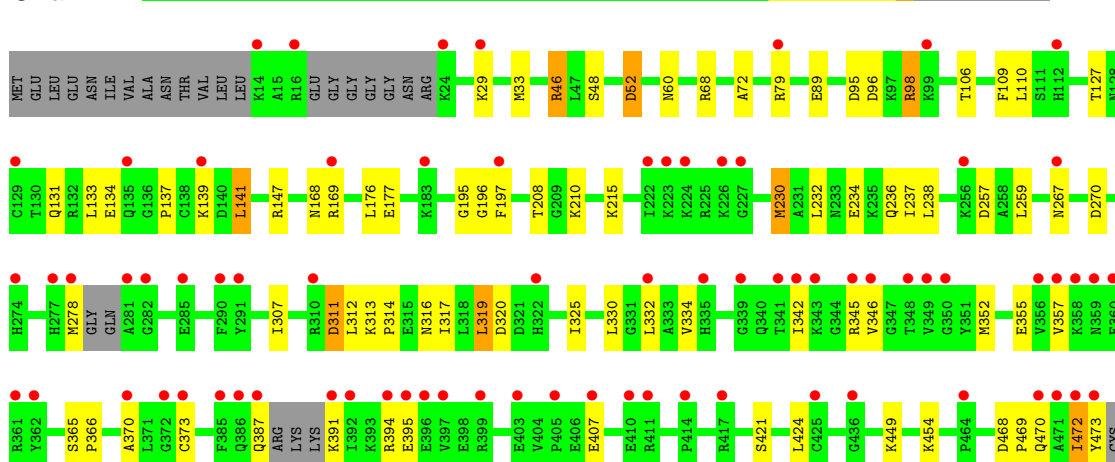
- Molecule 1: G protein-coupled receptor kinase 6

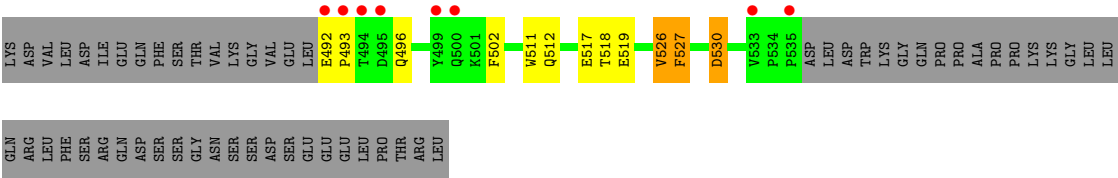
Chain A:



- Molecule 1: G protein-coupled receptor kinase 6

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.16Å 59.27Å 221.09Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.60) 97.3 (30.00-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.202 , 0.243 0.200 , 0.235	Depositor DCC
$R_{free}$ test set	2316 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 45983 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ANP, MG

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	1.06	4/4101 (0.1%)	1.02	15/5521 (0.3%)
1	B	0.74	0/4074	0.87	7/5488 (0.1%)
All	All	0.92	4/8175 (0.0%)	0.95	22/11009 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLU	CD-OE2	6.82	1.33	1.25
1	A	517	GLU	CD-OE1	6.80	1.33	1.25
1	A	91	GLU	CD-OE2	5.24	1.31	1.25
1	A	240	LYS	CD-CE	5.14	1.64	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	A	96	ASP	CB-CG-OD2	9.15	126.54	118.30
1	B	96	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	394	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	270	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	52	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	52	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	431	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	523	GLU	OE1-CD-OE2	5.92	130.41	123.30
1	A	257	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	95	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	68	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	530	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	468	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	270	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	230	MET	CG-SD-CE	5.25	108.60	100.20
1	A	449	LYS	CB-CA-C	-5.25	99.91	110.40
1	A	355	GLU	CB-CA-C	-5.21	99.99	110.40
1	A	455	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	311	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	321	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4011	0	4008	59	0
1	B	3984	0	3974	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	2	0
5	A	30	0	0	2	0
5	B	7	0	0	0	0
All	All	8106	0	8008	102	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (102) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:132:ARG:NH2	1:A:138:CYS:SG	2.42	0.93
1:A:319:LEU:CD2	1:A:325:ILE:HG22	2.00	0.92
1:B:133:LEU:HB2	1:B:141:LEU:HD21	1.57	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:319:LEU:HD22	1:B:325:ILE:HG22	1.58	0.84
1:A:133:LEU:HB2	1:A:141:LEU:HD21	1.66	0.75
1:A:150:HIS:ND1	5:A:592:HOH:O	2.20	0.74
1:B:106:THR:HG22	1:B:110:LEU:HD12	1.72	0.71
1:A:325:ILE:C	1:A:325:ILE:HD12	2.11	0.71
1:A:255:THR:HG22	1:A:257:ASP:H	1.58	0.69
1:A:68:ARG:NH2	1:A:85:ASP:OD1	2.28	0.67
1:A:314:PRO:HG3	1:A:374:LEU:HD13	1.78	0.65
1:A:319:LEU:HD22	1:A:325:ILE:HG22	1.78	0.64
1:B:127:THR:HG22	1:B:131:GLN:HE22	1.64	0.62
1:B:334:VAL:HG11	1:B:342:ILE:HD13	1.81	0.61
1:A:319:LEU:HD23	1:A:325:ILE:HG22	1.81	0.60
1:A:530:ASP:HB3	1:B:72:ALA:CB	2.31	0.60
1:A:30:TRP:HA	1:A:33:MET:HE3	1.83	0.60
1:B:325:ILE:HD12	1:B:325:ILE:C	2.21	0.59
1:A:473:TYR:N	1:A:473:TYR:HD2	2.00	0.59
1:B:127:THR:CG2	1:B:131:GLN:HE22	2.17	0.57
1:A:473:TYR:CD2	1:A:473:TYR:N	2.72	0.57
1:A:155:VAL:HG12	1:A:156:ALA:N	2.20	0.56
1:A:132:ARG:CZ	1:A:138:CYS:SG	2.94	0.55
1:B:232:LEU:HD11	1:B:236:GLN:NE2	2.22	0.55
1:A:255:THR:HG22	1:A:257:ASP:N	2.21	0.55
1:A:197:PHE:CD2	1:A:222:ILE:HD13	2.43	0.54
1:B:387:GLN:O	1:B:391:LYS:NZ	2.36	0.53
1:A:30:TRP:HA	1:A:33:MET:CE	2.39	0.52
1:A:54:HIS:ND1	1:A:58:GLU:OE1	2.38	0.52
1:B:320:ASP:OD1	1:B:320:ASP:C	2.48	0.52
1:A:383:SER:OG	5:A:604:HOH:O	2.19	0.51
1:B:313:LYS:HB2	1:B:314:PRO:HD2	1.94	0.50
1:A:14:LYS:HG3	1:A:29:LYS:HE3	1.94	0.50
1:B:352:MET:CE	1:B:357:VAL:HG12	2.41	0.50
1:A:45:LEU:O	1:A:46:ARG:C	2.49	0.50
1:B:352:MET:HE2	1:B:357:VAL:HG12	1.93	0.49
1:B:526:VAL:HG22	1:B:527:PHE:H	1.77	0.49
1:B:98:ARG:HD2	1:B:137:PRO:O	2.13	0.49
1:A:365:SER:OG	1:A:366:PRO:HD3	2.12	0.48
4:B:577:ANP:O2G	4:B:577:ANP:O3A	2.31	0.48
1:A:418:SER:O	1:A:422:GLN:HG3	2.13	0.48
1:B:259:LEU:HB3	1:B:502:PHE:CE2	2.48	0.48
1:A:244:ARG:HD2	1:A:457:GLY:O	2.13	0.48
1:A:527:PHE:CD1	1:A:527:PHE:C	2.87	0.48
1:B:60:ASN:HB3	1:B:512:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ASN:ND2	1:B:168:ASN:OD1	2.47	0.47
1:A:492:GLU:N	1:A:493:PRO:CD	2.77	0.47
1:B:139:LYS:HD2	1:B:454:LYS:NZ	2.29	0.47
1:B:208:THR:HB	1:B:518:THR:HG21	1.97	0.47
1:A:197:PHE:CE2	1:A:222:ILE:HD13	2.49	0.47
1:B:237:ILE:HG23	1:B:307:ILE:HD13	1.97	0.47
1:A:355:GLU:CG	1:A:428:PRO:HG3	2.45	0.47
1:A:530:ASP:HB3	1:B:72:ALA:HB3	1.96	0.47
1:B:492:GLU:N	1:B:493:PRO:CD	2.77	0.47
1:A:86:GLY:HA3	1:A:105:LEU:HD21	1.97	0.46
1:B:215:LYS:NZ	1:B:234:GLU:OE2	2.44	0.46
1:A:509:ILE:HB	1:A:510:PRO:HD3	1.98	0.46
1:B:373:CYS:SG	1:B:424:LEU:HD21	2.56	0.46
1:A:45:LEU:O	1:A:46:ARG:O	2.34	0.45
1:B:29:LYS:O	1:B:33:MET:HG3	2.16	0.45
1:A:341:THR:OG1	1:A:361:ARG:HD3	2.16	0.45
1:A:502:PHE:CD2	1:A:502:PHE:C	2.90	0.45
1:A:72:ALA:HB1	1:B:530:ASP:HB3	1.99	0.45
1:B:177:GLU:HB2	1:B:511:TRP:CZ3	2.52	0.45
1:B:238:LEU:HD21	1:B:330:LEU:HD13	1.98	0.45
1:A:409:SER:C	1:A:411:ARG:H	2.21	0.44
1:B:311:ASP:OD2	1:B:316:ASN:ND2	2.50	0.44
1:A:208:THR:HB	1:A:518:THR:HG21	2.00	0.44
1:B:210:LYS:NZ	1:B:517:GLU:OE1	2.33	0.44
1:A:355:GLU:HG3	1:A:428:PRO:HG3	2.00	0.43
1:A:72:ALA:CB	1:B:530:ASP:HB3	2.48	0.43
1:B:526:VAL:HG22	1:B:527:PHE:N	2.33	0.43
1:B:109:PHE:O	1:B:110:LEU:HD23	2.18	0.43
1:B:334:VAL:HG11	1:B:342:ILE:CD1	2.47	0.43
1:B:215:LYS:NZ	4:B:577:ANP:O2B	2.52	0.43
1:A:345:ARG:HG2	1:A:356:VAL:O	2.18	0.43
1:A:365:SER:N	1:A:366:PRO:CD	2.82	0.43
1:A:313:LYS:HB2	1:A:314:PRO:CD	2.49	0.42
1:A:15:ALA:O	1:A:16:ARG:HG3	2.20	0.42
1:B:267:ASN:HD21	1:B:472:ILE:HD12	1.83	0.42
1:A:285:GLU:O	1:A:286:ALA:C	2.56	0.42
1:A:240:LYS:HE2	1:A:305:GLU:HB3	2.01	0.42
1:A:125:LEU:HD21	1:A:144:GLU:HG3	2.01	0.42
1:B:518:THR:O	1:B:519:GLU:HB2	2.18	0.42
1:B:168:ASN:HD22	1:B:168:ASN:N	2.17	0.42
1:A:144:GLU:HA	1:A:144:GLU:OE1	2.20	0.42
1:B:195:GLY:O	1:B:197:PHE:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:312:LEU:HB3	1:B:370:ALA:CB	2.51	0.41
1:A:325:ILE:O	1:A:325:ILE:HD12	2.21	0.41
1:A:95:ASP:OD1	1:A:98:ARG:NH2	2.53	0.41
1:B:139:LYS:HD2	1:B:454:LYS:HZ2	1.84	0.41
1:A:93:THR:HB	1:A:98:ARG:HG3	2.03	0.41
1:A:430:GLU:O	1:A:435:ARG:NH1	2.54	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.91	0.41
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.20	0.41
1:A:156:ALA:HB3	1:A:157:PRO:HD3	2.03	0.41
1:A:338:GLU:H	1:A:338:GLU:HG2	1.68	0.41
1:B:311:ASP:HB2	1:B:332:LEU:HD12	2.04	0.40
1:A:89:GLU:O	1:A:93:THR:OG1	2.38	0.40
1:A:232:LEU:HD11	1:A:236:GLN:NE2	2.37	0.40
1:B:330:LEU:N	1:B:330:LEU:HD12	2.36	0.40
1:B:365:SER:N	1:B:366:PRO:CD	2.84	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	489/576 (85%)	458 (94%)	24 (5%)	7 (1%)	16	32
1	B	482/576 (84%)	459 (95%)	17 (4%)	6 (1%)	19	39
All	All	971/1152 (84%)	917 (94%)	41 (4%)	13 (1%)	18	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	449	LYS
1	A	526	VAL
1	B	141	LEU
1	B	196	GLY

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Mol	Chain	Res	Type
1	B	449	LYS
1	A	46	ARG
1	B	46	ARG
1	B	526	VAL
1	A	471	ALA
1	A	196	GLY
1	A	469	PRO
1	B	469	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	432/503 (86%)	398 (92%)	34 (8%)	18	34
1	B	430/503 (86%)	402 (94%)	28 (6%)	24	46
All	All	862/1006 (86%)	800 (93%)	62 (7%)	21	39

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	27	SER
1	A	48	SER
1	A	60	ASN
1	A	78	SER
1	A	96	ASP
1	A	104	ASN
1	A	106	THR
1	A	112	HIS
1	A	123	ARG
1	A	130	THR
1	A	135	GLN
1	A	138	CYS
1	A	169	ARG
1	A	248	SER
1	A	255	THR
1	A	277	HIS

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Mol	Chain	Res	Type
1	A	278	MET
1	A	280	GLN
1	A	359	ASN
1	A	361	ARG
1	A	374	LEU
1	A	382	GLN
1	A	389	LYS
1	A	394	ARG
1	A	396	GLU
1	A	411	ARG
1	A	472	ILE
1	A	473	TYR
1	A	474	CYS
1	A	494	THR
1	A	496	GLN
1	A	500	GLN
1	A	527	PHE
1	B	46	ARG
1	B	48	SER
1	B	52	ASP
1	B	79	ARG
1	B	89	GLU
1	B	95	ASP
1	B	98	ARG
1	B	134	GLU
1	B	147	ARG
1	B	169	ARG
1	B	230	MET
1	B	257	ASP
1	B	278	MET
1	B	317	ILE
1	B	319	LEU
1	B	345	ARG
1	B	346	VAL
1	B	355	GLU
1	B	394	ARG
1	B	395	GLU
1	B	407	GLU
1	B	421	SER
1	B	470	GLN
1	B	472	ILE
1	B	473	TYR

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Mol	Chain	Res	Type
1	B	496	GLN
1	B	527	PHE
1	B	530	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	168	ASN
1	A	335	HIS
1	A	359	ASN
1	A	387	GLN
1	A	513	ASN
1	B	108	ASN
1	B	131	GLN
1	B	168	ASN
1	B	387	GLN
1	B	500	GLN
1	B	513	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	ANP	A	577	2	33,33,33	3.54	8 (24%)	51,52,52	2.51	15 (29%)
3	PO4	A	579	-	4,4,4	0.27	0	6,6,6	0.37	0
4	ANP	B	577	2	33,33,33	3.31	7 (21%)	51,52,52	2.42	14 (27%)
3	PO4	B	579	-	4,4,4	0.32	0	6,6,6	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	577	2	-	1/18/38/38	0/1/3/3
3	PO4	A	579	-	-	0/0/0/0	0/0/0/0
4	ANP	B	577	2	-	0/18/38/38	0/1/3/3
3	PO4	B	579	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	577	ANP	PG-N3B	12.66	1.75	1.64
4	B	577	ANP	PG-N3B	12.65	1.75	1.64
4	B	577	ANP	PB-N3B	11.47	1.74	1.64
4	A	577	ANP	PB-N3B	11.36	1.74	1.64
4	A	577	ANP	PG-O1G	5.63	1.53	1.46
4	A	577	ANP	PB-O1B	5.14	1.52	1.46
4	A	577	ANP	PB-O3A	5.12	1.66	1.59
4	B	577	ANP	PG-O1G	4.65	1.51	1.46
4	B	577	ANP	PB-O1B	3.67	1.50	1.46
4	A	577	ANP	C4-N9	-3.21	1.33	1.37
4	B	577	ANP	C5-C4	2.52	1.46	1.40
4	B	577	ANP	PB-O3A	2.32	1.62	1.59
4	A	577	ANP	C2'-C1'	-2.31	1.50	1.53
4	A	577	ANP	PA-O3A	2.21	1.63	1.59
4	B	577	ANP	C4-N9	-2.00	1.34	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	577	ANP	N3-C2-N1	-10.21	120.18	128.71
4	B	577	ANP	PB-N3B-PG	-8.36	116.00	130.07
4	B	577	ANP	N3-C2-N1	-7.36	122.55	128.71
4	A	577	ANP	PB-N3B-PG	-6.45	119.22	130.07
4	B	577	ANP	N3-C4-N9	5.95	136.18	125.43
4	A	577	ANP	N3-C4-N9	5.33	135.06	125.43
4	A	577	ANP	O1B-PB-N3B	-4.69	104.75	111.83
4	B	577	ANP	O1G-PG-N3B	-4.36	105.24	111.83
4	A	577	ANP	C8-N9-C4	4.27	110.16	106.90
4	B	577	ANP	O4'-C1'-N9	3.99	112.15	108.44
4	A	577	ANP	O3G-PG-O2G	3.64	118.11	107.66
4	B	577	ANP	C5-C4-N3	-3.60	117.87	125.70
4	B	577	ANP	O2B-PB-O1B	3.32	117.56	109.89
4	B	577	ANP	C4-C5-N7	-3.29	106.70	109.52
4	B	577	ANP	C2-N3-C4	3.13	122.91	114.01
4	A	577	ANP	O2G-PG-N3B	-2.96	98.56	106.61
4	A	577	ANP	C2-N3-C4	2.83	122.05	114.01
4	B	577	ANP	O1B-PB-N3B	-2.72	107.72	111.83
4	A	577	ANP	C5-C4-N3	-2.70	119.82	125.70
4	B	577	ANP	C3'-C2'-C1'	2.59	104.97	100.91
4	B	577	ANP	PA-O3A-PB	-2.58	122.98	131.81
4	B	577	ANP	O3G-PG-O2G	2.57	115.03	107.66
4	A	577	ANP	C4-C5-N7	-2.52	107.36	109.52
4	A	577	ANP	C2-N1-C6	2.50	123.29	118.77
4	A	577	ANP	O3'-C3'-C2'	-2.35	104.18	111.83
4	A	577	ANP	O2'-C2'-C3'	-2.14	104.87	111.83
4	B	577	ANP	C8-N9-C4	2.12	108.52	106.90
4	A	577	ANP	O2A-PA-O5'	-2.08	98.01	108.51
4	A	577	ANP	C1'-N9-C4	-2.05	123.09	126.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	577	ANP	O1G-PG-N3B-PB

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	495/576 (85%)	0.66	44 (8%) <b>10</b> <b>7</b>	56, 67, 85, 106	0
1	B	492/576 (85%)	0.99	83 (16%) <b>2</b> <b>1</b>	58, 68, 85, 111	0
All	All	987/1152 (85%)	0.82	127 (12%) <b>4</b> <b>3</b>	56, 68, 85, 111	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	7.7
1	A	474	CYS	6.0
1	B	397	VAL	5.3
1	B	135	GLN	5.3
1	A	125	LEU	4.9
1	B	494	THR	4.7
1	B	349	VAL	4.7
1	B	470	GLN	4.6
1	A	473	TYR	4.6
1	B	277	HIS	4.5
1	B	385	PHE	4.3
1	B	342	ILE	4.3
1	B	386	GLN	4.1
1	B	345	ARG	4.0
1	B	392	ILE	3.9
1	B	391	LYS	3.8
1	B	14	LYS	3.8
1	B	394	ARG	3.7
1	B	387	GLN	3.7
1	B	139	LYS	3.7
1	A	371	LEU	3.7
1	A	370	ALA	3.7
1	A	373	CYS	3.6
1	B	278	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	472	ILE	3.5
1	B	403	GLU	3.4
1	A	530	ASP	3.4
1	B	356	VAL	3.4
1	A	471	ALA	3.3
1	A	469	PRO	3.3
1	B	360	GLU	3.3
1	B	500	GLN	3.3
1	A	470	GLN	3.3
1	A	135	GLN	3.2
1	B	535	PRO	3.2
1	B	267	ASN	3.2
1	B	407	GLU	3.2
1	B	24	LYS	3.0
1	B	493	PRO	3.0
1	B	223	LYS	3.0
1	A	372	GLY	3.0
1	B	285	GLU	3.0
1	A	296	CYS	3.0
1	B	414	PRO	2.9
1	A	140	ASP	2.9
1	A	295	ILE	2.9
1	B	222	ILE	2.9
1	B	361	ARG	2.9
1	B	472	ILE	2.9
1	B	197	PHE	2.9
1	A	369	TRP	2.9
1	B	79	ARG	2.8
1	A	312	LEU	2.8
1	B	112	HIS	2.8
1	B	373	CYS	2.8
1	A	24	LYS	2.7
1	B	227	GLY	2.7
1	A	374	LEU	2.7
1	B	226	LYS	2.7
1	B	464	PRO	2.7
1	B	396	GLU	2.7
1	A	375	LEU	2.7
1	A	292	ALA	2.7
1	B	339	GLY	2.6
1	B	471	ALA	2.6
1	B	16	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	166	TYR	2.6
1	A	281	ALA	2.6
1	B	348	THR	2.5
1	A	280	GLN	2.5
1	A	368	TRP	2.5
1	A	277	HIS	2.5
1	B	399	ARG	2.5
1	B	281	ALA	2.5
1	B	357	VAL	2.5
1	A	389	LYS	2.5
1	B	183	LYS	2.5
1	A	103	ARG	2.5
1	B	291	TYR	2.4
1	B	224	LYS	2.4
1	B	256	LYS	2.4
1	B	358	LYS	2.4
1	B	129	CYS	2.4
1	A	353	ALA	2.4
1	B	533	VAL	2.4
1	A	367	ASP	2.4
1	B	332	LEU	2.4
1	B	495	ASP	2.4
1	A	293	ALA	2.3
1	B	425	CYS	2.3
1	B	335	HIS	2.3
1	B	99	LYS	2.3
1	B	492	GLU	2.3
1	A	279	GLY	2.3
1	A	366	PRO	2.3
1	A	351	TYR	2.3
1	B	343	LYS	2.3
1	B	346	VAL	2.2
1	B	169	ARG	2.2
1	A	352	MET	2.2
1	A	316	ASN	2.2
1	A	226	LYS	2.2
1	A	328	SER	2.2
1	B	362	TYR	2.2
1	A	297	CYS	2.2
1	B	290	PHE	2.2
1	A	14	LYS	2.2
1	B	341	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	436	GLY	2.1
1	B	359	ASN	2.1
1	A	298	GLY	2.1
1	B	395	GLU	2.1
1	A	350	GLY	2.1
1	B	322	HIS	2.1
1	B	411	ARG	2.1
1	B	499	TYR	2.1
1	B	282	GLY	2.1
1	B	372	GLY	2.1
1	B	370	ALA	2.0
1	B	350	GLY	2.0
1	A	247	VAL	2.0
1	B	410	GLU	2.0
1	B	417	ARG	2.0
1	B	274	HIS	2.0
1	B	310	ARG	2.0
1	B	29	LYS	2.0
1	B	405	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	578	1/1	0.27	-0.02	87,87,87,87	0
2	MG	A	578	1/1	0.21	-0.37	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ANP	B	577	31/31	0.16	-0.91	60,63,92,93	0
3	PO4	A	579	5/5	0.14	-0.94	83,83,87,87	0
3	PO4	B	579	5/5	0.16	-1.30	91,93,95,97	0
4	ANP	A	577	31/31	0.18	-1.32	60,65,103,105	0

## 6.5 Other polymers

There are no such residues in this entry.