Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:15 AM GMT

PDB ID	:	2CCI
Title	:	CRYSTAL STRUCTURE OF PHOSPHO-CDK2 CYCLIN A IN COMPLEX WITH A PEPTIDE CONTAINING BOTH THE SUBSTRATE AND RECRUITMENT SITES OF CDC6
Authors	:	Cheng, K.Y.; Noble, M.E.M.; Skamnaki, V.; Brown, N.R.; Lowe, E.D.; Kontogiannis, L.; Shen, K.; Cole, P.A.; Siligardi, G.; Johnson, L.N.
Deposited on	:	2006-01-16
Resolution	:	2.70 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

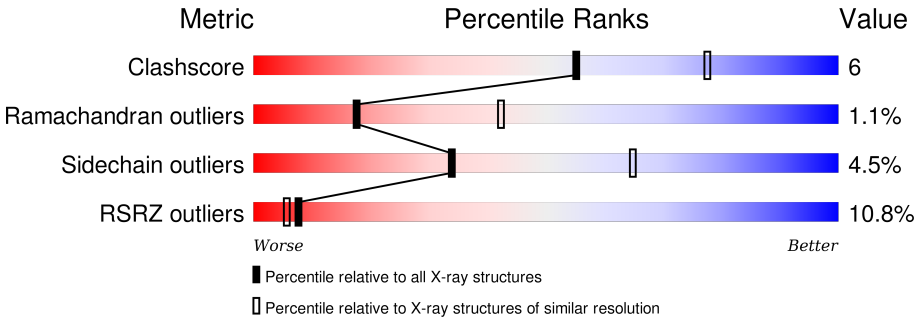
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 >=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 <=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	299	5% 79% 18%
1	C	299	19% 80% 17%
2	B	258	% 85% 14%
2	D	258	13% 80% 18%
3	F	30	23% 50% 10% 37%
3	I	30	20% 30% 13% 53%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9391 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called CELL DIVISION CONTROL PROTEIN 6 HOMOLOG.

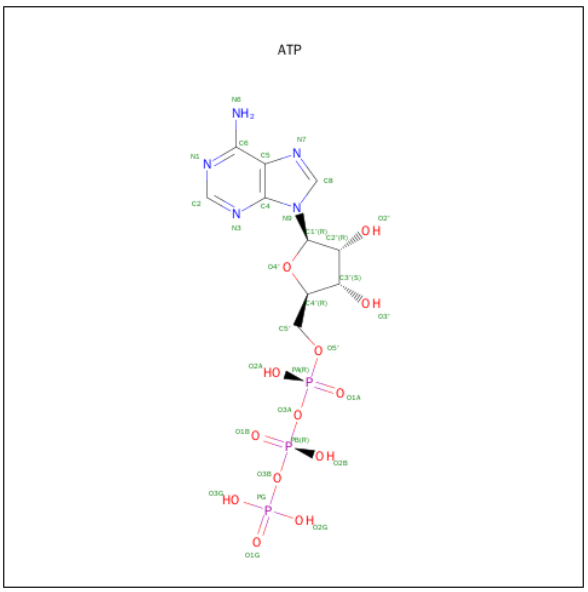
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	19	Total	C	N	O	0	0	0
			160	99	37	24			
3	I	14	Total	C	N	O	0	0	0
			114	73	25	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	67	HIS	PRO	ENGINEERED MUTATION	UNP Q99741
F	68	HIS	PRO	ENGINEERED MUTATION	UNP Q99741
F	69	ALA	CYS	ENGINEERED MUTATION	UNP Q99741
F	72	ARG	PRO	ENGINEERED MUTATION	UNP Q99741
I	69	ALA	CYS	ENGINEERED MUTATION	UNP Q99741
I	72	ARG	PRO	ENGINEERED MUTATION	UNP Q99741

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	23	Total	O	0	0
			23	23		
6	C	22	Total	O	0	0
			22	22		
6	D	12	Total	O	0	0
			12	12		
6	F	7	Total	O	0	0
			7	7		

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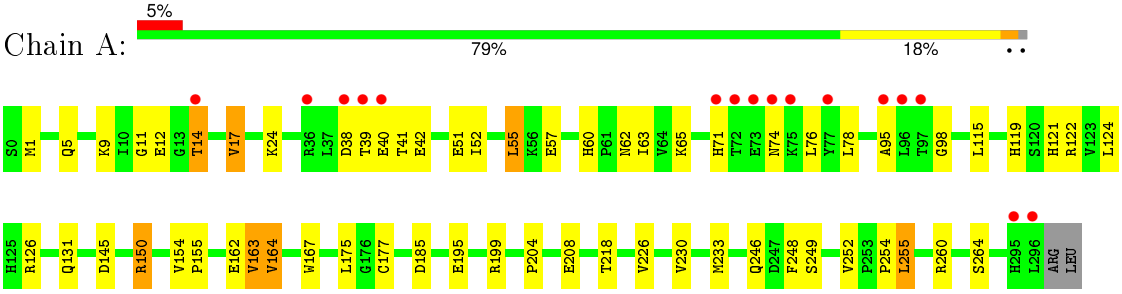
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	3	Total O 3 3	0	0

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 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.

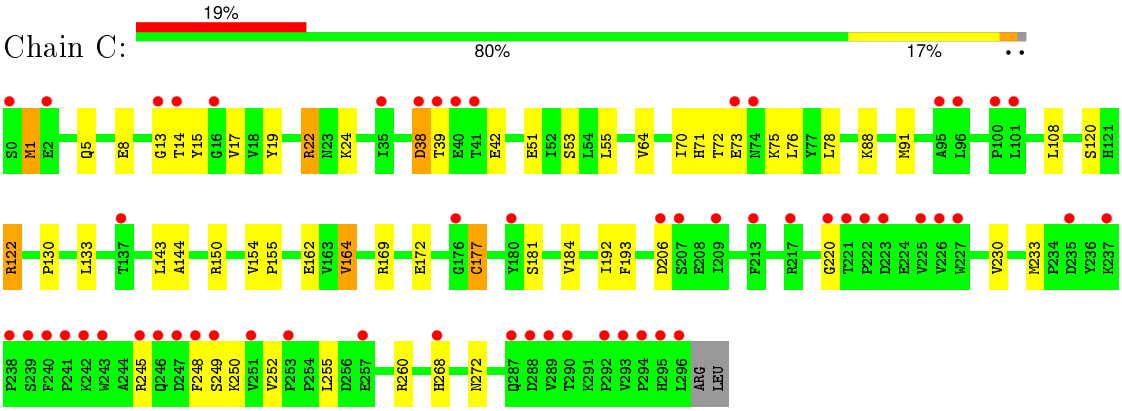
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



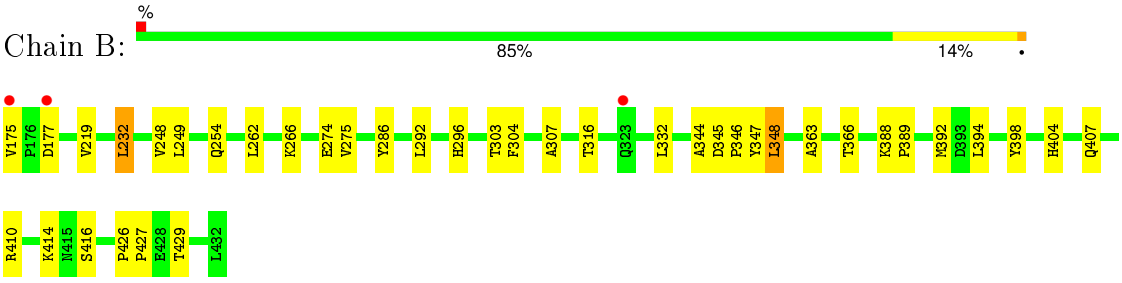
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C:



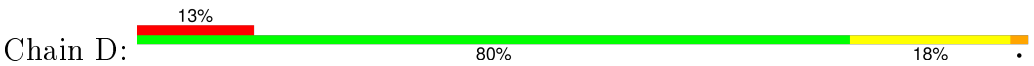
- Molecule 2: CYCLIN A2

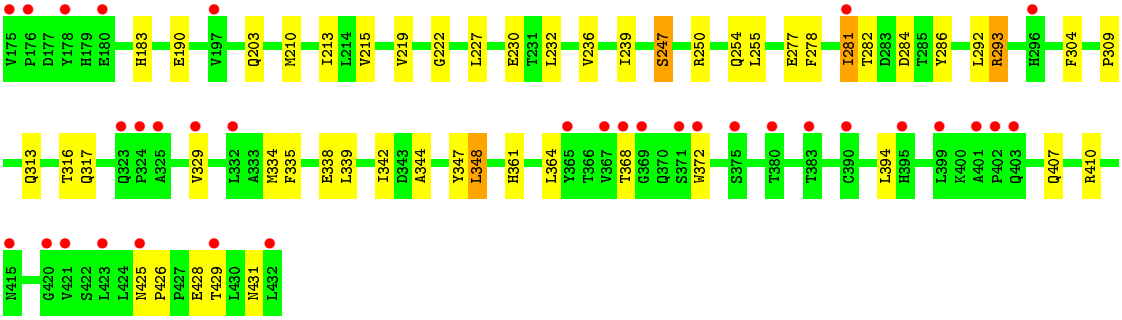
Chain B:



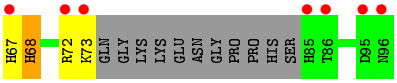
- Molecule 2: CYCLIN A2

Chain D:

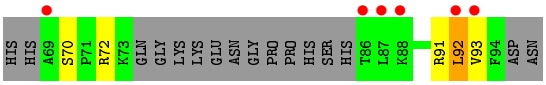




• Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG



• Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.42Å 114.39Å 170.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.92 – 2.70 37.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (94.92-2.70) 97.1 (37.02-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.261 , 0.321 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	3 of 39591 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	9391	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPO, MG, ATP

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	0/2438	0.59	1/3308 (0.0%)
1	C	0.39	0/2438	0.55	0/3308
2	B	0.43	0/2133	0.56	0/2897
2	D	0.37	0/2133	0.53	0/2897
3	F	0.37	0/163	0.50	0/215
3	I	0.43	0/114	0.60	0/148
All	All	0.41	0/9419	0.56	1/12773 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	LEU	CA-CB-CG	5.01	126.83	115.30

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	2388	0	2430	43	0
1	C	2388	0	2430	31	0
2	B	2083	0	2107	24	0
2	D	2083	0	2107	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	160	0	161	2	0
3	I	114	0	130	2	0
4	A	31	0	12	0	0
4	C	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	44	0	0	3	0
6	B	23	0	0	0	0
6	C	22	0	0	0	0
6	D	12	0	0	0	0
6	F	7	0	0	1	0
6	I	3	0	0	1	0
All	All	9391	0	9389	117	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 (117) 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)
2:D:203:GLN:HE22	2:D:247:SER:HA	1.22	1.05
1:A:154:VAL:O	2:B:316:THR:HG22	1.62	0.97
1:C:1:MET:HE1	1:C:70:ILE:HD13	1.51	0.90
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.54	0.89
1:A:5:GLN:HB2	1:A:24:LYS:HE3	1.66	0.77
2:B:366:THR:HG23	2:B:427:PRO:HD3	1.68	0.75
1:A:177:CYS:HB2	6:A:2023:HOH:O	1.87	0.75
1:A:95:ALA:HA	1:A:199:ARG:HH11	1.54	0.72
1:A:42:GLU:OE1	2:B:275:VAL:HG23	1.89	0.71
3:F:67:HIS:O	3:F:68:HIS:HB2	1.90	0.71
1:A:154:VAL:O	2:B:316:THR:CG2	2.39	0.71
1:C:1:MET:HE2	1:C:1:MET:HA	1.71	0.71
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.72	0.71
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.73	0.71
1:A:51:GLU:O	1:A:55:LEU:HB2	1.91	0.70
2:D:203:GLN:NE2	2:D:247:SER:HA	2.03	0.67
1:C:230:VAL:HA	1:C:233:MET:HE2	1.76	0.67
1:C:1:MET:CE	1:C:1:MET:HA	2.24	0.66
1:C:73:GLU:HG2	2:D:293:ARG:HH22	1.64	0.62
3:F:73:LYS:HA	6:F:2004:HOH:O	2.00	0.62
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLU:O	1:C:55:LEU:HB2	2.01	0.61
1:A:230:VAL:HG23	1:A:233:MET:HE1	1.82	0.61
2:B:248:VAL:HG12	2:B:249:LEU:O	2.03	0.58
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.57
1:A:252:VAL:HG12	1:A:254:PRO:HD2	1.86	0.57
1:C:64:VAL:HG23	1:C:143:LEU:O	2.04	0.57
1:A:177:CYS:SG	1:A:233:MET:SD	3.02	0.57
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.05	0.57
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.74	0.56
4:C:1297:ATP:O1G	4:C:1297:ATP:O1A	2.22	0.56
1:A:39:THR:HG22	1:A:40:GLU:HG2	1.87	0.56
2:D:347:TYR:OH	2:D:394:LEU:HA	2.06	0.56
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.87	0.55
1:A:1:MET:HA	1:A:1:MET:HE2	1.88	0.55
1:C:72:THR:HB	1:C:75:LYS:H	1.72	0.54
1:C:5:GLN:HB2	1:C:24:LYS:HE3	1.89	0.54
1:A:9:LYS:HD3	1:A:17:VAL:HG11	1.90	0.54
1:C:13:GLY:O	1:C:15:TYR:N	2.40	0.54
1:A:218:THR:HA	1:A:246:GLN:NE2	2.23	0.54
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.88	0.54
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.89	0.54
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.44	0.52
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.92	0.52
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.10	0.52
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.92	0.52
2:D:215:VAL:HG12	2:D:342:ILE:HD13	1.91	0.52
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.92	0.52
2:B:303:THR:O	2:B:304:PHE:HB2	2.10	0.51
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.93	0.51
1:C:130:PRO:HD3	1:C:192:ILE:HG12	1.94	0.50
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.93	0.50
1:A:60:HIS:HD2	1:A:62:ASN:H	1.60	0.49
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.95	0.49
2:D:230:GLU:OE2	2:D:313:GLN:NE2	2.40	0.49
2:B:416:SER:HB3	1:C:8:GLU:OE2	2.13	0.49
1:A:60:HIS:CD2	1:A:62:ASN:H	2.31	0.48
1:A:71:HIS:CE1	2:B:296:HIS:HD2	2.32	0.48
1:A:249:SER:HA	1:A:260:ARG:HD3	1.94	0.47
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.97	0.47
2:D:329:VAL:HG11	2:D:364:LEU:HD12	1.96	0.47
1:A:252:VAL:HB	1:A:255:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:CD	1:C:162:GLU:H	2.18	0.47
1:C:164:VAL:HB	1:C:169:ARG:HG3	1.97	0.47
1:A:162:GLU:CD	1:A:162:GLU:H	2.18	0.47
1:A:65:LYS:HE2	6:A:2009:HOH:O	2.14	0.46
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.50	0.46
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.82	0.45
1:A:71:HIS:NE2	2:B:296:HIS:HD2	2.12	0.45
2:B:347:TYR:OH	2:B:394:LEU:HA	2.16	0.45
2:D:277:GLU:O	2:D:281:ILE:HG13	2.16	0.45
1:A:60:HIS:HB3	1:A:63:ILE:HD12	1.98	0.45
2:D:213:ILE:HG22	3:I:92:LEU:HD22	1.99	0.45
1:A:126:ARG:NH2	1:A:150:ARG:HB3	2.31	0.44
1:C:220:GLY:HA3	1:C:245:ARG:HG2	1.99	0.44
1:C:181:SER:O	1:C:184:VAL:HG22	2.17	0.44
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.00	0.43
1:A:230:VAL:HA	1:A:233:MET:HE2	2.01	0.43
2:B:388:LYS:O	2:B:392:MET:HG2	2.18	0.43
2:D:250:ARG:HD3	6:I:2003:HOH:O	2.18	0.43
1:A:71:HIS:HA	1:A:76:LEU:HD12	1.99	0.43
1:C:88:LYS:HA	1:C:91:MET:HE2	2.00	0.43
1:C:154:VAL:HA	1:C:155:PRO:HA	1.86	0.43
1:C:5:GLN:HG2	1:C:22:ARG:NH1	2.34	0.43
2:D:190:GLU:N	2:D:309:PRO:HG2	2.33	0.43
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.01	0.43
2:D:254:GLN:HE21	2:D:282:THR:HG22	1.83	0.43
1:C:38:ASP:HB2	1:C:39:THR:H	1.59	0.43
1:A:41:THR:HB	1:A:42:GLU:H	1.73	0.43
1:C:17:VAL:HB	1:C:19:TYR:CE2	2.53	0.43
1:C:172:GLU:O	1:C:177:CYS:HB2	2.19	0.42
1:A:230:VAL:HG23	1:A:233:MET:CE	2.50	0.42
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.96	0.42
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.54	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.54	0.42
2:D:278:PHE:HA	2:D:281:ILE:HD11	2.00	0.42
2:D:210:MET:HE1	2:D:250:ARG:HB3	2.01	0.42
2:B:410:ARG:O	2:B:414:LYS:HG3	2.18	0.42
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.37	0.42
1:C:53:SER:HB3	2:D:304:PHE:O	2.20	0.42
2:D:334:MET:O	2:D:338:GLU:HB2	2.20	0.41
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.55	0.41
2:D:361:HIS:HB2	2:D:372:TRP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:HA2	1:A:199:ARG:NE	2.36	0.41
2:B:404:HIS:O	2:B:407:GLN:NE2	2.54	0.41
1:A:208:GLU:HG3	6:A:2029:HOH:O	2.19	0.41
1:A:195:GLU:O	1:A:199:ARG:HA	2.21	0.41
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.02	0.41
1:C:249:SER:HA	1:C:260:ARG:HD2	2.02	0.41
1:C:122:ARG:O	1:C:122:ARG:HD2	2.21	0.41
1:C:71:HIS:HD2	1:C:76:LEU:HD13	1.86	0.40
1:A:162:GLU:CD	1:A:162:GLU:N	2.75	0.40
1:A:248:PHE:CZ	1:A:264:SER:HA	2.56	0.40
2:D:236:VAL:HA	2:D:239:ILE:HD12	2.03	0.40
3:I:91:ARG:O	3:I:91:ARG:HG2	2.21	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.88	0.40
2:B:254:GLN:HB3	2:B:286:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/299 (98%)	270 (92%)	18 (6%)	6 (2%)	9 24
1	C	294/299 (98%)	266 (90%)	26 (9%)	2 (1%)	26 55
2	B	256/258 (99%)	246 (96%)	9 (4%)	1 (0%)	39 69
2	D	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	39 69
3	F	15/30 (50%)	13 (87%)	1 (7%)	1 (7%)	1 2
3	I	10/30 (33%)	6 (60%)	3 (30%)	1 (10%)	1 0
All	All	1125/1174 (96%)	1040 (92%)	73 (6%)	12 (1%)	17 42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
2	B	177	ASP
1	C	14	THR
1	A	11	GLY
1	A	164	VAL
1	C	164	VAL
3	I	92	LEU
1	A	14	THR
3	F	68	HIS
1	A	38	ASP
1	A	145	ASP
2	D	281	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	250 (96%)	11 (4%)	36	68
1	C	261/263 (99%)	245 (94%)	16 (6%)	23	49
2	B	232/232 (100%)	226 (97%)	6 (3%)	54	83
2	D	232/232 (100%)	223 (96%)	9 (4%)	39	70
3	F	17/26 (65%)	16 (94%)	1 (6%)	24	51
3	I	12/26 (46%)	9 (75%)	3 (25%)	1	2
All	All	1015/1042 (97%)	969 (96%)	46 (4%)	34	65

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	VAL
1	A	55	LEU
1	A	74	ASN
1	A	121	HIS
1	A	122	ARG
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	150	ARG
1	A	163	VAL
1	A	226	VAL
1	A	255	LEU
2	B	175	VAL
2	B	232	LEU
2	B	274	GLU
2	B	292	LEU
2	B	348	LEU
2	B	429	THR
1	C	1	MET
1	C	22	ARG
1	C	38	ASP
1	C	42	GLU
1	C	78	LEU
1	C	120	SER
1	C	122	ARG
1	C	150	ARG
1	C	177	CYS
1	C	206	ASP
1	C	248	PHE
1	C	250	LYS
1	C	252	VAL
1	C	255	LEU
1	C	268	HIS
1	C	272	ASN
2	D	247	SER
2	D	284	ASP
2	D	292	LEU
2	D	293	ARG
2	D	348	LEU
2	D	368	THR
2	D	428	GLU
2	D	429	THR
2	D	431	ASN
3	F	72	ARG
3	I	70	SER
3	I	72	ARG
3	I	93	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	62	ASN
1	A	84	HIS
1	A	119	HIS
1	A	246	GLN
1	A	265	GLN
1	A	287	GLN
2	B	183	HIS
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	403	GLN
2	B	425	ASN
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	85	GLN
2	D	233	HIS
2	D	317	GLN
2	D	425	ASN
3	F	85	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	TPO	A	160	1	8,10,11	2.95	3 (37%)	7,14,16	0.80	0
1	TPO	C	160	1	8,10,11	3.02	3 (37%)	7,14,16	0.91	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
1	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O2P	4.17	1.69	1.54
1	A	160	TPO	P-O3P	4.25	1.70	1.54
1	C	160	TPO	P-O3P	4.29	1.70	1.54
1	C	160	TPO	P-O2P	4.34	1.70	1.54
1	A	160	TPO	P-O1P	5.66	1.69	1.51
1	C	160	TPO	P-O1P	5.88	1.70	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
4	ATP	A	1297	5	24,33,33	1.05	2 (8%)	31,52,52	1.78	5 (16%)
4	ATP	C	1297	5	24,33,33	0.97	1 (4%)	31,52,52	1.72	5 (16%)

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	ATP	A	1297	5	-	0/18/38/38	0/3/3/3
4	ATP	C	1297	5	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297	ATP	O4'-C1'	2.10	1.43	1.41
4	A	1297	ATP	C5-C4	3.29	1.47	1.40
4	C	1297	ATP	C5-C4	3.32	1.48	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1297	ATP	N3-C2-N1	-6.84	123.65	128.89
4	C	1297	ATP	N3-C2-N1	-6.06	124.25	128.89
4	C	1297	ATP	C2'-C1'-N9	-4.43	107.52	114.29
4	A	1297	ATP	PA-O3A-PB	-3.66	122.44	132.73
4	A	1297	ATP	PB-O3B-PG	-2.84	123.14	132.67
4	C	1297	ATP	C4-C5-N7	-2.75	106.95	109.48
4	A	1297	ATP	C4-C5-N7	-2.58	107.10	109.48
4	C	1297	ATP	PB-O3B-PG	-2.23	125.19	132.67
4	C	1297	ATP	PA-O3A-PB	-2.18	126.61	132.73
4	A	1297	ATP	C2'-C1'-N9	-2.07	111.12	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1297	ATP	1	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^{th} 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^2)	Q<0.9
1	A	296/299 (98%)	0.66	16 (5%) 29 28	30, 35, 46, 51	0
1	C	296/299 (98%)	1.22	57 (19%) 2 1	30, 38, 46, 48	0
2	B	258/258 (100%)	0.36	3 (1%) 81 81	31, 36, 41, 48	0
2	D	258/258 (100%)	1.03	34 (13%) 4 4	30, 37, 44, 49	0
3	F	19/30 (63%)	1.61	7 (36%) 0 0	42, 45, 56, 57	0
3	I	14/30 (46%)	1.91	6 (42%) 0 0	53, 61, 66, 66	0
All	All	1141/1174 (97%)	0.85	123 (10%) 8 6	30, 37, 46, 66	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	7.8
1	C	39	THR	7.3
1	A	40	GLU	6.7
1	C	248	PHE	5.9
2	D	175	VAL	5.6
1	A	73	GLU	5.2
1	A	71	HIS	5.1
1	C	245	ARG	5.0
3	I	86	THR	5.0
1	C	247	ASP	4.9
1	A	74	ASN	4.9
2	D	323	GLN	4.9
1	C	40	GLU	4.8
1	C	137	THR	4.5
1	C	293	VAL	4.5
1	C	213	PHE	4.4
1	C	288	ASP	4.4
1	C	241	PRO	4.3
1	C	73	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	95	ALA	4.3
1	C	74	ASN	4.3
2	D	367	VAL	4.2
1	C	0	SER	4.1
2	D	432	LEU	3.9
1	C	296	LEU	3.7
1	C	295	HIS	3.7
1	A	295	HIS	3.7
1	C	287	GLN	3.6
1	C	13	GLY	3.6
2	D	178	TYR	3.4
2	B	175	VAL	3.4
1	C	246	GLN	3.4
1	C	238	PRO	3.3
1	C	243	TRP	3.3
1	C	217	ARG	3.2
1	C	101	LEU	3.2
1	C	16	GLY	3.2
2	D	180	GLU	3.2
2	D	371	SER	3.2
2	D	176	PRO	3.1
1	C	251	VAL	3.1
1	C	235	ASP	3.1
3	F	72	ARG	3.0
1	C	100	PRO	3.0
3	F	85	HIS	3.0
1	C	242	LYS	3.0
3	I	93	VAL	3.0
1	C	294	PRO	3.0
2	D	425	ASN	3.0
1	C	221	THR	2.9
1	C	289	VAL	2.9
1	C	207	SER	2.9
2	D	372	TRP	2.9
2	D	402	PRO	2.9
2	D	324	PRO	2.8
3	F	67	HIS	2.8
1	C	240	PHE	2.8
2	D	429	THR	2.8
1	A	96	LEU	2.8
2	D	383	THR	2.8
1	C	239	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	395	HIS	2.7
2	D	375	SER	2.7
2	D	197	VAL	2.7
1	C	223	ASP	2.7
2	D	401	ALA	2.7
1	C	96	LEU	2.6
1	A	38	ASP	2.6
2	D	420	GLY	2.6
1	C	290	THR	2.6
2	D	281	ILE	2.6
3	I	69	ALA	2.6
3	F	95	ASP	2.6
1	C	209	ILE	2.6
1	A	14	THR	2.6
2	D	421	VAL	2.6
3	F	96	ASN	2.5
1	C	225	VAL	2.5
1	C	268	HIS	2.5
1	A	36	ARG	2.5
1	C	226	VAL	2.4
1	A	97	THR	2.4
1	C	227	TRP	2.4
1	C	14	THR	2.4
1	A	77	TYR	2.4
2	D	403	GLN	2.4
2	B	177	ASP	2.4
1	C	237	LYS	2.4
1	C	253	PRO	2.3
1	C	2	GLU	2.3
1	A	75	LYS	2.3
2	D	368	THR	2.3
1	C	249	SER	2.3
1	C	222	PRO	2.3
1	C	180	TYR	2.3
1	A	72	THR	2.3
1	C	38	ASP	2.3
2	D	380	THR	2.3
1	A	296	LEU	2.3
2	D	296	HIS	2.2
2	D	369	GLY	2.2
1	A	95	ALA	2.2
1	C	206	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	257	GLU	2.2
1	C	176	GLY	2.2
2	D	415	ASN	2.2
2	D	423	LEU	2.2
3	I	87	LEU	2.2
2	D	399	LEU	2.1
3	F	73	LYS	2.1
2	D	365	TYR	2.1
2	D	329	VAL	2.1
3	F	86	THR	2.1
3	I	92	LEU	2.1
1	C	35	ILE	2.1
2	D	390	CYS	2.1
2	D	325	ALA	2.1
1	C	220	GLY	2.1
3	I	88	LYS	2.0
2	B	323	GLN	2.0
1	C	41	THR	2.0
2	D	332	LEU	2.0
1	C	292	PRO	2.0

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^{th} 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^2)	Q<0.9
1	TPO	C	160	11/12	0.91	0.17	-	35,36,36,36	0
1	TPO	A	160	11/12	0.92	0.22	-	31,33,33,33	0

6.3 Carbohydrates (i)

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^{th} 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^2)	Q<0.9
4	ATP	A	1297	31/31	0.90	0.19	-0.49	35,37,58,58	0
4	ATP	C	1297	31/31	0.91	0.18	-0.67	32,36,55,56	0
5	MG	C	1298	1/1	0.88	0.16	-1.80	43,43,43,43	0
5	MG	A	1298	1/1	0.89	0.08	-1.87	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.