Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:56 PM GMT

PDB ID	:	4QFR
Title	:	Structure of AMPK in complex with Cl-A769662 activator and STAUROSPORINE inhibitor
Authors	:	Calabrese, M.F.; Kurumbail, R.G.
Deposited on	:	2014-05-21
Resolution	:	3.34 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:

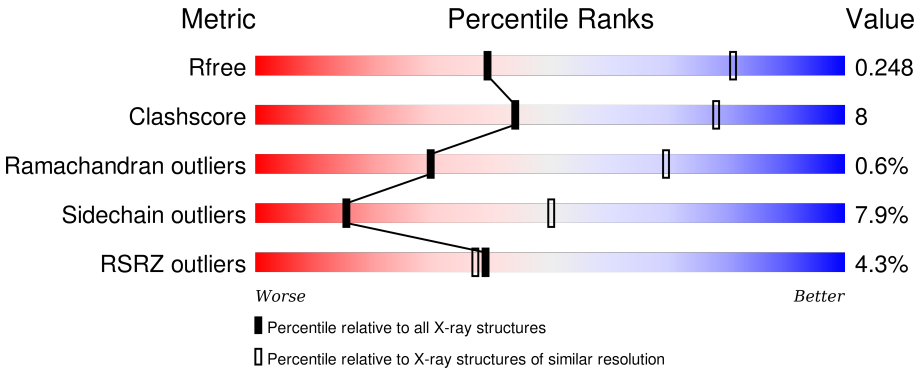
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.34 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	503	2% 59% 12% 28%
2	B	204	2% 58% 19% 22%
3	C	330	6% 64% 17% 15%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	604	-	-	-	X
5	CL	B	301	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6516 atoms, of which 26 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
1	A	362	Total	C	N	O	P	S	0	0	0
			2943	1888	514	522	1	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P54645
A	517	ALA	-	SEE REMARK 999	UNP P54645
A	518	SER	-	SEE REMARK 999	UNP P54645
A	519	GLY	-	SEE REMARK 999	UNP P54645
A	520	GLY	-	SEE REMARK 999	UNP P54645
A	521	PRO	-	SEE REMARK 999	UNP P54645
A	522	GLY	-	SEE REMARK 999	UNP P54645
A	523	GLY	-	SEE REMARK 999	UNP P54645
A	524	SER	-	SEE REMARK 999	UNP P54645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1245	810	209	223	3			

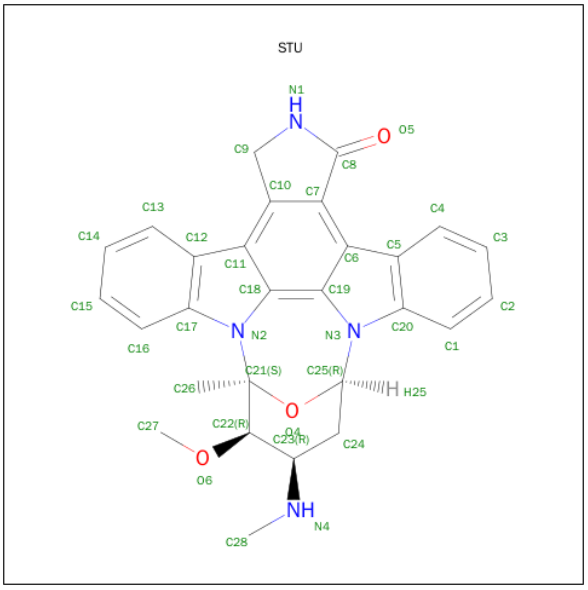
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	EXPRESSION TAG	UNP P80386
B	108	ASP	SER	ENGINEERED MUTATION	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	279	Total	C	N	O	S	0	0	0
			2157	1402	362	387	6			

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).

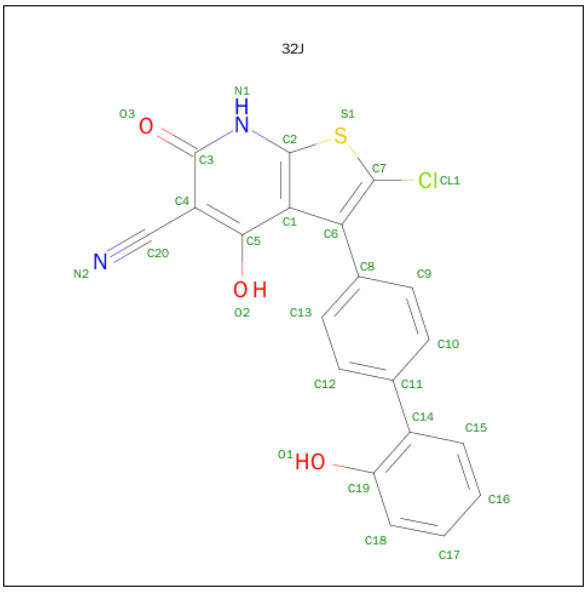


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			61	28	26	4	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

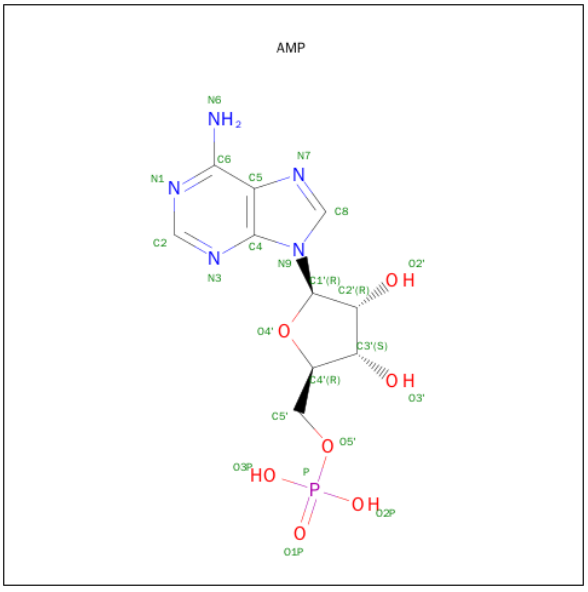
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	4	Total	Cl	0	0
			4	4		

- Molecule 6 is 2-CHLORO-4-HYDROXY-3-(2'-HYDROXYBIPHENYL-4-YL)-6-OXO-6,7-DIHYDROTHIENO[2,3-B]PYRIDINE-5-CARBONITRILE (three-letter code: 32J) (formula: $C_{20}H_{11}ClN_2O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	S	0	0
			27	20	1	2	3	1		

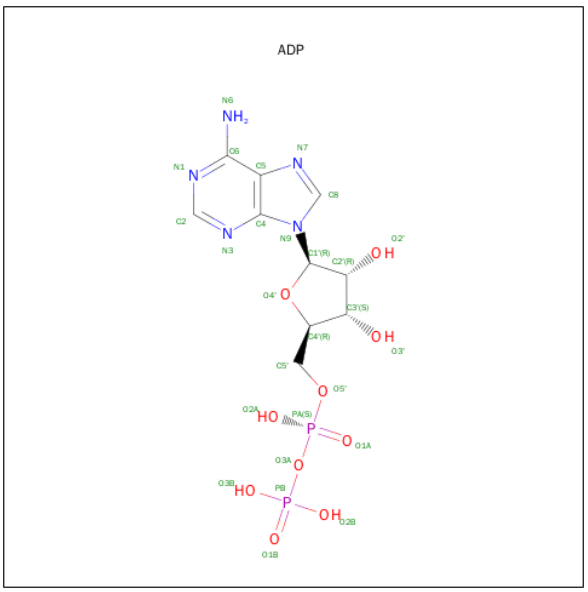
- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

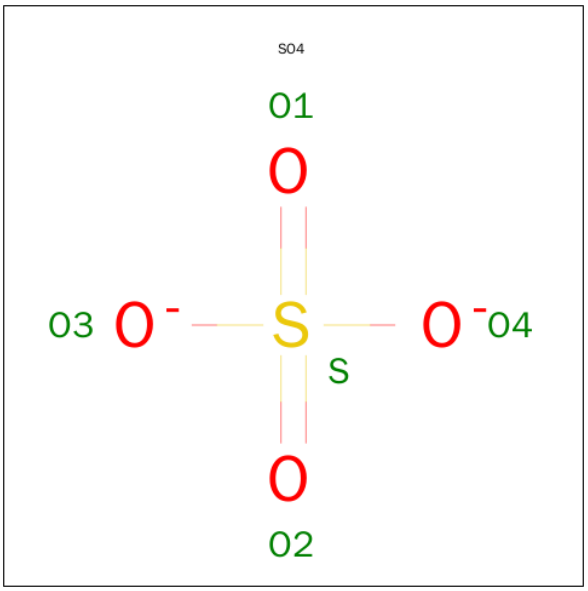
- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



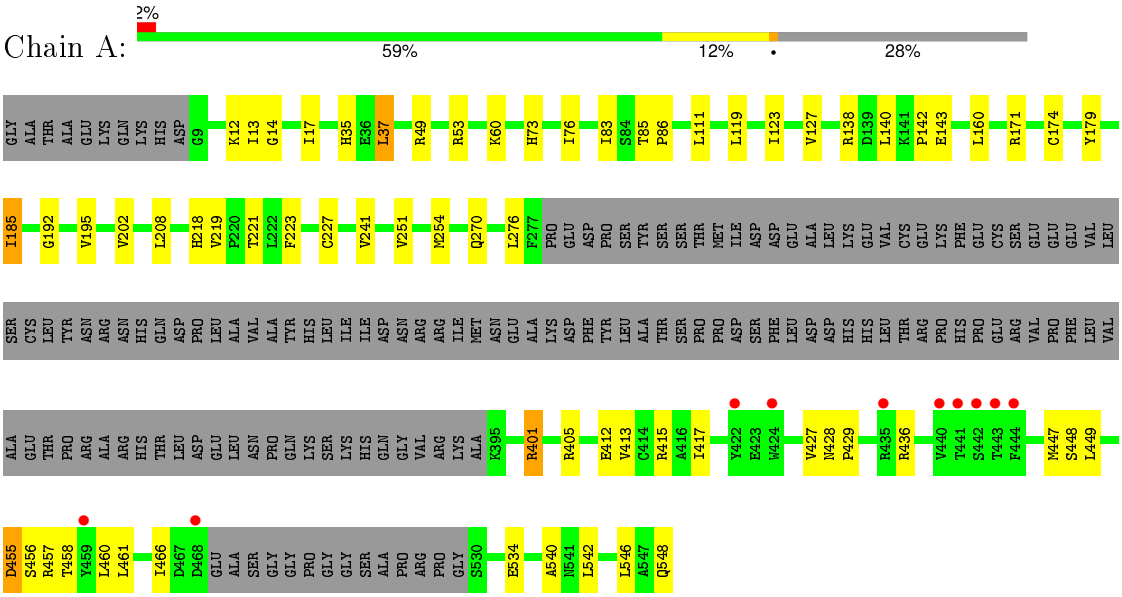
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	O	S		0	0
			5	4	1			

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.

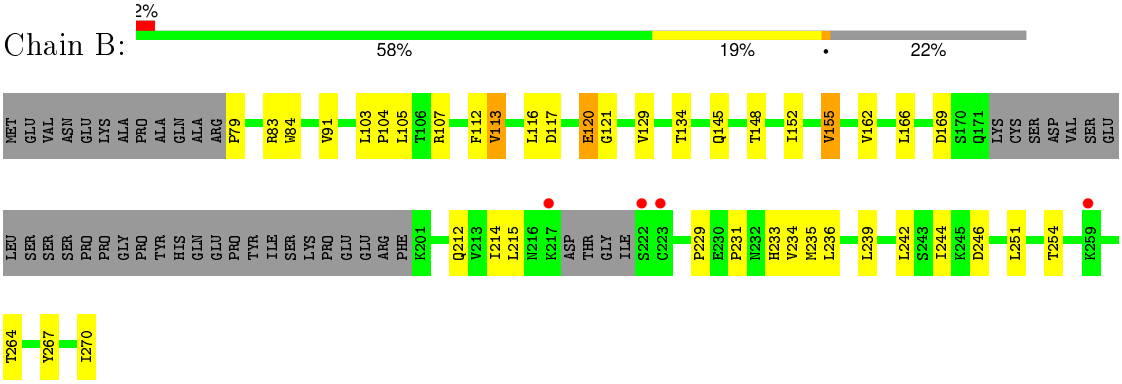
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1

Chain A:



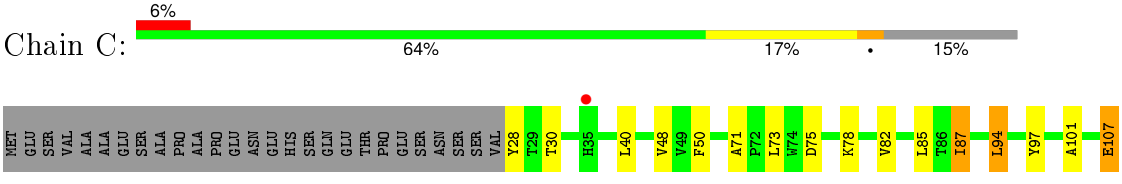
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

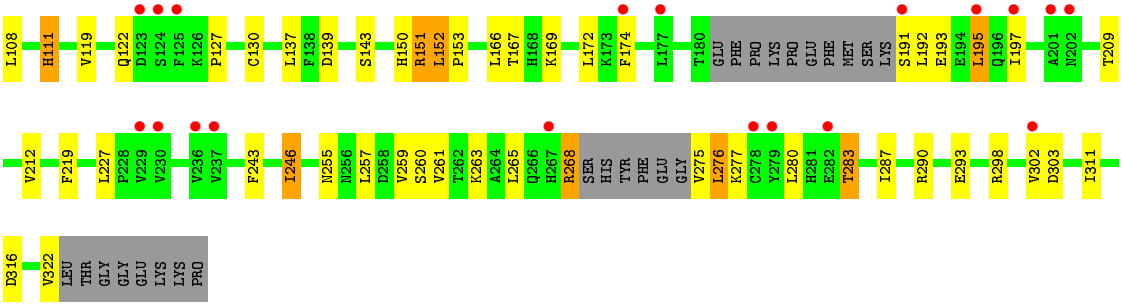
Chain B:



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

Chain C:




L108 H111 V119 Q122 D123 S124 F125 K126 P127 C130 L137 F138 D139 S143 H150 R151 L152 P153 L166 T167 H168 K169 L172 K173 F174 L177 T180 GLU PHE PRO LYS PRO GLU PHE MET SER LYS S191 L192 E193 E194 L195 Q196 I197 A201 N202 T209
V212 F219 L227 P228 V229 V230 V236 V237 F243 I246 N255 N256 L257 D258 V259 S260 V261 T262 K263 A264 L265 Q266 H267 R268 SER HIS TYR PHE GLU GLY V275 L276 K277 C278 Y279 L280 H281 E282 T283 I287 R290 E293 R298 V302 D303 I311
D316 V322 LEU THR GLY GLY GLU LYS LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.62Å 124.62Å 402.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 3.34 29.85 – 3.34	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.85-3.34) 96.6 (29.85-3.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 3.31Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.210 , 0.249 0.205 , 0.248	Depositor DCC
R_{free} test set	1352 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	84.1	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 97.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 27060 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6516	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: ADP, STU, TPO, CL, 32J, SO4, 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	0.51	0/2997	0.77	1/4040 (0.0%)
2	B	0.52	0/1279	0.75	0/1745
3	C	0.46	0/2197	0.67	0/2995
All	All	0.49	0/6473	0.73	1/8780 (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	14	GLY	N-CA-C	-5.92	98.29	113.10

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	2943	0	2974	37	0
2	B	1245	0	1232	18	0
3	C	2157	0	2171	45	0
4	A	35	26	26	6	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	46	0	24	3	0
8	C	27	0	12	1	0
9	C	5	0	0	0	0
All	All	6490	26	6448	103	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 8.

All (103) 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)
3:C:152:LEU:HD12	3:C:153:PRO:N	1.54	1.21
3:C:152:LEU:HD12	3:C:153:PRO:CD	1.77	1.12
3:C:152:LEU:CD1	3:C:153:PRO:HD2	1.89	1.03
3:C:152:LEU:HD12	3:C:153:PRO:HD2	1.47	0.95
3:C:151:ARG:NH1	3:C:167:THR:HG21	1.95	0.81
4:A:601:STU:H16	4:A:601:STU:H261	1.60	0.80
3:C:243:PHE:HB3	7:C:402:AMP:H5'1	1.64	0.80
3:C:152:LEU:HD13	3:C:153:PRO:HD2	1.66	0.76
3:C:152:LEU:CD1	3:C:153:PRO:CD	2.53	0.74
3:C:130:CYS:HA	3:C:152:LEU:HD11	1.71	0.73
3:C:193:GLU:HB2	3:C:280:LEU:HB3	1.75	0.69
4:A:601:STU:C17	4:A:601:STU:H273	2.25	0.67
1:A:218:HIS:CD2	1:A:221:THR:HG23	2.31	0.66
3:C:191:SER:HA	3:C:283:THR:HA	1.79	0.65
1:A:455:ASP:HB2	1:A:458:THR:HG22	1.79	0.64
3:C:152:LEU:C	3:C:152:LEU:HD12	2.15	0.63
3:C:275:VAL:HG21	3:C:277:LYS:HE3	1.80	0.62
1:A:160:LEU:HD13	1:A:174:CYS:HB2	1.82	0.62
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.82	0.61
1:A:455:ASP:HB3	1:A:457:ARG:H	1.66	0.61
2:B:79:PRO:HA	2:B:117:ASP:HA	1.84	0.60
3:C:97:TYR:HB3	3:C:107:GLU:HG3	1.83	0.60
3:C:40:LEU:HD21	3:C:174:PHE:HB2	1.84	0.60
3:C:150:HIS:ND1	8:C:403:ADP:O2A	2.35	0.59
2:B:120:GLU:HA	2:B:155:VAL:HG13	1.84	0.58
3:C:169:LYS:NZ	7:C:402:AMP:O1P	2.28	0.58
2:B:107:ARG:HD3	2:B:112:PHE:CZ	2.39	0.57
1:A:218:HIS:HD2	1:A:221:THR:HG23	1.68	0.57
3:C:107:GLU:O	3:C:111:HIS:HB2	2.04	0.57
2:B:214:ILE:HB	2:B:229:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:CYS:HA	3:C:152:LEU:CD1	2.34	0.57
3:C:151:ARG:NH1	3:C:167:THR:CG2	2.66	0.57
2:B:121:GLY:H	2:B:155:VAL:HG13	1.70	0.56
1:A:540:ALA:HB2	2:B:251:LEU:HD11	1.86	0.56
2:B:244:ILE:HG21	2:B:270:ILE:HD11	1.89	0.55
3:C:219:PHE:CE1	3:C:227:LEU:HG	2.43	0.53
1:A:413:VAL:O	1:A:417:ILE:HG13	2.08	0.53
1:A:449:LEU:HD23	1:A:461:LEU:HD21	1.91	0.53
3:C:209:THR:HA	3:C:260:SER:HB2	1.91	0.53
1:A:179:TYR:HD2	1:A:202:VAL:HG23	1.72	0.53
2:B:233:HIS:HA	2:B:236:LEU:HD12	1.90	0.53
1:A:119:LEU:O	1:A:123:ILE:HD12	2.10	0.52
2:B:162:VAL:O	2:B:166:LEU:HG	2.11	0.51
4:A:601:STU:H273	4:A:601:STU:C16	2.40	0.50
3:C:152:LEU:CD1	3:C:153:PRO:O	2.59	0.50
1:A:179:TYR:CD2	1:A:202:VAL:HG23	2.46	0.49
2:B:103:LEU:HD12	2:B:104:PRO:HD2	1.94	0.49
2:B:267:TYR:HB2	3:C:50:PHE:HD1	1.77	0.49
3:C:75:ASP:HB3	3:C:78:LYS:HB2	1.93	0.49
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.93	0.48
3:C:152:LEU:HD11	3:C:153:PRO:O	2.13	0.48
1:A:49:ARG:O	1:A:53:ARG:HG2	2.14	0.48
3:C:265:LEU:HD22	3:C:268:ARG:NH1	2.29	0.48
1:A:12:LYS:HG2	1:A:17:ILE:HG22	1.96	0.48
1:A:436:ARG:HH22	1:A:534:GLU:HG2	1.78	0.48
1:A:401:ARG:O	1:A:548:GLN:HB3	2.14	0.47
3:C:152:LEU:CD1	3:C:153:PRO:N	2.49	0.47
4:A:601:STU:C16	4:A:601:STU:H261	2.30	0.47
3:C:40:LEU:HD12	3:C:137:LEU:HD11	1.97	0.47
1:A:73:HIS:HB3	1:A:76:ILE:HD12	1.97	0.46
3:C:151:ARG:CZ	3:C:167:THR:HG21	2.45	0.46
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.56	0.46
1:A:192:GLY:O	1:A:195:VAL:HG22	2.16	0.46
3:C:151:ARG:CZ	3:C:167:THR:CG2	2.94	0.46
3:C:97:TYR:OH	3:C:119:VAL:HG11	2.16	0.46
3:C:107:GLU:H	3:C:107:GLU:HG2	1.29	0.45
1:A:179:TYR:HA	1:A:202:VAL:HG21	1.99	0.45
1:A:127:VAL:HG22	1:A:140:LEU:HD21	1.99	0.44
3:C:260:SER:H	3:C:263:LYS:HD2	1.82	0.44
3:C:197:ILE:HG22	3:C:316:ASP:HB3	1.98	0.44
2:B:231:PRO:HG3	2:B:254:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:HD2	1:A:221:THR:H	1.64	0.43
3:C:276:LEU:HB2	7:C:402:AMP:N1	2.33	0.43
1:A:179:TYR:CD2	1:A:202:VAL:CG2	3.01	0.43
1:A:143:GLU:HB3	4:A:601:STU:H281	1.99	0.43
3:C:192:LEU:HD13	3:C:287:ILE:HD13	2.01	0.43
1:A:13:ILE:HD11	1:A:83:ILE:HG21	2.01	0.43
2:B:84:TRP:CE2	2:B:129:VAL:HG21	2.54	0.42
3:C:303:ASP:OD1	3:C:303:ASP:C	2.55	0.42
3:C:195:LEU:HD22	3:C:197:ILE:HD11	2.00	0.42
2:B:83:ARG:HG3	2:B:113:VAL:HG22	2.00	0.42
1:A:179:TYR:HD2	1:A:202:VAL:CG2	2.31	0.42
1:A:254:MET:CE	2:B:212:GLN:HG3	2.49	0.42
1:A:219:VAL:HG13	1:A:223:PHE:CE1	2.54	0.42
1:A:428:ASN:HB3	1:A:429:PRO:HD2	2.02	0.42
3:C:212:VAL:HG23	3:C:259:VAL:O	2.20	0.42
4:A:601:STU:C16	4:A:601:STU:C26	2.95	0.42
2:B:91:VAL:HG12	2:B:105:LEU:HD12	2.02	0.42
1:A:35:HIS:HE1	1:A:37:LEU:HD12	1.85	0.42
1:A:142:PRO:HD2	1:A:179:TYR:CZ	2.55	0.42
1:A:448:SER:HB3	1:A:466:ILE:HD11	2.01	0.41
1:A:412:GLU:HA	1:A:415:ARG:HE	1.85	0.41
3:C:48:VAL:O	3:C:71:ALA:HB1	2.20	0.41
3:C:101:ALA:HA	3:C:255:ASN:O	2.20	0.41
6:A:606:32J:CL1	6:A:606:32J:C13	3.05	0.41
1:A:208:LEU:HD11	1:A:241:VAL:HG21	2.02	0.41
1:A:455:ASP:HB2	1:A:458:THR:H	1.85	0.41
1:A:227:CYS:O	1:A:251:VAL:HG11	2.21	0.41
1:A:85:THR:HB	1:A:86:PRO:HD2	2.03	0.41
1:A:218:HIS:CD2	1:A:221:THR:H	2.39	0.40
3:C:94:LEU:HG	3:C:257:LEU:HD11	2.02	0.40
2:B:145:GLN:H	2:B:145:GLN:CD	2.24	0.40
3:C:87:ILE:HG23	3:C:246:ILE:HG23	2.03	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	355/503 (71%)	333 (94%)	21 (6%)	1 (0%)	46 81
2	B	153/204 (75%)	137 (90%)	15 (10%)	1 (1%)	26 67
3	C	273/330 (83%)	250 (92%)	20 (7%)	3 (1%)	17 57
All	All	781/1037 (75%)	720 (92%)	56 (7%)	5 (1%)	30 69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	GLU
3	C	122	GLN
3	C	127	PRO
1	A	427	VAL
3	C	293	GLU

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	325/448 (72%)	309 (95%)	16 (5%)	31 69
2	B	137/185 (74%)	123 (90%)	14 (10%)	9 35
3	C	232/299 (78%)	207 (89%)	25 (11%)	8 32
All	All	694/932 (74%)	639 (92%)	55 (8%)	15 50

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	60	LYS
1	A	111	LEU
1	A	138	ARG

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Mol	Chain	Res	Type
1	A	171	ARG
1	A	185	ILE
1	A	270	GLN
1	A	276	LEU
1	A	401	ARG
1	A	405	ARG
1	A	447	MET
1	A	455	ASP
1	A	456	SER
1	A	460	LEU
1	A	542	LEU
1	A	546	LEU
2	B	113	VAL
2	B	116	LEU
2	B	134	THR
2	B	148	THR
2	B	152	ILE
2	B	155	VAL
2	B	169	ASP
2	B	215	LEU
2	B	234	VAL
2	B	235	MET
2	B	239	LEU
2	B	242	LEU
2	B	246	ASP
2	B	264	THR
3	C	28	TYR
3	C	30	THR
3	C	82	VAL
3	C	87	ILE
3	C	94	LEU
3	C	107	GLU
3	C	108	LEU
3	C	111	HIS
3	C	139	ASP
3	C	143	SER
3	C	151	ARG
3	C	152	LEU
3	C	166	LEU
3	C	172	LEU
3	C	195	LEU
3	C	246	ILE

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Mol	Chain	Res	Type
3	C	261	VAL
3	C	268	ARG
3	C	276	LEU
3	C	283	THR
3	C	290	ARG
3	C	298	ARG
3	C	302	VAL
3	C	311	ILE
3	C	322	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	403	GLN
1	A	548	GLN
2	B	212	GLN
2	B	216	ASN
3	C	168	HIS
3	C	221	GLN

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	0.88	1 (12%)	7,14,16	1.86	3 (42%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-2.11	1.53	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	TPO	O3P-P-O1P	-2.90	101.24	110.58
1	A	172	TPO	O-C-CA	-2.08	119.94	125.44
1	A	172	TPO	O3P-P-O2P	2.84	118.20	107.38

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	STU	A	601	-	27,42,42	2.31	9 (33%)	23,68,68	1.82	7 (30%)
6	32J	A	606	-	26,30,30	0.85	2 (7%)	27,44,44	2.52	2 (7%)
7	AMP	C	401	-	20,25,25	0.54	0	22,38,38	0.54	0
7	AMP	C	402	-	20,25,25	0.64	0	22,38,38	0.94	1 (4%)
8	ADP	C	403	-	22,29,29	0.70	0	27,45,45	0.99	1 (3%)
9	SO4	C	404	-	4,4,4	0.21	0	6,6,6	0.08	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	STU	A	601	-	-	0/4/42/42	0/0/8/8
6	32J	A	606	-	-	0/9/10/10	0/4/4/4
7	AMP	C	401	-	-	0/6/26/26	0/3/3/3
7	AMP	C	402	-	-	0/6/26/26	0/3/3/3
8	ADP	C	403	-	-	0/12/32/32	0/3/3/3
9	SO4	C	404	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	606	32J	C6-C1	2.33	1.45	1.42
6	A	606	32J	C3-N1	2.56	1.37	1.33
4	A	601	STU	O5-C8	2.77	1.28	1.23
4	A	601	STU	C7-C10	2.83	1.46	1.40
4	A	601	STU	C6-C19	3.13	1.46	1.42
4	A	601	STU	C19-C18	3.29	1.49	1.41
4	A	601	STU	C7-C6	3.62	1.49	1.43
4	A	601	STU	C11-C18	3.96	1.47	1.42
4	A	601	STU	C5-C20	4.49	1.48	1.41
4	A	601	STU	C10-C11	4.49	1.49	1.42
4	A	601	STU	C12-C17	4.64	1.49	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	606	32J	C4-C3-N1	-12.31	114.87	124.19
4	A	601	STU	C1-C20-C5	-2.84	116.64	120.73
4	A	601	STU	C16-C17-C12	-2.67	116.89	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	402	AMP	O2P-P-O1P	-2.41	102.81	110.58
4	A	601	STU	O5-C8-C7	-2.20	124.94	128.62
4	A	601	STU	C1-C20-N3	2.03	134.62	132.18
4	A	601	STU	C13-C12-C17	2.65	122.74	119.39
4	A	601	STU	C4-C5-C20	2.96	123.13	119.39
6	A	606	32J	C6-C1-C2	3.83	110.59	107.54
8	C	403	ADP	O3A-PA-O5'	3.83	113.11	102.94
4	A	601	STU	C16-C17-N2	4.56	137.79	132.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	STU	6	0
6	A	606	32J	1	0
7	C	402	AMP	3	0
8	C	403	ADP	1	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	361/503 (71%)	-0.02	10 (2%)	56	56	43, 76, 158, 182	0
2	B	159/204 (77%)	0.07	4 (2%)	61	60	61, 89, 129, 152	0
3	C	279/330 (84%)	0.26	20 (7%)	18	18	72, 135, 181, 194	0
All	All	799/1037 (77%)	0.10	34 (4%)	39	37	43, 94, 171, 194	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	230	VAL	5.4
1	A	444	PHE	4.9
3	C	177	LEU	3.7
3	C	197	ILE	3.7
1	A	441	THR	3.6
3	C	191	SER	3.5
3	C	123	ASP	3.3
3	C	278	CYS	3.2
3	C	236	VAL	3.1
3	C	201	ALA	3.1
2	B	217	LYS	2.9
2	B	222	SER	2.8
3	C	302	VAL	2.8
1	A	442	SER	2.8
3	C	237	VAL	2.7
3	C	35	HIS	2.6
1	A	424	TRP	2.4
3	C	124	SER	2.4
3	C	279	TYR	2.4
1	A	435	ARG	2.4
2	B	223	CYS	2.4
3	C	195	LEU	2.4
1	A	440	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	422	TYR	2.3
3	C	174	PHE	2.3
1	A	443	THR	2.3
3	C	125	PHE	2.3
3	C	282	GLU	2.2
3	C	267	HIS	2.2
1	A	468	ASP	2.1
2	B	259	LYS	2.1
3	C	229	VAL	2.1
1	A	459	TYR	2.1
3	C	202	ASN	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	0.97	0.12	-	81,82,86,89	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	CL	B	301	1/1	0.85	0.53	9.77	90,90,90,90	0
5	CL	A	604	1/1	0.99	0.33	3.98	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	32J	A	606	27/27	0.94	0.23	0.67	57,65,82,91	0
7	AMP	C	401	23/23	0.87	0.29	0.57	143,169,171,171	0
4	STU	A	601	35/35	0.97	0.24	0.57	54,59,70,72	0
8	ADP	C	403	27/27	0.83	0.29	0.42	166,179,185,188	0
7	AMP	C	402	23/23	0.79	0.25	-0.33	154,169,181,182	0
9	SO4	C	404	5/5	0.78	0.56	-	200,202,202,203	0
5	CL	A	603	1/1	0.75	0.08	-	112,112,112,112	0
5	CL	A	605	1/1	0.86	0.16	-	84,84,84,84	0
5	CL	A	602	1/1	0.96	0.18	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.