Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:23 PM GMT

PDB ID	:	4EOO
Title	:	Thr 160 phosphorylated CDK2 Q131E - human cyclin A3 complex with ATP
Authors	:	Echalier, A.; Cot, E.; Camasses, A.; Hodimont, E.; Hoh, F.; Sheinerman, F.; Krasinska, L.; Fisher, D.
Deposited on	:	2012-04-14
Resolution	:	2.10 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 ⓘ symbol.

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

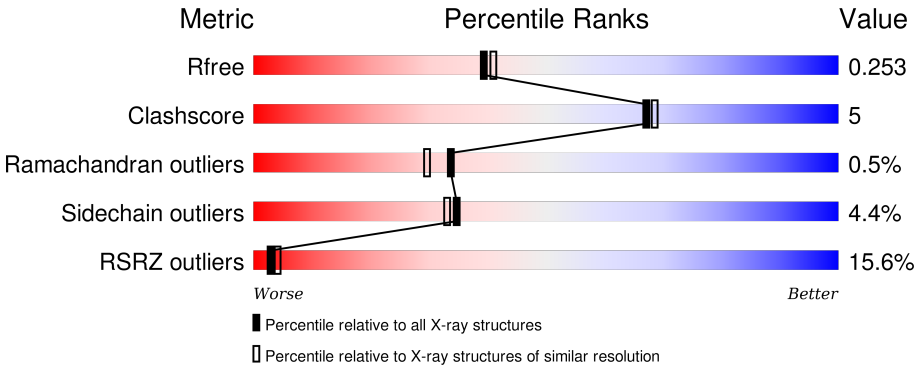
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	6% 83% 15% ••
1	C	299	27% 83% 14% •
2	B	258	9% 90% 9% •
2	D	258	19% 84% 13% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SGM	B	502	-	-	-	X
5	SGM	D	501	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9456 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	P	S	0	3	0
			2398	1555	410	424	1	8			
1	C	298	Total	C	N	O	P	S	0	1	0
			2402	1558	407	428	1	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
A	131	GLU	GLN	ENGINEERED MUTATION	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941
C	131	GLU	GLN	ENGINEERED MUTATION	UNP P24941

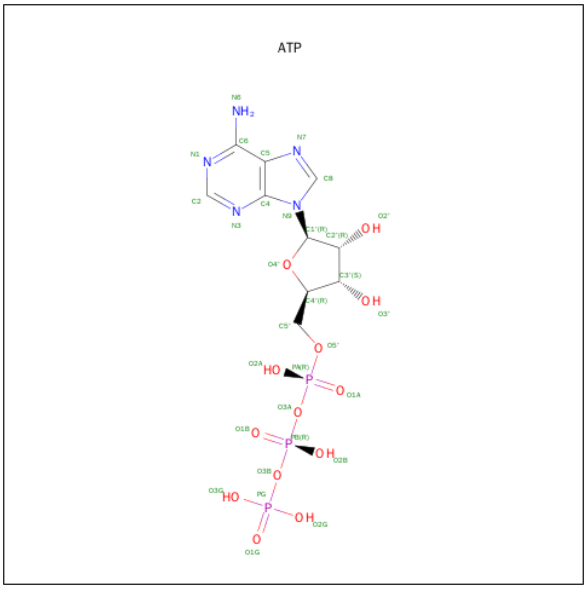
- Molecule 2 is a protein called Cyclin-A2.

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	254	Total	C	N	O	S	0	1	0
			2063	1335	338	379	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

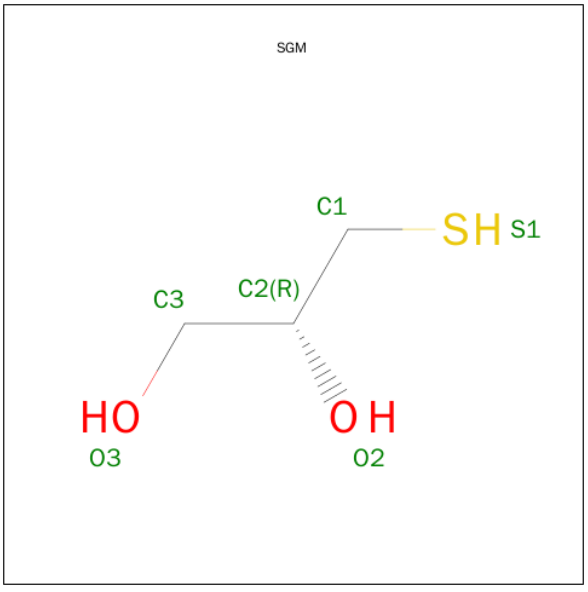
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- 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 MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			6	3	2	1		
5	D	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 6 is water.

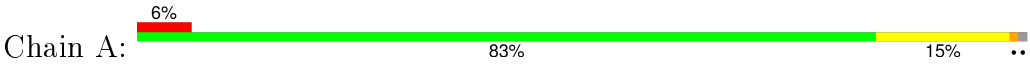
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	154	Total	O	0	0
			154	154		
6	B	118	Total	O	0	0
			118	118		
6	C	82	Total	O	0	0
			82	82		
6	D	79	Total	O	0	0
			79	79		

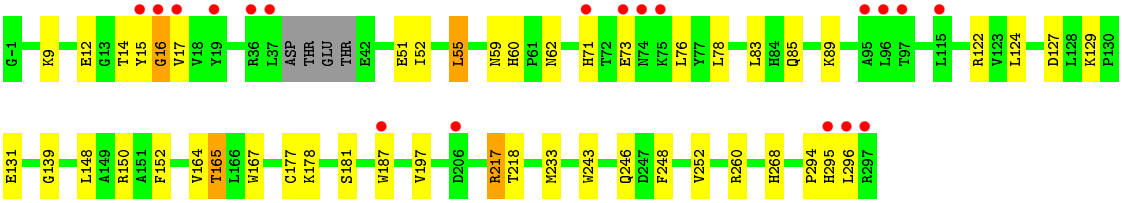
3 Residue-property plots (i)

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: Cyclin-dependent kinase 2

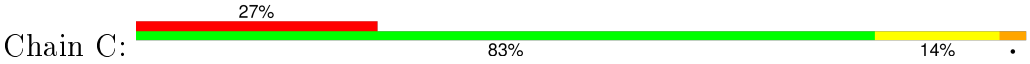
Chain A:

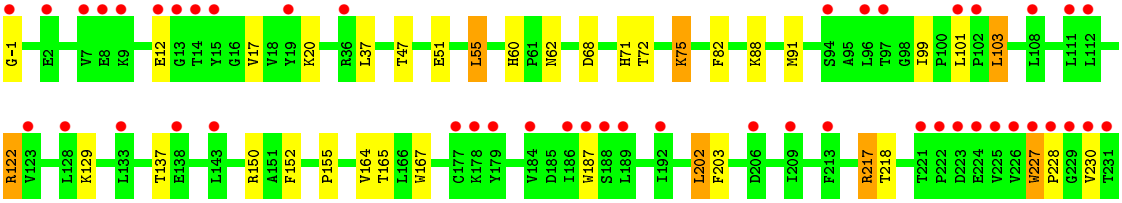




- Molecule 1: Cyclin-dependent kinase 2

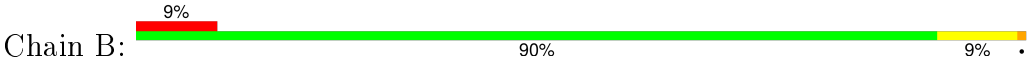
Chain C:

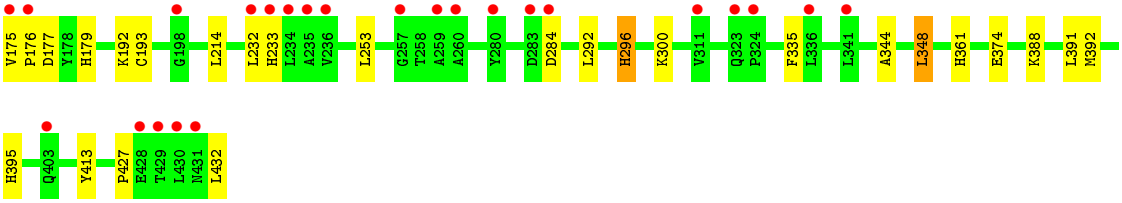




- Molecule 2: Cyclin-A2

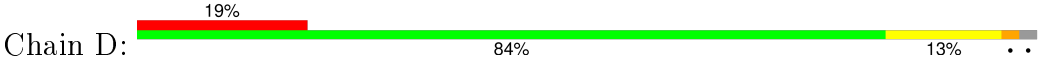
Chain B:

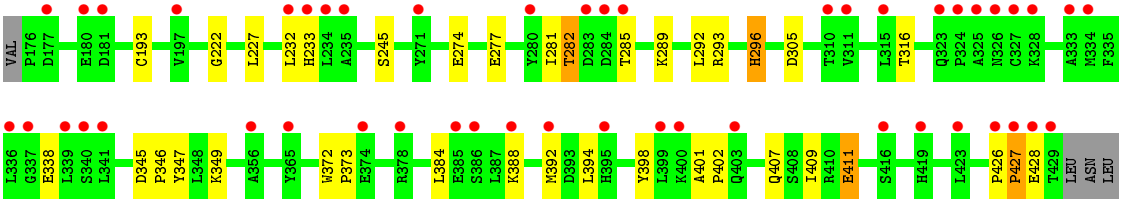




- Molecule 2: Cyclin-A2

Chain D:




VAL P176 D177 E180 D181 C193 V197 G222 L227 L232 H233 L234 A235 S245 Y271 E274 E277 Y280 T281 T282 D283 D284 T285 K289 L292 R293 H296 D305 T310 W311 L315 T316 Q323 P324 A325 N326 C327 K328 A333 N334 F335
L336 G337 E338 L339 S340 L341 D345 P346 Y347 L348 K349 A356 Y365 W372 P373 E374 R378 L384 E385 S386 L387 K388 M392 D393 L394 H395 Y398 L399 K400 A401 P402 Q403 Q407 S408 I409 R410 E411 S416 H419 L423 P426 P427 E428 T429 LEU ASN LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.11Å 134.49Å 148.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.10 29.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.79-2.10) 98.6 (29.79-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.253 0.214 , 0.253	Depositor DCC
R_{free} test set	4381 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 86124 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9456	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, SGM, 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	0.53	3/2448 (0.1%)	0.61	1/3318 (0.0%)
1	C	0.48	3/2453 (0.1%)	0.57	0/3328
2	B	0.46	0/2133	0.56	0/2897
2	D	0.44	0/2113	0.51	0/2867
All	All	0.48	6/9147 (0.1%)	0.57	1/12410 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	TRP	CD2-CE2	5.44	1.47	1.41
1	A	187	TRP	CD2-CE2	5.29	1.47	1.41
1	C	167	TRP	CD2-CE2	5.28	1.47	1.41
1	A	167	TRP	CD2-CE2	5.27	1.47	1.41
1	C	187	TRP	CD2-CE2	5.08	1.47	1.41
1	C	227	TRP	CD2-CE2	5.02	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	ARG	NE-CZ-NH1	-6.02	117.29	120.30

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	2398	0	2433	30	1
1	C	2402	0	2437	26	0
2	B	2083	0	2107	16	0
2	D	2063	0	2083	21	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	12	2	0
4	C	31	0	12	0	0
5	B	6	0	8	2	0
5	D	6	0	8	2	0
6	A	154	0	0	7	1
6	B	118	0	0	1	0
6	C	82	0	0	1	0
6	D	79	0	0	1	0
All	All	9456	0	9100	87	1

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 5.

All (87) 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:B:193:CYS:SG	5:B:502:SGM:S1	2.34	0.87
2:B:176:PRO:HD2	2:B:179:HIS:CE1	2.13	0.84
2:D:274:GLU:HG2	2:D:277:GLU:HG3	1.62	0.82
1:C:71:HIS:HD2	2:D:296:HIS:CE1	2.03	0.76
1:A:148:LEU:HG	6:A:422:HOH:O	1.84	0.76
1:A:15:TYR:N	1:A:16:GLY:HA3	2.01	0.76
1:A:60:HIS:HD2	1:A:62:ASN:H	1.37	0.70
1:C:60:HIS:HD2	1:C:62:ASN:H	1.37	0.70
1:C:218:THR:HA	1:C:246:GLN:NE2	2.08	0.69
1:A:60:HIS:CD2	1:A:62:ASN:H	2.10	0.69
1:C:60:HIS:CD2	1:C:62:ASN:H	2.11	0.68
2:D:193:CYS:SG	5:D:501:SGM:S1	2.64	0.67
2:B:175:VAL:HB	2:B:176:PRO:CD	2.25	0.67
2:D:407:GLN:O	2:D:411:GLU:HG2	1.97	0.65
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.66	0.64
2:B:175:VAL:HB	2:B:176:PRO:HD2	1.82	0.62
1:A:15:TYR:N	1:A:16:GLY:CA	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:HD2	2:B:179:HIS:NE2	2.16	0.61
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.02	0.60
1:C:227:TRP:O	1:C:230:VAL:HG23	2.01	0.60
1:A:252:VAL:HB	6:A:408:HOH:O	2.01	0.59
1:A:260:ARG:HD3	6:A:409:HOH:O	2.01	0.59
1:C:51:GLU:O	1:C:55:LEU:HB2	2.02	0.59
1:A:268:HIS:HD2	6:A:519:HOH:O	1.85	0.58
1:A:15:TYR:H	1:A:16:GLY:HA3	1.68	0.58
1:C:72:THR:HB	1:C:75:LYS:H	1.69	0.57
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.86	0.57
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.87	0.56
1:A:15:TYR:H	1:A:16:GLY:CA	2.19	0.55
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.22	0.55
2:B:233:HIS:HE1	6:B:651:HOH:O	1.88	0.55
1:A:83:LEU:O	4:A:302:ATP:H2	1.90	0.54
1:A:85:GLN:HG3	1:A:89:LYS:HE3	1.91	0.53
1:A:177:CYS:HB2	1:A:233:MET:CE	2.37	0.53
1:C:88:LYS:HA	1:C:91:MET:HE2	1.90	0.53
1:A:131:GLU:HG3	6:A:550:HOH:O	2.08	0.52
1:A:218:THR:HA	1:A:246:GLN:HE21	1.74	0.52
1:C:47:THR:HG23	6:C:467:HOH:O	2.10	0.52
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.92	0.52
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.46	0.51
1:C:129:LYS:NZ	1:C:165:THR:HG21	2.26	0.51
1:A:268:HIS:CE1	6:A:476:HOH:O	2.63	0.50
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.42	0.50
1:C:241:PRO:HB2	1:C:243:TRP:NE1	2.26	0.50
2:D:289:LYS:O	2:D:293[B]:ARG:HG3	2.12	0.50
1:C:-1:GLY:HA3	1:C:68:ASP:OD2	2.11	0.50
1:A:9:LYS:NZ	1:A:12:GLU:OE2	2.41	0.49
1:A:181:SER:HB3	6:A:489:HOH:O	2.11	0.49
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.58	0.49
4:A:302:ATP:O3B	4:A:302:ATP:H5'2	2.12	0.49
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.49	0.48
1:A:9:LYS:HE2	1:A:12:GLU:HG3	1.96	0.48
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.49	0.47
2:B:176:PRO:HB2	2:B:177:ASP:O	2.14	0.47
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.97	0.46
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.94	0.46
2:D:347:TYR:OH	2:D:394:LEU:HA	2.16	0.46
1:C:277:ALA:O	1:C:281:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.51	0.45
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.51	0.45
1:C:12:GLU:HA	1:C:17:VAL:HG12	1.99	0.44
2:B:388:LYS:O	2:B:392:MET:HG2	2.17	0.44
1:C:253:PRO:HG2	1:C:254:PRO:HD3	2.00	0.44
1:C:71:HIS:CD2	2:D:296:HIS:HE1	2.35	0.43
2:D:372:TRP:HA	2:D:373:PRO:HD3	1.86	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.85	0.43
1:C:155:PRO:HD2	2:D:316:THR:HB	2.01	0.43
1:A:51:GLU:O	1:A:55:LEU:HB2	2.19	0.43
2:D:282:THR:OG1	2:D:282:THR:O	2.35	0.43
1:C:217:ARG:O	1:C:246:GLN:NE2	2.37	0.42
2:D:426:PRO:HA	2:D:427:PRO:HD3	1.86	0.42
2:B:395:HIS:HE1	2:B:427:PRO:O	2.03	0.42
1:C:240:PHE:HA	1:C:241:PRO:HD3	1.92	0.42
1:C:99:ILE:HG23	1:C:103:LEU:HD12	2.03	0.41
2:D:338:GLU:HG2	2:D:409:ILE:HD13	2.03	0.41
2:D:233:HIS:HE1	6:D:644:HOH:O	2.03	0.41
2:D:305:ASP:HB3	5:D:501:SGM:H12	2.03	0.41
2:D:388:LYS:O	2:D:392:MET:HG2	2.21	0.41
1:C:20:LYS:HE3	1:C:82:PHE:CZ	2.56	0.41
1:A:71:HIS:HD1	2:B:300:LYS:HG3	1.86	0.41
1:C:283:HIS:HA	1:C:284:PRO:HD2	1.91	0.40
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.56	0.40
1:A:139:GLY:HA2	1:A:294:PRO:HD3	2.03	0.40
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.03	0.40
2:B:192:LYS:HB3	5:B:502:SGM:H31	2.04	0.40
2:D:346:PRO:O	2:D:349:LYS:HG2	2.22	0.40
1:A:295:HIS:CD2	1:A:296:LEU:HG	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH1	6:A:516:HOH:O[4_445]	2.06	0.14

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	293/299 (98%)	279 (95%)	12 (4%)	2 (1%)	26	21
1	C	296/299 (99%)	283 (96%)	11 (4%)	2 (1%)	26	21
2	B	256/258 (99%)	252 (98%)	4 (2%)	0	100	100
2	D	253/258 (98%)	246 (97%)	6 (2%)	1 (0%)	39	37
All	All	1098/1114 (99%)	1060 (96%)	33 (3%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
1	A	16	GLY
2	D	427	PRO
1	C	228	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	261/262 (100%)	250 (96%)	11 (4%)	36	35
1	C	262/262 (100%)	247 (94%)	15 (6%)	25	22
2	B	232/232 (100%)	225 (97%)	7 (3%)	48	51
2	D	229/232 (99%)	218 (95%)	11 (5%)	31	29
All	All	984/988 (100%)	940 (96%)	44 (4%)	35	32

All (44) 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	59[A]	ASN
1	A	59[B]	ASN
1	A	73	GLU
1	A	122	ARG
1	A	150	ARG
1	A	165	THR
1	A	178	LYS
1	A	248	PHE
2	B	232	LEU
2	B	284	ASP
2	B	292	LEU
2	B	296	HIS
2	B	348	LEU
2	B	374	GLU
2	B	432	LEU
1	C	37	LEU
1	C	55	LEU
1	C	75	LYS
1	C	101	LEU
1	C	103	LEU
1	C	122	ARG
1	C	137	THR
1	C	150	ARG
1	C	202	LEU
1	C	217	ARG
1	C	242	LYS
1	C	246	GLN
1	C	247	ASP
1	C	255	LEU
1	C	281	LEU
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	282	THR
2	D	285	THR
2	D	292	LEU
2	D	296	HIS
2	D	384	LEU
2	D	398	TYR

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Mol	Chain	Res	Type
2	D	411	GLU
2	D	428	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	246	GLN
2	B	254	GLN
2	B	296	HIS
2	B	312	ASN
2	B	395	HIS
1	C	59	ASN
1	C	60	HIS
1	C	71	HIS
1	C	85	GLN
1	C	211	GLN
2	D	179	HIS
2	D	254	GLN
2	D	296	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	0.72	0	7,14,16	1.40	0
1	TPO	C	160	1	8,10,11	0.67	0	7,14,16	1.39	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
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

There are no bond length outliers.

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 7 ligands modelled in this entry, 3 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	ATP	A	302	3	24,33,33	1.05	2 (8%)	31,52,52	1.94	4 (12%)
5	SGM	B	502	-	5,5,5	0.50	0	5,5,5	0.50	0
4	ATP	C	301	3	24,33,33	1.09	2 (8%)	31,52,52	1.89	4 (12%)
5	SGM	D	501	-	5,5,5	0.43	0	5,5,5	0.53	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	ATP	A	302	3	-	0/18/38/38	0/3/3/3
5	SGM	B	502	-	-	0/4/4/4	0/0/0/0
4	ATP	C	301	3	-	0/18/38/38	0/3/3/3
5	SGM	D	501	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	ATP	O4'-C1'	2.32	1.44	1.41
4	C	301	ATP	O4'-C1'	2.35	1.44	1.41
4	A	302	ATP	C5-C4	3.13	1.47	1.40
4	C	301	ATP	C5-C4	3.28	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	301	ATP	N3-C2-N1	-7.21	123.38	128.89
4	A	302	ATP	N3-C2-N1	-6.71	123.75	128.89
4	A	302	ATP	C2'-C1'-N9	-5.79	105.44	114.29
4	C	301	ATP	C2'-C1'-N9	-4.37	107.61	114.29
4	C	301	ATP	PB-O3B-PG	-3.36	121.41	132.67
4	A	302	ATP	C4-C5-N7	-3.00	106.72	109.48
4	C	301	ATP	C4-C5-N7	-2.64	107.05	109.48
4	A	302	ATP	PB-O3B-PG	-2.56	124.07	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	ATP	2	0
5	B	502	SGM	2	0
5	D	501	SGM	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^{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	294/299 (98%)	0.45	19 (6%) 22 29	17, 28, 62, 80	0
1	C	297/299 (99%)	1.44	81 (27%) 1 1	31, 53, 98, 116	0
2	B	258/258 (100%)	0.62	24 (9%) 11 15	19, 32, 51, 78	0
2	D	254/258 (98%)	1.06	48 (18%) 2 2	25, 50, 82, 96	0
All	All	1103/1114 (99%)	0.90	172 (15%) 3 4	17, 40, 82, 116	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	VAL	10.5
1	C	226	VAL	9.1
1	C	295[A]	HIS	9.1
2	B	175	VAL	9.0
1	A	95	ALA	8.4
1	C	15	TYR	8.0
1	A	96	LEU	7.8
1	C	234	PRO	7.6
1	C	233	MET	7.4
1	C	236	TYR	6.5
1	A	15	TYR	5.9
1	C	250	LYS	5.6
2	D	284	ASP	5.4
2	D	423	LEU	5.4
2	D	323	GLN	5.4
2	D	280	TYR	5.3
1	C	13	GLY	5.3
2	D	283	ASP	5.3
1	C	14	THR	5.2
1	C	287	GLN	5.2
1	C	244	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	249	SER	4.8
1	C	235	ASP	4.8
1	C	243	TRP	4.7
2	D	416	SER	4.7
1	C	247	ASP	4.6
2	D	392	MET	4.6
1	C	189	LEU	4.5
1	C	232	SER	4.5
1	C	228	PRO	4.4
2	D	399	LEU	4.4
1	C	251	VAL	4.4
1	C	293	VAL	4.4
2	B	284	ASP	4.4
2	D	429	THR	4.3
2	D	327	CYS	4.3
1	C	223	ASP	4.3
1	C	296	LEU	4.2
1	C	256	ASP	4.2
1	C	138	GLU	4.2
2	D	378	ARG	4.1
1	C	213	PHE	4.1
1	C	248	PHE	4.1
1	C	282	ALA	4.1
1	C	128	LEU	4.0
1	C	273	LYS	4.0
1	C	97	THR	3.9
1	A	73	GLU	3.9
1	A	36	ARG	3.9
2	B	431	ASN	3.8
1	C	12	GLU	3.8
1	C	19	TYR	3.7
1	C	229	GLY	3.6
1	C	-1	GLY	3.6
1	C	36	ARG	3.6
1	A	97	THR	3.5
2	D	271	TYR	3.5
1	C	184	VAL	3.5
2	D	419	HIS	3.4
1	C	230	VAL	3.4
2	B	260	ALA	3.4
1	C	231	THR	3.4
2	B	341	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	337	GLY	3.3
2	D	395	HIS	3.2
2	D	428	GLU	3.2
1	A	296	LEU	3.2
1	C	188	SER	3.1
2	B	236	VAL	3.1
1	C	288	ASP	3.1
2	B	323	GLN	3.1
1	C	227	TRP	3.0
1	A	37	LEU	3.0
2	D	324	PRO	3.0
2	B	283	ASP	3.0
1	C	102	PRO	3.0
1	C	177	CYS	3.0
2	D	235	ALA	3.0
1	A	297	ARG	2.9
1	C	222	PRO	2.9
2	D	232	LEU	2.9
1	C	179	TYR	2.9
2	B	280	TYR	2.9
2	D	177	ASP	2.9
2	D	400	LYS	2.9
2	D	311	VAL	2.9
1	C	246	GLN	2.9
2	B	232	LEU	2.9
1	C	284	PRO	2.9
1	C	240	PHE	2.8
2	D	341	LEU	2.8
2	D	197	VAL	2.8
1	C	258	ASP	2.8
1	C	187	TRP	2.8
1	C	192	ILE	2.8
1	A	295	HIS	2.8
2	D	426	PRO	2.7
2	D	336	LEU	2.7
2	D	339	LEU	2.7
1	C	209	ILE	2.7
1	C	2	GLU	2.7
2	B	234	LEU	2.7
2	D	365	TYR	2.7
1	C	241	PRO	2.7
2	D	326	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	255	LEU	2.6
2	D	385	GLU	2.6
1	C	257	GLU	2.6
2	D	334	MET	2.6
2	D	180	GLU	2.6
2	B	176	PRO	2.5
1	C	133	LEU	2.5
2	D	427	PRO	2.5
2	D	285	THR	2.5
2	D	310	THR	2.5
1	C	178	LYS	2.5
2	B	403	GLN	2.5
1	A	19	TYR	2.5
1	C	101	LEU	2.5
1	C	245	ARG	2.5
2	D	340	SER	2.5
2	B	198	GLY	2.5
2	B	336	LEU	2.4
1	A	16	GLY	2.4
1	A	74	ASN	2.4
2	B	324	PRO	2.4
1	C	143	LEU	2.4
2	D	233	HIS	2.4
1	C	224	GLU	2.4
2	D	315	LEU	2.4
2	D	328	LYS	2.4
2	D	388	LYS	2.3
2	D	386	SER	2.3
1	A	17	VAL	2.3
1	C	123	VAL	2.3
1	C	108	LEU	2.3
1	C	112	LEU	2.3
2	B	259	ALA	2.3
2	B	428	GLU	2.3
2	D	234	LEU	2.3
2	B	429	THR	2.2
2	D	356	ALA	2.2
2	D	403	GLN	2.2
2	B	233	HIS	2.2
1	C	253	PRO	2.2
2	D	374	GLU	2.2
1	C	7	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	181	ASP	2.2
2	D	333	ALA	2.2
1	C	291	LYS	2.2
1	C	111	LEU	2.2
2	B	430	LEU	2.1
1	C	254	PRO	2.1
1	C	206	ASP	2.1
1	C	272	ASN	2.1
1	C	96	LEU	2.1
1	C	9	LYS	2.1
1	C	260	ARG	2.1
1	C	186	ILE	2.1
1	A	71	HIS	2.1
2	B	235	ALA	2.1
1	A	187	TRP	2.1
1	A	115	LEU	2.1
2	B	257	GLY	2.1
1	A	206[A]	ASP	2.1
1	C	8	GLU	2.0
1	C	94	SER	2.0
1	C	221	THR	2.0
1	A	75	LYS	2.0
2	D	325	ALA	2.0
2	B	311	VAL	2.0
1	C	242	LYS	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	0.96	0.11	-	41,45,51,51	0
1	TPO	A	160	11/12	0.99	0.08	-	22,22,23,24	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
5	SGM	D	501	6/6	0.81	0.37	5.12	59,61,64,65	0
5	SGM	B	502	6/6	0.91	0.27	4.38	48,50,52,57	0
4	ATP	A	302	31/31	0.94	0.14	-0.15	29,36,52,52	4
4	ATP	C	301	31/31	0.92	0.15	-0.42	43,54,58,59	4
3	MG	B	501	1/1	0.96	0.10	-0.73	40,40,40,40	0
3	MG	A	301	1/1	0.92	0.06	-	37,37,37,37	0
3	MG	C	302	1/1	0.80	0.07	-	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.