



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 05:09 PM EDT

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 : unknown  
Resolution : 2.60 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 : rb-20030345  
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) : rb-20030345

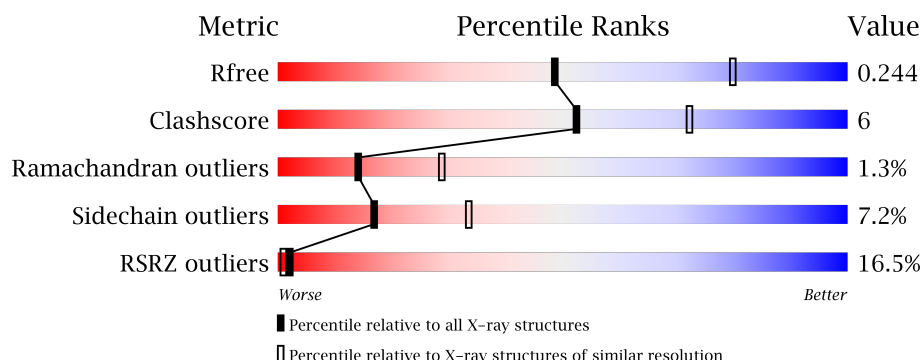
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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. 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	576	<div> <div>8%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	576	<div> <div>20%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8106 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 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			

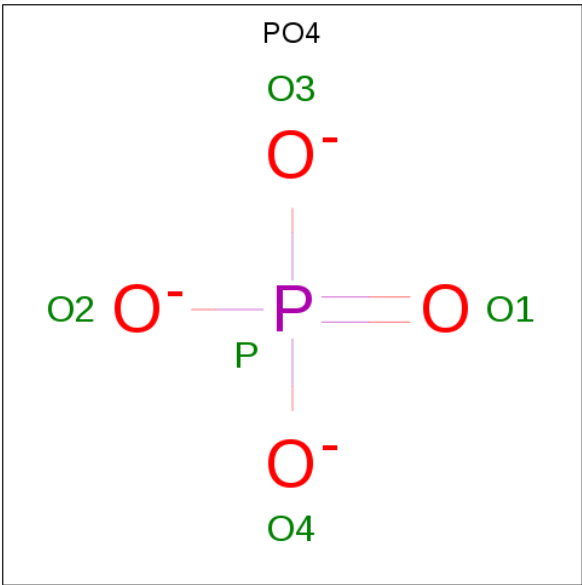
There are 10 discrepancies between the modelled and reference sequences:

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).

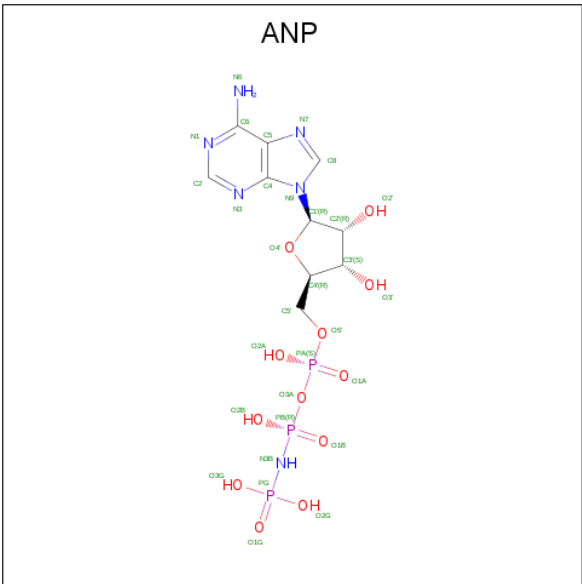
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- 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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

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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		

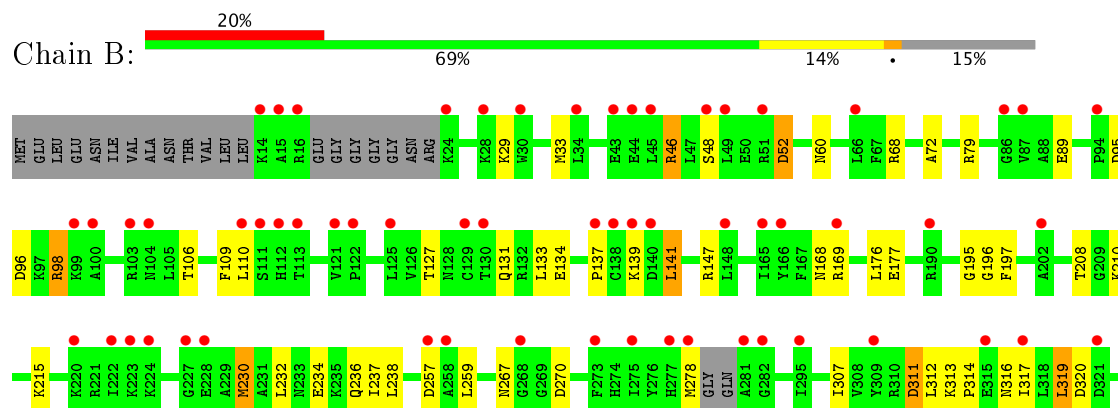
### 3 Residue-property plots [i](#)

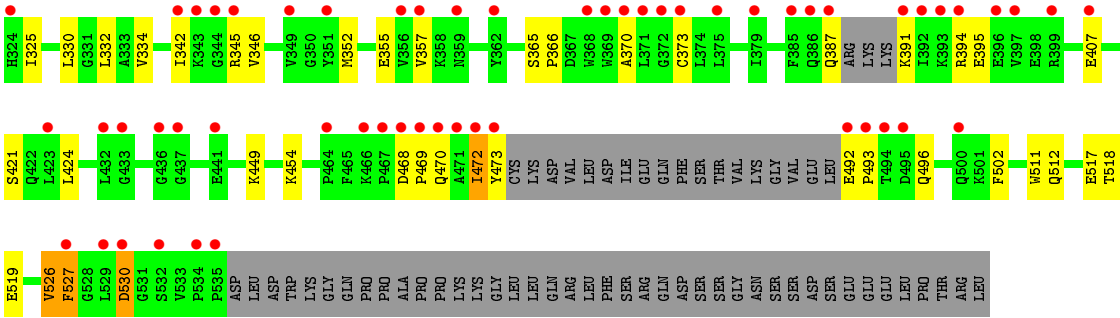
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: G protein-coupled receptor kinase 6



- Molecule 1: G protein-coupled receptor kinase 6





## 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 0.208 , 0.244	Depositor DCC
$R_{free}$ test set	2317 reflections (5.31%)	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> )	0.30 , 81.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	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.

<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: 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 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	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

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 6.

All (102) 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: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	Interatomic distance (Å)	Clash overlap (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:C	1:B:325:ILE:HD12	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:A:14:LYS:HG3	1:A:29:LYS:HE3	1.94	0.50
1:A:45:LEU:O	1:A:46:ARG:C	2.49	0.50
1:B:313:LYS:HB2	1:B:314:PRO:HD2	1.94	0.50
1:B:352:MET:CE	1:B:357:VAL:HG12	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASN:HB3	1:B:512:GLN:OE1	2.14	0.48
1:A:492:GLU:N	1:A:493:PRO:CD	2.77	0.47
1:A:168:ASN:ND2	1:B:168:ASN:OD1	2.47	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:238:LEU:HD21	1:B:330:LEU:HD13	1.98	0.45
1:B:177:GLU:HB2	1:B:511:TRP:CZ3	2.52	0.45
1:A:208:THR:HB	1:A:518:THR:HG21	2.00	0.44
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: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:A:285:GLU:O	1:A:286:ALA:C	2.56	0.42
1:B:267:ASN:HD21	1:B:472:ILE:HD12	1.83	0.42
1:A:125:LEU:HD21	1:A:144:GLU:HG3	2.01	0.42
1:A:240:LYS:HE2	1:A:305:GLU:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:396:GLU:HA	1:A:396:GLU:OE1	2.20	0.41
1:A:430:GLU:O	1:A:435:ARG:NH1	2.54	0.41
1:A:93:THR:HB	1:A:98:ARG:HG3	2.03	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.91	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:A:89:GLU:O	1:A:93:THR:OG1	2.38	0.40
1:B:311:ASP:HB2	1:B:332:LEU:HD12	2.04	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%)	13	26
1	B	482/576 (84%)	459 (95%)	17 (4%)	6 (1%)	15	32
All	All	971/1152 (84%)	917 (94%)	41 (4%)	13 (1%)	14	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LEU

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Mol	Chain	Res	Type
1	A	449	LYS
1	A	526	VAL
1	B	141	LEU
1	B	196	GLY
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%)	14	28
1	B	430/503 (86%)	402 (94%)	28 (6%)	20	39
All	All	862/1006 (86%)	800 (93%)	62 (7%)	17	33

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

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	138	CYS
1	A	169	ARG
1	A	248	SER
1	A	255	THR
1	A	277	HIS
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

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Mol	Chain	Res	Type
1	B	395	GLU
1	B	407	GLU
1	B	421	SER
1	B	470	GLN
1	B	472	ILE
1	B	473	TYR
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 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

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	29,33,33	2.43	7 (24%)	28,52,52	2.57	9 (32%)
3	PO4	A	579	-	4,4,4	0.80	0	6,6,6	1.39	1 (16%)
4	ANP	B	577	2	29,33,33	2.01	6 (20%)	28,52,52	2.13	8 (28%)
3	PO4	B	579	-	4,4,4	0.58	0	6,6,6	1.31	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	-	1/13/38/38	0/3/3/3
3	PO4	A	579	-	-	0/0/0/0	0/0/0/0
4	ANP	B	577	2	-	0/13/38/38	0/3/3/3
3	PO4	B	579	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	577	ANP	C2'-C1'	-2.18	1.50	1.53
4	A	577	ANP	O4'-C1'	2.14	1.44	1.41
4	B	577	ANP	C5-C4	2.52	1.46	1.40
4	B	577	ANP	PB-O3A	2.69	1.62	1.59
4	B	577	ANP	PB-O1B	4.04	1.50	1.46
4	A	577	ANP	PB-N3B	4.11	1.74	1.63
4	B	577	ANP	PB-N3B	4.14	1.74	1.63
4	B	577	ANP	PG-N3B	4.53	1.75	1.63
4	A	577	ANP	PG-N3B	4.53	1.75	1.63
4	B	577	ANP	PG-O1G	5.10	1.51	1.46
4	A	577	ANP	PB-O1B	5.64	1.52	1.46
4	A	577	ANP	PB-O3A	5.90	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	577	ANP	PG-O1G	6.18	1.53	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	577	ANP	N3-C2-N1	-9.97	120.18	128.86
4	B	577	ANP	N3-C2-N1	-7.24	122.55	128.86
4	A	577	ANP	O1B-PB-N3B	-4.71	104.75	111.79
4	B	577	ANP	O1G-PG-N3B	-4.38	105.24	111.79
4	B	577	ANP	C4-C5-N7	-2.80	106.70	109.41
4	B	577	ANP	O1B-PB-N3B	-2.72	107.72	111.79
4	B	577	ANP	PA-O3A-PB	-2.66	122.98	132.38
4	A	577	ANP	O3'-C3'-C2'	-2.39	104.18	111.83
4	A	577	ANP	O2'-C2'-C3'	-2.17	104.87	111.83
4	A	577	ANP	O2A-PA-O5'	-2.15	98.01	108.14
4	A	577	ANP	C4-C5-N7	-2.12	107.36	109.41
4	A	577	ANP	C1'-N9-C4	-2.05	123.09	126.64
4	B	577	ANP	O2A-PA-O1A	2.00	122.65	112.28
3	A	579	PO4	O4-P-O2	2.25	116.17	107.90
4	A	577	ANP	C2-N1-C6	2.58	123.29	118.77
4	B	577	ANP	O3G-PG-O2G	2.62	115.03	107.69
4	B	577	ANP	O2B-PB-O1B	3.70	117.56	109.87
4	A	577	ANP	O3G-PG-O2G	3.72	118.11	107.69

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	577	ANP	2	0

## 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%)	0.83	47 (9%) <b>9</b> <b>5</b>	56, 67, 85, 106	0
1	B	492/576 (85%)	1.36	116 (23%) <b>1</b> <b>0</b>	58, 68, 85, 111	0
All	All	987/1152 (85%)	1.09	163 (16%) <b>2</b> <b>1</b>	56, 68, 85, 111	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	13.9
1	B	391	LYS	9.2
1	B	222	ILE	7.3
1	B	281	ALA	6.9
1	B	282	GLY	6.7
1	B	387	GLN	6.0
1	B	535	PRO	5.8
1	B	258	ALA	5.6
1	A	470	GLN	5.6
1	A	474	CYS	5.5
1	A	469	PRO	5.5
1	B	129	CYS	5.5
1	B	392	ILE	5.4
1	A	140	ASP	5.2
1	B	138	CYS	5.1
1	A	530	ASP	5.1
1	B	394	ARG	5.1
1	B	396	GLU	4.9
1	B	342	ILE	4.8
1	B	44	GLU	4.8
1	B	278	MET	4.8
1	B	436	GLY	4.8
1	B	349	VAL	4.7
1	B	500	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	28	LYS	4.7
1	B	494	THR	4.6
1	B	103	ARG	4.5
1	B	375	LEU	4.4
1	A	14	LYS	4.3
1	B	530	ASP	4.3
1	B	121	VAL	4.3
1	B	104	ASN	4.2
1	B	257	ASP	4.2
1	B	399	ARG	4.2
1	A	95	ASP	4.1
1	B	356	VAL	4.1
1	B	493	PRO	4.1
1	B	139	LYS	3.9
1	B	344	GLY	3.9
1	B	223	LYS	3.9
1	A	473	TYR	3.8
1	B	357	VAL	3.8
1	B	24	LYS	3.7
1	B	470	GLN	3.6
1	B	110	LEU	3.6
1	A	373	CYS	3.6
1	B	86	GLY	3.6
1	B	165	ILE	3.6
1	A	494	THR	3.6
1	A	135	GLN	3.6
1	B	130	THR	3.6
1	B	166	TYR	3.5
1	A	128	ASN	3.5
1	B	386	GLN	3.5
1	B	14	LYS	3.5
1	B	220	LYS	3.4
1	B	125	LEU	3.4
1	A	277	HIS	3.3
1	B	277	HIS	3.3
1	A	472	ILE	3.3
1	B	43	GLU	3.3
1	B	371	LEU	3.3
1	B	140	ASP	3.2
1	B	495	ASP	3.2
1	B	534	PRO	3.2
1	B	227	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	262	VAL	3.2
1	B	48	SER	3.2
1	B	317	ILE	3.2
1	B	385	PHE	3.2
1	B	468	ASP	3.2
1	B	471	ALA	3.1
1	B	492	GLU	3.1
1	B	30	TRP	3.1
1	B	111	SER	3.1
1	B	228	GLU	3.0
1	B	351	TYR	3.0
1	B	464	PRO	3.0
1	B	309	TYR	3.0
1	B	372	GLY	3.0
1	A	125	LEU	3.0
1	B	368	TRP	2.9
1	A	256	LYS	2.9
1	B	273	PHE	2.9
1	A	370	ALA	2.9
1	B	407	GLU	2.8
1	B	137	PRO	2.8
1	A	279	GLY	2.8
1	A	493	PRO	2.8
1	B	99	LYS	2.8
1	A	16	ARG	2.8
1	B	373	CYS	2.8
1	B	45	LEU	2.8
1	B	112	HIS	2.8
1	B	345	ARG	2.8
1	B	441	GLU	2.8
1	B	469	PRO	2.7
1	A	226	LYS	2.7
1	B	370	ALA	2.7
1	A	496	GLN	2.7
1	B	529	LEU	2.7
1	B	393	LYS	2.7
1	A	213	ALA	2.7
1	B	437	GLY	2.7
1	A	372	GLY	2.7
1	B	275	ILE	2.6
1	B	66	LEU	2.6
1	A	165	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	2.6
1	A	44	GLU	2.6
1	A	468	ASP	2.5
1	A	214	CYS	2.5
1	A	410	GLU	2.5
1	B	432	LEU	2.5
1	B	122	PRO	2.4
1	B	202	ALA	2.4
1	B	224	LYS	2.4
1	B	51	ARG	2.4
1	B	343	LYS	2.4
1	B	369	TRP	2.4
1	B	315	GLU	2.4
1	A	143	GLN	2.4
1	B	362	TYR	2.4
1	A	24	LYS	2.4
1	B	466	LYS	2.4
1	A	374	LEU	2.4
1	B	359	ASN	2.4
1	B	472	ILE	2.4
1	B	527	PHE	2.3
1	B	49	LEU	2.3
1	B	148	LEU	2.3
1	B	397	VAL	2.3
1	B	379	ILE	2.3
1	B	87	VAL	2.3
1	B	268	GLY	2.2
1	A	124	GLN	2.2
1	A	169	ARG	2.2
1	A	136	GLY	2.2
1	B	467	PRO	2.2
1	B	532	SER	2.2
1	B	94	PRO	2.2
1	B	16	ARG	2.2
1	B	190	ARG	2.2
1	A	497	ASP	2.2
1	B	15	ALA	2.2
1	B	423	LEU	2.2
1	A	368	TRP	2.2
1	B	324	HIS	2.2
1	B	433	GLY	2.1
1	B	169	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	351	TYR	2.1
1	A	263	LEU	2.1
1	A	317	ILE	2.1
1	B	295	ILE	2.1
1	A	127	THR	2.1
1	A	258	ALA	2.1
1	A	390	LYS	2.1
1	A	495	ASP	2.1
1	A	203	CYS	2.1
1	B	34	LEU	2.1
1	B	321	ASP	2.1
1	B	100	ALA	2.1
1	B	113	THR	2.1

## 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	PO4	A	579	5/5	0.83	0.34	0.07	83,83,87,87	0
3	PO4	B	579	5/5	0.89	0.31	-0.33	91,93,95,97	0
4	ANP	A	577	31/31	0.90	0.19	-1.00	60,65,103,105	0
4	ANP	B	577	31/31	0.91	0.16	-2.74	60,63,92,93	0
2	MG	A	578	1/1	0.90	0.16	-	92,92,92,92	0
2	MG	B	578	1/1	0.74	0.25	-	87,87,87,87	0



## 6.5 Other polymers

There are no such residues in this entry.