Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NPI
Title	:	Clp1-ATP-Pcf11 complex
Authors	:	Noble, C.G.; Beuth, B.; Taylor, I.A.
Deposited on	:	2006-10-27
Resolution	:	2.95 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:

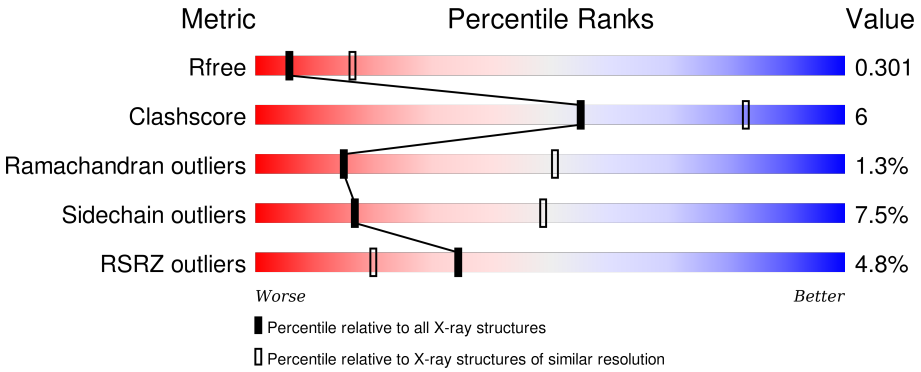
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	460	6% 74% 17% • 7%
1	B	460	3% 73% 18% • 7%
2	C	110	17% • 80%
2	D	110	2% 18% 5% 77%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7437 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 Protein CLP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	Se	0	0	0
			3412	2193	571	636	6	6			
1	B	428	Total	C	N	O	S	Se	0	0	0
			3412	2193	571	636	6	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MSE	-	MODIFIED RESIDUE	UNP Q08685
A	-13	GLY	-	CLONING ARTIFACT	UNP Q08685
A	-12	SER	-	CLONING ARTIFACT	UNP Q08685
A	-11	SER	-	CLONING ARTIFACT	UNP Q08685
A	-10	HIS	-	EXPRESSION TAG	UNP Q08685
A	-9	HIS	-	EXPRESSION TAG	UNP Q08685
A	-8	HIS	-	EXPRESSION TAG	UNP Q08685
A	-7	HIS	-	EXPRESSION TAG	UNP Q08685
A	-6	HIS	-	EXPRESSION TAG	UNP Q08685
A	-5	HIS	-	EXPRESSION TAG	UNP Q08685
A	-4	SER	-	CLONING ARTIFACT	UNP Q08685
A	-3	GLN	-	CLONING ARTIFACT	UNP Q08685
A	-2	ASP	-	CLONING ARTIFACT	UNP Q08685
A	-1	PRO	-	CLONING ARTIFACT	UNP Q08685
A	0	ASN	-	CLONING ARTIFACT	UNP Q08685
A	1	SER	-	CLONING ARTIFACT	UNP Q08685
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q08685
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q08685
A	118	MSE	MET	MODIFIED RESIDUE	UNP Q08685
A	206	MSE	MET	MODIFIED RESIDUE	UNP Q08685
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q08685
A	436	MSE	MET	MODIFIED RESIDUE	UNP Q08685
B	-14	MSE	-	MODIFIED RESIDUE	UNP Q08685
B	-13	GLY	-	CLONING ARTIFACT	UNP Q08685
B	-12	SER	-	CLONING ARTIFACT	UNP Q08685

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	SER	-	CLONING ARTIFACT	UNP Q08685
B	-10	HIS	-	EXPRESSION TAG	UNP Q08685
B	-9	HIS	-	EXPRESSION TAG	UNP Q08685
B	-8	HIS	-	EXPRESSION TAG	UNP Q08685
B	-7	HIS	-	EXPRESSION TAG	UNP Q08685
B	-6	HIS	-	EXPRESSION TAG	UNP Q08685
B	-5	HIS	-	EXPRESSION TAG	UNP Q08685
B	-4	SER	-	CLONING ARTIFACT	UNP Q08685
B	-3	GLN	-	CLONING ARTIFACT	UNP Q08685
B	-2	ASP	-	CLONING ARTIFACT	UNP Q08685
B	-1	PRO	-	CLONING ARTIFACT	UNP Q08685
B	0	ASN	-	CLONING ARTIFACT	UNP Q08685
B	1	SER	-	CLONING ARTIFACT	UNP Q08685
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q08685
B	112	MSE	MET	MODIFIED RESIDUE	UNP Q08685
B	118	MSE	MET	MODIFIED RESIDUE	UNP Q08685
B	206	MSE	MET	MODIFIED RESIDUE	UNP Q08685
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q08685
B	436	MSE	MET	MODIFIED RESIDUE	UNP Q08685

- Molecule 2 is a protein called Protein PCF11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	0	0	0
			189	120	31	38			
2	D	25	Total	C	N	O	0	0	0
			212	133	36	43			

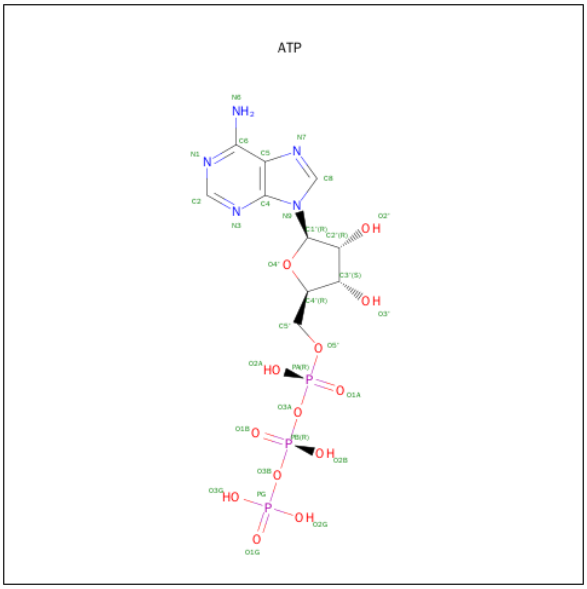
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	560	MSE	MET	MODIFIED RESIDUE	UNP P39081
D	560	MSE	MET	MODIFIED RESIDUE	UNP P39081

- 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		

- 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	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

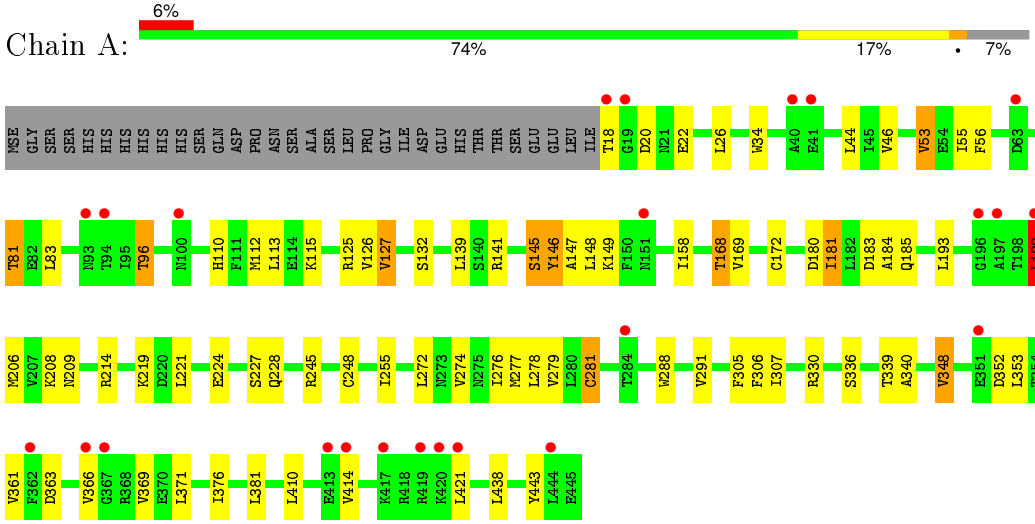
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	77	Total	O	0	0
			77	77		
5	C	7	Total	O	0	0
			7	7		
5	D	7	Total	O	0	0
			7	7		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

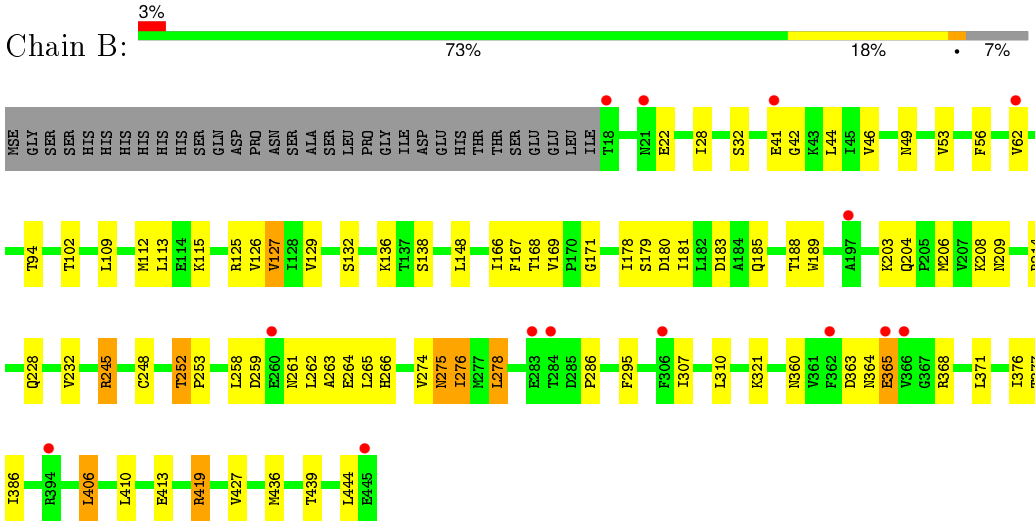
- Molecule 1: Protein CLP1

Chain A:



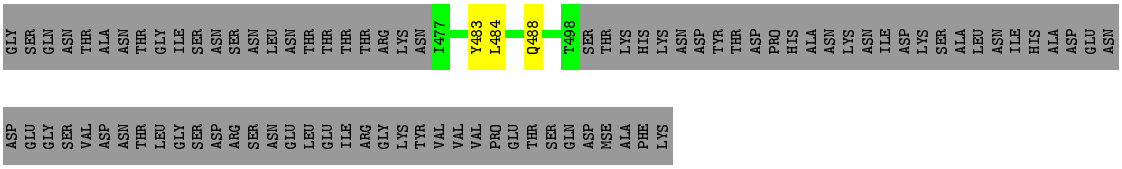
- Molecule 1: Protein CLP1

Chain B:

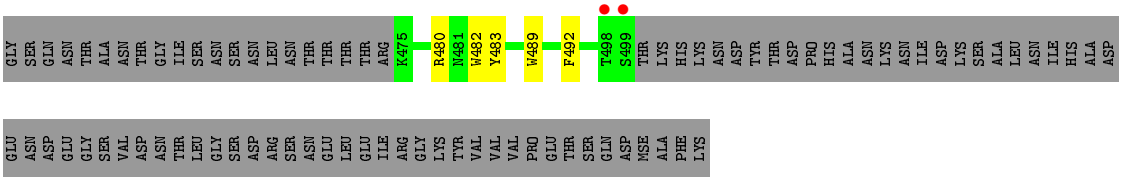


- Molecule 2: Protein PCF11

Chain C:



- Molecule 2: Protein PCF11



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.97Å 94.99Å 181.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.95 14.95 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.0 (15.00-2.95) 90.0 (14.95-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.303 0.257 , 0.301	Depositor DCC
R_{free} test set	1493 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 29533 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7437	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: 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	0.33	0/3483	0.54	1/4729 (0.0%)
1	B	0.33	0/3483	0.56	0/4729
2	C	0.34	0/194	0.43	0/263
2	D	0.35	0/217	0.43	0/293
All	All	0.33	0/7377	0.55	1/10014 (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	199	LEU	CA-CB-CG	5.24	127.35	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	3412	0	3451	44	0
1	B	3412	0	3451	47	0
2	C	189	0	168	2	0
2	D	212	0	192	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	A	57	0	0	0	0
5	B	77	0	0	7	0
5	C	7	0	0	0	0
5	D	7	0	0	0	0
All	All	7437	0	7286	92	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 (92) 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:148:LEU:HD11	1:A:180:ASP:HA	1.46	0.95
1:B:109:LEU:HD21	1:B:278:LEU:HD11	1.55	0.89
1:B:148:LEU:HD11	1:B:180:ASP:HA	1.56	0.85
1:B:125:ARG:H	1:B:275:ASN:HD21	1.26	0.84
1:B:376:ILE:HG23	1:B:381:LEU:HD12	1.63	0.78
1:A:172:CYS:HB3	1:A:209:ASN:HA	1.69	0.73
1:A:168:THR:HG22	1:A:169:VAL:H	1.53	0.73
1:B:127:VAL:HG22	1:B:274:VAL:HG11	1.73	0.69
1:B:180:ASP:HB2	5:B:2508:HOH:O	1.93	0.67
1:B:406:LEU:HD22	2:D:482:TRP:HB3	1.82	0.60
1:A:278:LEU:HD22	1:A:307:ILE:HD11	1.84	0.59
1:A:360:ASN:HB2	1:A:363:ASP:HB2	1.84	0.59
1:A:168:THR:HG23	2:C:483:TYR:OH	2.01	0.59
1:A:53:VAL:HG13	1:A:81:THR:HG21	1.84	0.58
1:A:376:ILE:HG23	1:A:381:LEU:HD12	1.86	0.57
1:B:360:ASN:HB2	1:B:363:ASP:HB2	1.87	0.56
1:B:214:ARG:HD3	5:B:2527:HOH:O	2.05	0.56
1:A:127:VAL:HG22	1:A:274:VAL:HG11	1.87	0.56
1:A:279:VAL:HG21	1:A:291:VAL:HG11	1.87	0.55
1:A:34:TRP:O	1:A:96:THR:O	2.25	0.55
1:A:278:LEU:HD23	1:A:305:PHE:HB2	1.87	0.55
1:A:279:VAL:HG12	1:A:281:CYS:HB2	1.87	0.55
1:A:353:LEU:HD23	1:A:355:ILE:HD11	1.87	0.55
1:B:168:THR:HG23	2:D:483:TYR:OH	2.06	0.55
1:A:110:HIS:HE1	1:A:147:ALA:HA	1.73	0.54
1:B:427:VAL:HG22	2:D:480:ARG:O	2.07	0.53
2:C:484:LEU:HD22	2:C:488:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLN:HE21	1:B:413:GLU:HA	1.73	0.52
1:A:183:ASP:OD1	1:A:185:GLN:HG2	2.10	0.52
1:B:125:ARG:N	1:B:275:ASN:HD21	2.02	0.52
1:B:263:ALA:HA	1:B:266:HIS:HD2	1.75	0.51
1:B:129:VAL:HA	5:B:2509:HOH:O	2.11	0.50
1:B:360:ASN:HB3	1:B:363:ASP:H	1.75	0.50
1:B:208:LYS:HD2	1:B:228:GLN:HE21	1.76	0.50
1:B:46:VAL:HG13	1:B:83:LEU:HD13	1.94	0.50
1:A:336:SER:H	1:A:339:THR:HB	1.78	0.49
1:A:125:ARG:HG2	1:A:248:CYS:HB3	1.95	0.48
1:A:56:PHE:CZ	1:A:74:PRO:HD2	2.49	0.48
1:A:46:VAL:HG13	1:A:83:LEU:HD13	1.95	0.48
1:A:224:GLU:HG3	1:A:369:VAL:HG11	1.96	0.48
1:A:20:ASP:OD2	1:A:22:GLU:HG2	2.14	0.48
1:B:208:LYS:HD2	1:B:228:GLN:HG3	1.95	0.47
1:A:410:LEU:CD1	1:A:443:TYR:HD2	2.26	0.47
1:B:148:LEU:HD11	1:B:180:ASP:CA	2.36	0.47
1:B:166:ILE:HG22	1:B:167:PHE:CD1	2.49	0.47
1:B:56:PHE:CE2	1:B:138:SER:HB3	2.50	0.46
1:A:208:LYS:HD2	1:A:228:GLN:HG3	1.98	0.46
1:B:439:THR:HG21	5:B:2517:HOH:O	2.14	0.46
1:B:406:LEU:CD2	2:D:482:TRP:HB3	2.46	0.46
1:B:204:GLN:HG3	2:D:492:PHE:CE2	2.51	0.46
1:A:348:VAL:O	1:A:421:LEU:N	2.48	0.45
1:B:102:THR:HG21	1:B:310:LEU:HA	1.99	0.45
1:A:110:HIS:CE1	1:A:147:ALA:HA	2.52	0.45
1:B:381:LEU:HD22	1:B:386:ILE:HD11	1.98	0.45
1:B:206:MSE:HB2	2:D:489:TRP:CE2	2.52	0.45
1:B:102:THR:HB	5:B:2544:HOH:O	2.18	0.44
1:B:252:THR:HG22	1:B:253:PRO:HD2	1.99	0.44
1:B:262:LEU:HB3	1:B:265:LEU:HD12	1.99	0.44
1:B:109:LEU:HD22	1:B:307:ILE:HD11	2.00	0.44
1:A:146:TYR:CB	1:A:149:LYS:HB3	2.48	0.44
1:B:87:CYS:HA	1:B:88:PRO:HD3	1.89	0.44
1:B:126:VAL:HG13	1:B:276:ILE:HG12	2.01	0.43
1:B:168:THR:HG22	1:B:169:VAL:HG22	2.00	0.43
1:A:141:ARG:O	1:A:145:SER:HB2	2.19	0.43
1:B:360:ASN:H	1:B:364:ASN:HD22	1.65	0.42
1:B:28:ILE:HD11	1:B:32:SER:O	2.18	0.42
1:B:188:THR:O	1:B:189:TRP:HB2	2.18	0.42
1:B:183:ASP:OD1	1:B:185:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:CE1	1:A:146:TYR:O	2.73	0.42
1:B:148:LEU:HD13	1:B:178:ILE:HG22	2.02	0.42
1:A:148:LEU:CD1	1:A:180:ASP:HA	2.32	0.42
1:A:79:GLU:HG3	1:A:80:GLU:H	1.85	0.42
1:B:125:ARG:HA	1:B:248:CYS:HB3	2.02	0.42
1:A:146:TYR:HB3	1:A:149:LYS:HB3	2.01	0.42
1:A:127:VAL:HG23	1:A:277:MSE:HG3	2.02	0.41
1:B:386:ILE:CG2	1:B:436:MSE:HB3	2.50	0.41
1:A:181:ILE:H	1:A:181:ILE:HG13	1.58	0.41
1:B:148:LEU:CD1	1:B:180:ASP:HA	2.41	0.41
1:A:55:ILE:HD12	1:A:184:ALA:HB1	2.03	0.41
1:A:348:VAL:HG13	1:A:352:ASP:HB2	2.03	0.41
1:A:126:VAL:HA	1:A:276:ILE:O	2.21	0.41
1:A:199:LEU:H	1:A:199:LEU:HD13	1.86	0.41
1:A:288:TRP:CZ3	1:A:306:PHE:HB3	2.56	0.41
1:A:414:VAL:HA	1:A:421:LEU:HD23	2.04	0.40
1:B:258:LEU:HD22	1:B:264:GLU:HG2	2.04	0.40
1:B:171:GLY:HA3	5:B:2517:HOH:O	2.20	0.40
1:B:245:ARG:HD3	5:B:2513:HOH:O	2.20	0.40
1:A:193:LEU:HD23	1:A:202:ASN:HB2	2.02	0.40
1:A:125:ARG:HG2	1:A:248:CYS:CB	2.51	0.40
1:B:265:LEU:HB2	1:B:295:PHE:CZ	2.57	0.40
1:A:126:VAL:HG13	1:A:276:ILE:HG12	2.03	0.40
1:A:158:ILE:HD13	1:A:272:LEU:HD22	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	426/460 (93%)	380 (89%)	42 (10%)	4 (1%)	21 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	426/460 (93%)	394 (92%)	24 (6%)	8 (2%)	10 40
2	C	20/110 (18%)	20 (100%)	0	0	100 100
2	D	23/110 (21%)	23 (100%)	0	0	100 100
All	All	895/1140 (78%)	817 (91%)	66 (7%)	12 (1%)	15 51

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	419	ARG
1	B	42	GLY
1	B	62	VAL
1	B	261	ASN
1	A	96	THR
1	A	340	ALA
1	A	81	THR
1	B	41	GLU
1	B	209	ASN
1	B	365	GLU
1	B	286	PRO
1	A	366	VAL

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	385/407 (95%)	356 (92%)	29 (8%)	17 49
1	B	385/407 (95%)	353 (92%)	32 (8%)	14 43
2	C	20/97 (21%)	20 (100%)	0	100 100
2	D	23/97 (24%)	23 (100%)	0	100 100
All	All	813/1008 (81%)	752 (92%)	61 (8%)	17 49

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	26	LEU
1	A	44	LEU
1	A	53	VAL
1	A	112	MSE
1	A	113	LEU
1	A	115	LYS
1	A	127	VAL
1	A	132	SER
1	A	139	LEU
1	A	145	SER
1	A	146	TYR
1	A	168	THR
1	A	181	ILE
1	A	199	LEU
1	A	203	LYS
1	A	206	MSE
1	A	214	ARG
1	A	219	LYS
1	A	221	LEU
1	A	227	SER
1	A	245	ARG
1	A	255	ILE
1	A	281	CYS
1	A	330	ARG
1	A	348	VAL
1	A	361	VAL
1	A	371	LEU
1	A	438	LEU
1	B	22	GLU
1	B	44	LEU
1	B	49	ASN
1	B	53	VAL
1	B	94	THR
1	B	112	MSE
1	B	113	LEU
1	B	115	LYS
1	B	127	VAL
1	B	132	SER
1	B	136	LYS
1	B	179	SER
1	B	181	ILE
1	B	203	LYS

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Mol	Chain	Res	Type
1	B	219	LYS
1	B	221	LEU
1	B	232	VAL
1	B	245	ARG
1	B	252	THR
1	B	259	ASP
1	B	275	ASN
1	B	276	ILE
1	B	278	LEU
1	B	321	LYS
1	B	365	GLU
1	B	368	ARG
1	B	371	LEU
1	B	377	THR
1	B	406	LEU
1	B	410	LEU
1	B	419	ARG
1	B	444	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	110	HIS
1	A	120	ASN
1	A	133	GLN
1	A	154	GLN
1	A	242	GLN
1	A	273	ASN
1	A	302	ASN
1	A	364	ASN
1	B	49	ASN
1	B	120	ASN
1	B	228	GLN
1	B	266	HIS
1	B	267	HIS
1	B	273	ASN
1	B	275	ASN
1	B	364	ASN
1	B	382	GLN
2	C	488	GLN
2	D	476	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	600	3	24,33,33	0.99	1 (4%)	31,52,52	2.04	4 (12%)
4	ATP	B	1600	3	24,33,33	1.06	1 (4%)	31,52,52	1.83	4 (12%)

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	600	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1600	3	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ATP	C5-C4	3.10	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1600	ATP	C5-C4	3.29	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	600	ATP	N3-C2-N1	-7.60	123.08	128.89
4	B	1600	ATP	N3-C2-N1	-6.82	123.67	128.89
4	A	600	ATP	PA-O3A-PB	-4.74	119.43	132.73
4	B	1600	ATP	PA-O3A-PB	-4.12	121.16	132.73
4	A	600	ATP	PB-O3B-PG	-3.42	121.19	132.67
4	A	600	ATP	C4-C5-N7	-3.03	106.69	109.48
4	B	1600	ATP	C4-C5-N7	-2.94	106.78	109.48
4	B	1600	ATP	PB-O3B-PG	-2.29	124.99	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	422/460 (91%)	0.26	27 (6%) 23 12	26, 55, 90, 133	0
1	B	422/460 (91%)	-0.04	14 (3%) 50 31	25, 45, 69, 98	0
2	C	22/110 (20%)	0.05	0 100 100	31, 42, 62, 77	0
2	D	25/110 (22%)	0.31	2 (8%) 15 8	27, 39, 71, 90	0
All	All	891/1140 (78%)	0.12	43 (4%) 34 20	25, 49, 84, 133	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	499	SER	6.4
1	A	284	THR	6.2
1	A	18	THR	5.1
1	B	18	THR	3.6
1	A	197	ALA	3.3
1	A	420	LYS	3.3
1	B	62	VAL	3.2
1	A	366	VAL	3.1
1	A	100	ASN	3.0
1	A	419	ARG	2.9
1	B	366	VAL	2.8
1	A	417	LYS	2.8
1	B	41	GLU	2.7
1	B	445	GLU	2.7
1	A	360	ASN	2.7
1	B	197	ALA	2.6
1	A	63	ASP	2.5
1	A	362	PHE	2.5
1	A	41	GLU	2.4
1	B	394	ARG	2.4
1	A	94	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	284	THR	2.4
1	A	359	SER	2.3
1	A	196	GLY	2.3
1	A	367	GLY	2.3
1	A	151	ASN	2.3
1	A	93	ASN	2.2
1	A	351	GLU	2.2
1	A	40	ALA	2.2
1	A	19	GLY	2.2
1	A	414	VAL	2.2
1	A	444	LEU	2.2
1	A	413	GLU	2.1
1	B	306	PHE	2.1
1	A	421	LEU	2.1
1	A	80	GLU	2.1
1	B	260	GLU	2.1
1	B	21	ASN	2.1
1	A	199	LEU	2.1
1	B	283	GLU	2.0
1	B	365	GLU	2.0
2	D	498	THR	2.0
1	B	362	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	600	31/31	0.96	0.19	-0.25	41,44,45,45	0
4	ATP	B	1600	31/31	0.97	0.15	-0.55	37,39,40,41	0
3	MG	A	1500	1/1	0.95	0.12	-0.97	27,27,27,27	0
3	MG	B	2500	1/1	0.95	0.10	-2.27	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.