Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:31 PM GMT

PDB ID	:	4CFH
Title	:	Structure of an active form of mammalian AMPK
Authors	:	Xiao, B.; Sanders, M.J.; Underwood, E.; Heath, R.; Mayer, F.; Carmena, D.; Jing, C.; Walker, P.A.; Eccleston, J.F.; Haire, L.F.; Saiu, P.; Howell, S.A.; Aasland, R.; Martin, S.R.; Carling, D.; Gamblin, S.J.
Deposited on	:	2013-11-18
Resolution	:	3.24 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:

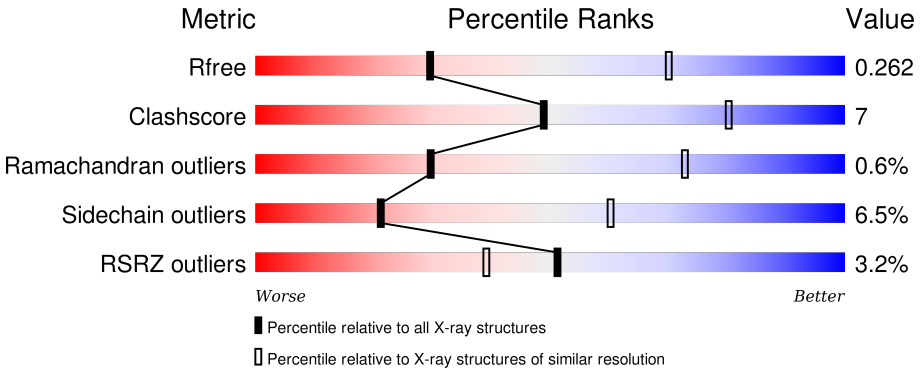
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.24 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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	493	4% 62% 17% • 18%
2	B	87	61% 17% • 21%
3	C	27	70% 7% 22%
4	E	330	2% 67% 22% • 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6429 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 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	402	3217	2059	565	576	1	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP P54645
A	-17	SER	-	EXPRESSION TAG	UNP P54645
A	-16	HIS	-	EXPRESSION TAG	UNP P54645
A	-15	HIS	-	EXPRESSION TAG	UNP P54645
A	-14	HIS	-	EXPRESSION TAG	UNP P54645
A	-13	HIS	-	EXPRESSION TAG	UNP P54645
A	-12	HIS	-	EXPRESSION TAG	UNP P54645
A	-11	HIS	-	EXPRESSION TAG	UNP P54645
A	-10	SER	-	EXPRESSION TAG	UNP P54645
A	-9	SER	-	EXPRESSION TAG	UNP P54645
A	-8	GLY	-	EXPRESSION TAG	UNP P54645
A	-7	LEU	-	EXPRESSION TAG	UNP P54645
A	-6	GLU	-	EXPRESSION TAG	UNP P54645
A	-5	VAL	-	EXPRESSION TAG	UNP P54645
A	-4	LEU	-	EXPRESSION TAG	UNP P54645
A	-3	PHE	-	EXPRESSION TAG	UNP P54645
A	-2	GLN	-	EXPRESSION TAG	UNP P54645
A	-1	GLY	-	EXPRESSION TAG	UNP P54645
A	0	PRO	-	EXPRESSION TAG	UNP P54645
A	1	MET	-	EXPRESSION TAG	UNP P54645
A	471	LEU	-	SEE REMARK 999	UNP P54645
A	472	GLU	-	SEE REMARK 999	UNP P54645
A	473	VAL	-	SEE REMARK 999	UNP P54645
A	474	LEU	-	SEE REMARK 999	UNP P54645

- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-

2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			550	360	92	95	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	MET	-	EXPRESSION TAG	UNP O43741

- Molecule 3 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	S	0	0	0
			164	107	26	29	2			

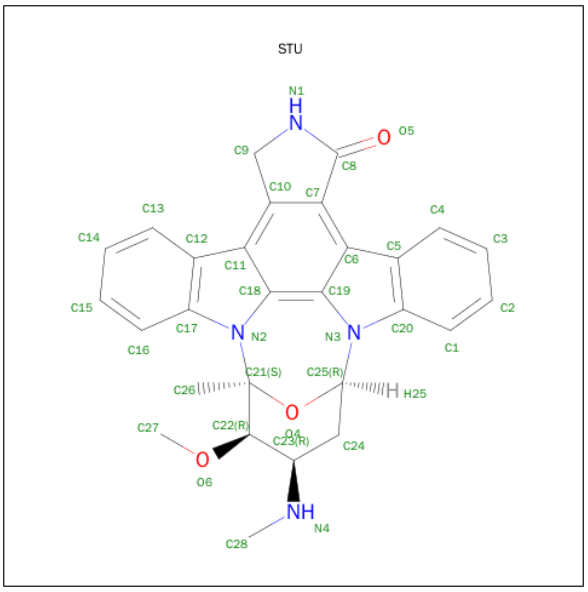
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	522	PHE	-	SEE REMARK 999	UNP P54645
C	523	GLN	-	SEE REMARK 999	UNP P54645

- Molecule 4 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1.

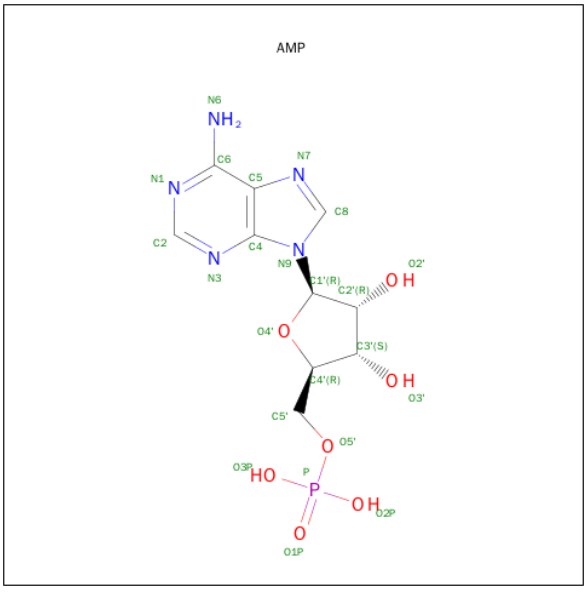
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	301	Total	C	N	O	S	0	0	0
			2417	1568	403	439	7			

- Molecule 5 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



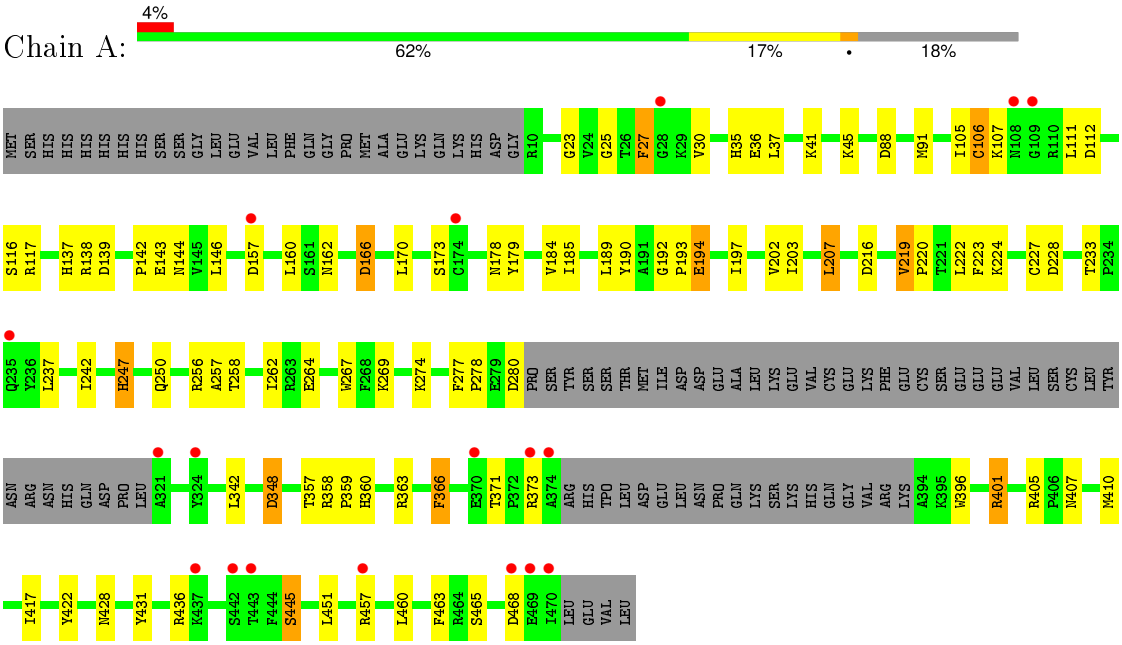
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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.

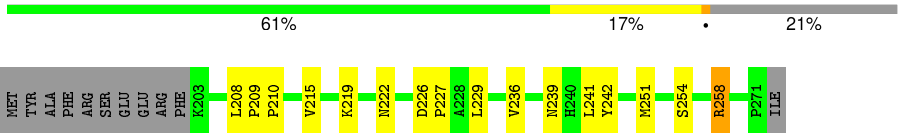
• Molecule 1: 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1

Chain A:



• Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-2

Chain B:

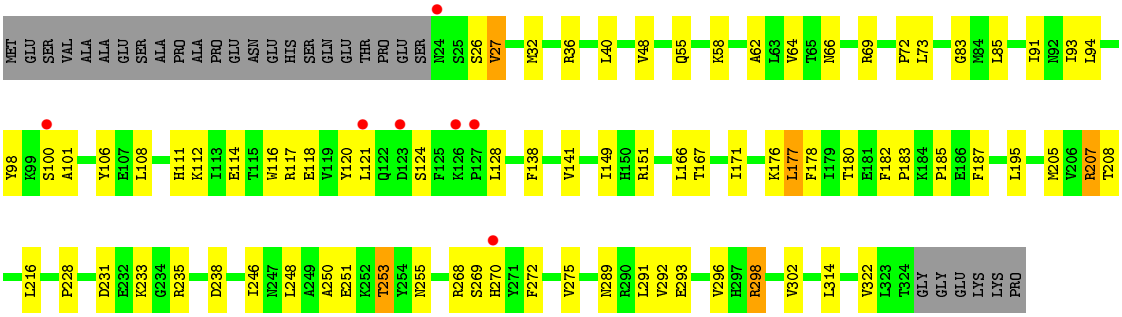


• Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1

Chain C:

• Molecule 4: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1

Chain E:


MET GLU SER VAL ALA ALA GLU SER ALA PRO ALA PRO GLU ASN GLU HIS SER GLN GLU THR PRO GLU SER N24 S25 S26 V27 M32 R36 L40 V48 Q55 K58 A62 L63 V64 T65 M66 R69 F72 L73 G83 M84 L85 I91 N92 I93 L94
Y98 K99 S100 A101 Y106 E107 L108 H111 K112 I113 E114 T115 W116 R117 E118 Y119 Y120 L121 Q122 D123 S124 F125 K126 P127 L128 F138 V141 I149 H150 R151 L166 T167 I171 K176 L177 F178 I179 T180 E181 F182 P183 K184 P185 E186 F187 L195 M205 V206 R207 T208
L216 P228 D231 E232 K233 G234 R235 D238 I246 N247 L248 A249 A250 E251 K252 T253 Y254 N255 R268 S269 H270 Y271 F272 V275 N289 R290 L291 V292 E293 V296 H297 R298 V302 L314 V322 L323 T324 GLY GLY GLU LYS LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.92Å 133.92Å 141.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.53 – 3.24 29.53 – 3.24	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.53-3.24) 86.9 (29.53-3.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.233 , 0.268 0.225 , 0.262	Depositor DCC
R_{free} test set	943 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	110.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 19628 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6429	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, STU, AMP

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	0.22	0/3282	0.42	0/4440
2	B	0.22	0/565	0.42	0/772
3	C	0.22	0/167	0.36	0/223
4	E	0.23	0/2468	0.42	0/3353
All	All	0.23	0/6482	0.42	0/8788

There are no bond length outliers.

There are no bond angle outliers.

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	3217	0	3182	53	0
2	B	550	0	585	10	0
3	C	164	0	165	0	0
4	E	2417	0	2477	36	0
5	A	35	0	26	4	0
6	E	46	0	24	2	0
All	All	6429	0	6459	93	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 7.

All (93) 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:23:GLY:HA3	1:A:30:VAL:HB	1.70	0.72
1:A:264:GLU:HA	1:A:269:LYS:HE3	1.75	0.68
1:A:363:ARG:HB3	2:B:227:PRO:HG3	1.76	0.67
1:A:142:PRO:HD3	1:A:203:ILE:HG12	1.76	0.66
1:A:417:ILE:HG23	1:A:422:TYR:HB2	1.77	0.65
4:E:93:ILE:HG21	4:E:108:LEU:HD13	1.77	0.65
2:B:226:ASP:HB3	2:B:229:LEU:HG	1.76	0.65
4:E:73:LEU:HD21	4:E:85:LEU:HB2	1.79	0.64
1:A:139:ASP:HB2	1:A:160:LEU:HD12	1.80	0.64
1:A:348:ASP:N	1:A:348:ASP:OD1	2.29	0.63
1:A:143:GLU:HB3	5:A:1550:STU:H281	1.79	0.63
1:A:179:TYR:HA	1:A:202:VAL:HG21	1.80	0.62
5:A:1550:STU:H16	5:A:1550:STU:H261	1.81	0.62
1:A:45:LYS:HB3	1:A:91:MET:HB2	1.81	0.61
1:A:185:ILE:HD13	1:A:223:PHE:HB3	1.83	0.60
4:E:69:ARG:NH2	6:E:1325:AMP:O2P	2.33	0.58
1:A:139:ASP:O	1:A:144:ASN:ND2	2.34	0.58
1:A:463:PHE:HB2	2:B:241:LEU:HB3	1.86	0.57
1:A:233:THR:HG21	1:A:242:ILE:HG23	1.86	0.57
4:E:40:LEU:HD12	4:E:166:LEU:HD11	1.86	0.57
1:A:358:ARG:HD2	1:A:359:PRO:HD2	1.87	0.57
1:A:138:ARG:NH1	1:A:190:TYR:OH	2.37	0.56
1:A:277:PHE:HB3	1:A:278:PRO:HD2	1.87	0.56
1:A:363:ARG:NH1	2:B:222:ASN:O	2.39	0.56
1:A:436:ARG:NH1	1:A:445:SER:OG	2.40	0.55
4:E:289:ASN:O	4:E:293:GLU:HG2	2.07	0.54
4:E:32:MET:O	4:E:138:PHE:N	2.42	0.53
1:A:35:HIS:CE1	1:A:37:LEU:HB2	2.43	0.53
1:A:105:ILE:O	1:A:107:LYS:N	2.42	0.53
1:A:360:HIS:HB3	1:A:363:ARG:HG2	1.90	0.53
1:A:117:ARG:NH1	1:A:267:TRP:O	2.37	0.53
1:A:166:ASP:OD1	1:A:166:ASP:N	2.41	0.52
1:A:166:ASP:OD2	2:B:258:ARG:NH1	2.42	0.52
1:A:105:ILE:HG22	1:A:106:CYS:H	1.74	0.52
1:A:428:ASN:HB2	1:A:431:TYR:HB3	1.90	0.52
4:E:91:ILE:HG23	4:E:216:LEU:HD22	1.91	0.52
1:A:173:SER:HA	1:A:184:VAL:HG13	1.92	0.51
4:E:205:MET:HB3	4:E:228:PRO:HG2	1.92	0.51
4:E:94:LEU:O	4:E:98:TYR:HB2	2.10	0.51
4:E:177:LEU:HB3	4:E:178:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:207:ARG:HH21	4:E:231:ASP:HA	1.76	0.51
4:E:187:PHE:HB2	4:E:195:LEU:HD21	1.93	0.49
1:A:216:ASP:HB3	1:A:222:LEU:HB2	1.94	0.48
1:A:396:TRP:HB2	2:B:215:VAL:HG11	1.94	0.48
1:A:219:VAL:HG23	1:A:220:PRO:HD3	1.95	0.48
1:A:25:GLY:H	5:A:1550:STU:C26	2.27	0.48
4:E:27:VAL:HG11	4:E:185:PRO:HG3	1.95	0.48
4:E:233:LYS:HB2	4:E:235:ARG:HG3	1.96	0.47
1:A:422:TYR:CE1	1:A:436:ARG:HG3	2.50	0.47
4:E:55:GLN:HA	4:E:112:LYS:HA	1.97	0.47
1:A:366:PHE:HD1	4:E:64:VAL:HG13	1.80	0.46
2:B:208:LEU:HD12	2:B:209:PRO:HD2	1.97	0.46
2:B:209:PRO:HA	2:B:210:PRO:HD3	1.78	0.46
4:E:149:ILE:HG12	4:E:151:ARG:H	1.81	0.46
4:E:58:LYS:HB2	4:E:58:LYS:HE3	1.81	0.46
4:E:100:SER:HA	4:E:101:ALA:HA	1.53	0.45
1:A:137:HIS:NE2	1:A:157:ASP:O	2.47	0.45
4:E:248:LEU:HA	4:E:253:THR:HG23	1.98	0.45
4:E:298:ARG:NH1	6:E:1325:AMP:O1P	2.32	0.45
1:A:192:GLY:N	1:A:194:GLU:OE2	2.48	0.45
4:E:176:LYS:HG2	4:E:292:VAL:HG21	1.98	0.45
1:A:250:GLN:HB2	1:A:256:ARG:HA	1.97	0.45
1:A:162:ASN:ND2	1:A:170:LEU:HD22	2.32	0.45
1:A:233:THR:HB	1:A:237:LEU:HD23	2.00	0.44
4:E:180:THR:HG22	4:E:182:PHE:H	1.82	0.44
1:A:258:THR:O	1:A:262:ILE:HG13	2.18	0.44
4:E:138:PHE:CE1	4:E:322:VAL:HG23	2.52	0.44
1:A:410:MET:HE3	1:A:451:LEU:HB2	1.99	0.44
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.58	0.43
4:E:251:GLU:HB2	4:E:253:THR:HG22	2.00	0.43
1:A:465:SER:HB3	2:B:239:ASN:HB3	2.01	0.43
4:E:141:VAL:HG22	4:E:171:ILE:HD13	2.00	0.43
1:A:247:HIS:CG	1:A:257:ALA:HB2	2.54	0.43
4:E:62:ALA:O	4:E:66:ASN:ND2	2.43	0.43
4:E:117:ARG:O	4:E:121:LEU:HB3	2.18	0.43
2:B:242:TYR:O	2:B:254:SER:N	2.52	0.43
4:E:269:SER:OG	4:E:270:HIS:N	2.52	0.43
4:E:83:GLY:HA2	4:E:128:LEU:HD13	2.00	0.43
1:A:193:PRO:O	1:A:197:ILE:HG12	2.20	0.42
4:E:93:ILE:HG12	4:E:116:TRP:CZ2	2.55	0.42
4:E:48:VAL:O	4:E:72:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:HB3	1:A:460:LEU:HD23	2.01	0.41
4:E:246:ILE:O	4:E:250:ALA:N	2.52	0.41
1:A:36:GLU:HG3	1:A:37:LEU:HD13	2.02	0.41
1:A:146:LEU:HD21	5:A:1550:STU:H241	2.03	0.41
1:A:274:LYS:HG3	1:A:280:ASP:H	1.86	0.41
1:A:116:SER:HB2	1:A:207:LEU:HB3	2.01	0.41
4:E:180:THR:O	4:E:183:PRO:HD2	2.21	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.95	0.41
1:A:373:ARG:HA	1:A:373:ARG:HD3	1.91	0.41
4:E:238:ASP:OD1	4:E:268:ARG:NH2	2.54	0.41
1:A:468:ASP:OD1	1:A:468:ASP:N	2.54	0.41
4:E:114:GLU:O	4:E:118:GLU:HG3	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	395/493 (80%)	358 (91%)	35 (9%)	2 (0%)	34 75
2	B	67/87 (77%)	61 (91%)	6 (9%)	0	100 100
3	C	19/27 (70%)	19 (100%)	0	0	100 100
4	E	299/330 (91%)	280 (94%)	16 (5%)	3 (1%)	19 62
All	All	780/937 (83%)	718 (92%)	57 (7%)	5 (1%)	30 73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	26	SER
1	A	27	PHE
1	A	106	CYS

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Mol	Chain	Res	Type
4	E	27	VAL
4	E	124	SER

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	346/446 (78%)	323 (93%)	23 (7%)	21 60
2	B	66/81 (82%)	62 (94%)	4 (6%)	23 63
3	C	18/23 (78%)	16 (89%)	2 (11%)	8 32
4	E	274/299 (92%)	257 (94%)	17 (6%)	23 63
All	All	704/849 (83%)	658 (94%)	46 (6%)	21 60

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

Mol	Chain	Res	Type
1	A	27	PHE
1	A	41	LYS
1	A	88	ASP
1	A	111	LEU
1	A	112	ASP
1	A	166	ASP
1	A	178	ASN
1	A	189	LEU
1	A	194	GLU
1	A	207	LEU
1	A	219	VAL
1	A	224	LYS
1	A	228	ASP
1	A	247	HIS
1	A	348	ASP
1	A	357	THR
1	A	366	PHE
1	A	371	THR
1	A	401	ARG

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Mol	Chain	Res	Type
1	A	405	ARG
1	A	407	ASN
1	A	445	SER
1	A	457	ARG
2	B	219	LYS
2	B	236	VAL
2	B	251	MET
2	B	258	ARG
3	C	537	GLU
3	C	542	LEU
4	E	36	ARG
4	E	106	TYR
4	E	111	HIS
4	E	120	TYR
4	E	167	THR
4	E	177	LEU
4	E	207	ARG
4	E	208	THR
4	E	253	THR
4	E	255	ASN
4	E	272	PHE
4	E	275	VAL
4	E	291	LEU
4	E	296	VAL
4	E	298	ARG
4	E	302	VAL
4	E	314	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	172	1	8,10,11	0.94	0	7,14,16	1.22	1 (14%)

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	172	1	-	0/8/11/13	0/0/0/0

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	172	TPO	O-C-CA	-2.39	119.12	125.44

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)

3 ligands 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	$\#\|Z\| > 2$
5	STU	A	1550	-	27,42,42	0.82	0	23,68,68	1.43	4 (17%)
6	AMP	E	1325	-	20,25,25	0.96	1 (5%)	22,38,38	1.74	2 (9%)
6	AMP	E	1326	-	20,25,25	0.94	1 (5%)	22,38,38	1.76	2 (9%)

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
5	STU	A	1550	-	-	0/4/42/42	0/0/8/8
6	AMP	E	1325	-	-	0/6/26/26	0/3/3/3
6	AMP	E	1326	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1326	AMP	C5-C4	3.06	1.47	1.40
6	E	1325	AMP	C5-C4	3.17	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1326	AMP	N3-C2-N1	-6.51	123.91	128.89
6	E	1325	AMP	N3-C2-N1	-6.49	123.93	128.89
5	A	1550	STU	C27-O6-C22	-3.71	107.29	114.39
6	E	1325	AMP	C4-C5-N7	-3.08	106.64	109.48
6	E	1326	AMP	C4-C5-N7	-3.02	106.70	109.48
5	A	1550	STU	C3-C4-C5	-2.21	116.98	120.79
5	A	1550	STU	O5-C8-C7	-2.02	125.24	128.62
5	A	1550	STU	C13-C12-C17	2.21	122.19	119.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1550	STU	4	0
6	E	1325	AMP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	401/493 (81%)	0.18	18 (4%) 37 26	66, 108, 156, 196	0
2	B	69/87 (79%)	-0.06	0 100 100	62, 82, 134, 178	0
3	C	21/27 (77%)	-0.08	0 100 100	72, 96, 130, 166	0
4	E	301/330 (91%)	-0.03	7 (2%) 64 52	61, 89, 157, 199	0
All	All	792/937 (84%)	0.07	25 (3%) 51 39	61, 97, 157, 199	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	ILE	4.8
4	E	123	ASP	4.6
1	A	374	ALA	4.0
1	A	174	CYS	3.9
1	A	109	GLY	3.7
1	A	469	GLU	3.5
4	E	24	ASN	3.1
4	E	270	HIS	3.0
4	E	100	SER	2.7
1	A	437	LYS	2.7
4	E	121	LEU	2.6
1	A	235	GLN	2.6
1	A	373	ARG	2.6
1	A	443	THR	2.5
4	E	126	LYS	2.5
1	A	108	ASN	2.3
1	A	324	TYR	2.3
4	E	127	PRO	2.3
1	A	370	GLU	2.2
1	A	321	ALA	2.2
1	A	457	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLY	2.1
1	A	468	ASP	2.1
1	A	157	ASP	2.0
1	A	442	SER	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	A	172	11/12	0.94	0.13	-	77,107,118,121	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	STU	A	1550	35/35	0.95	0.21	-0.42	84,110,121,126	0
6	AMP	E	1325	23/23	0.94	0.22	-0.42	67,74,79,89	0
6	AMP	E	1326	23/23	0.95	0.19	-0.53	75,80,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.