Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:25 AM GMT

PDB ID	:	3AR4
Title	:	Calcium pump crystal structure with bound ATP and TG in the absence of Ca2+
Authors	:	Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on	:	2010-11-24
Resolution	:	2.15 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:

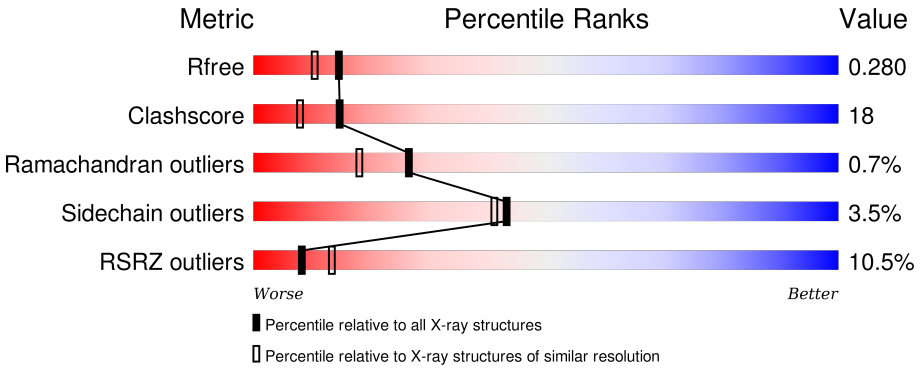
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	995	10% 66% 32%

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	TG1	A	1003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PTY	A	1011	-	-	-	X
6	PTY	A	1012	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8188 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.

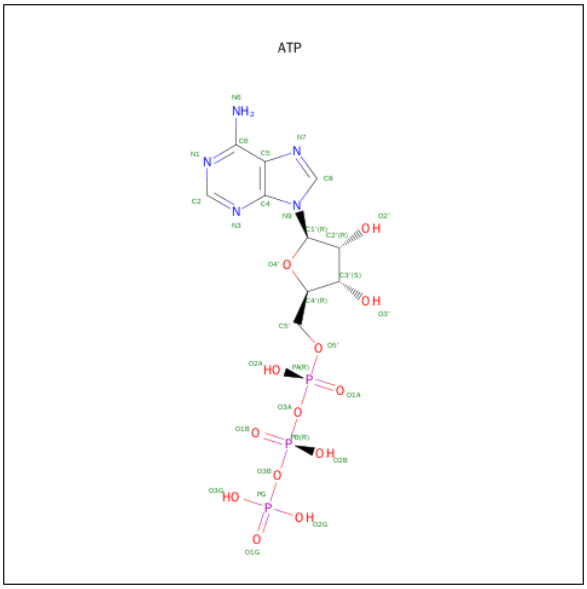
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	ACE	-	ACETYLATION	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

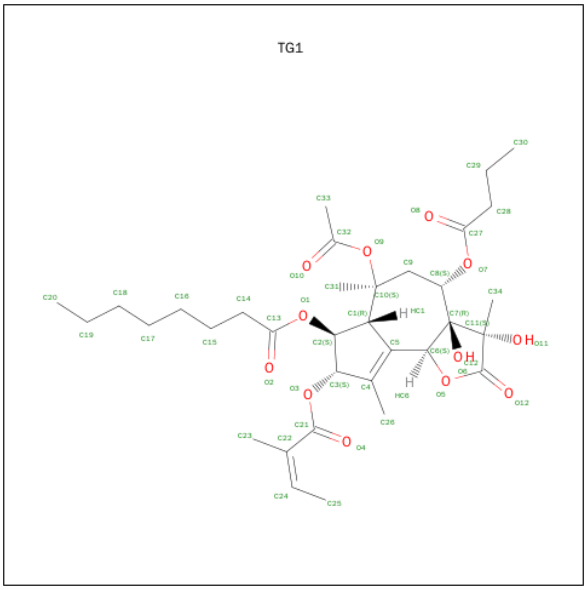
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

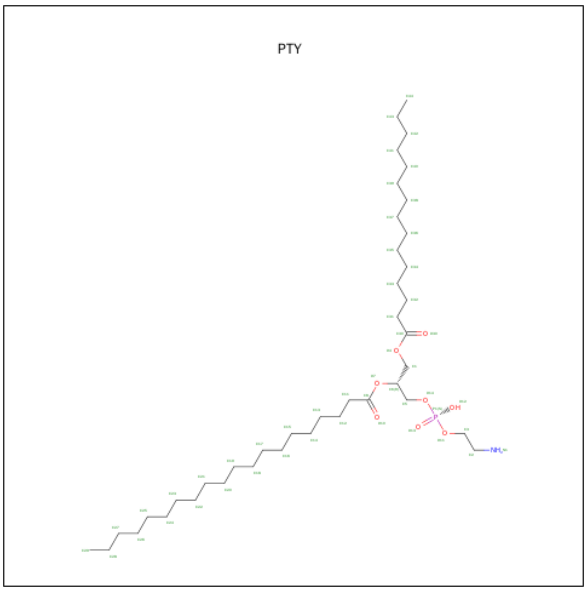
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: $C_{34}H_{50}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 46 34 12	0	0

- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 7 is water.

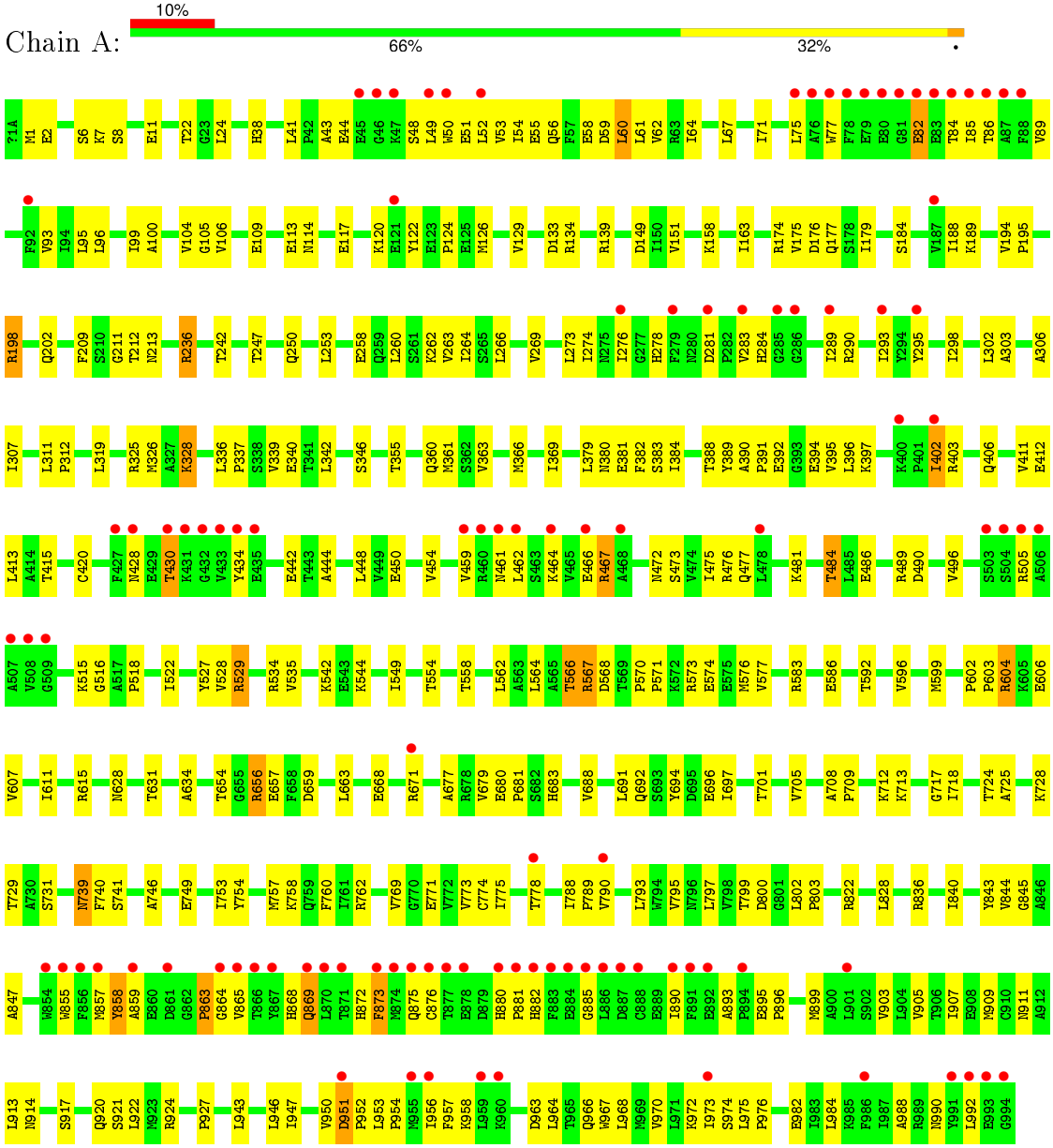
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	377	Total	O	0	0
			377	377		

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.38Å 71.38Å 590.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.15 51.32 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (14.97-2.15) 99.4 (51.32-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.16Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.281 0.237 , 0.280	Depositor DCC
R_{free} test set	4264 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 84932 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8188	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, TG1, PTY, ACE, NA, 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	0.34	0/7813	0.58	0/10594

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	7674	0	7765	279	0
2	A	31	0	12	3	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	46	0	50	2	0
6	A	57	0	33	1	0
7	A	377	0	0	16	0
All	All	8188	0	7860	279	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 18.

All (279) 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:328:LYS:NZ	1:A:328:LYS:HA	1.88	0.87
1:A:290:ARG:HH12	1:A:875:GLN:HG2	1.39	0.87
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.59	0.84
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.60	0.84
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.61	0.83
1:A:85:ILE:HG23	1:A:86:THR:HG22	1.61	0.82
1:A:462:LEU:HB3	1:A:466:GLU:HB2	1.63	0.81
1:A:963:ASP:H	1:A:966:GLN:NE2	1.80	0.79
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.62	0.79
1:A:963:ASP:H	1:A:966:GLN:HE21	1.29	0.78
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.66	0.78
1:A:273:LEU:HD23	1:A:276:ILE:HD11	1.66	0.77
1:A:739:ASN:HD22	1:A:740:PHE:N	1.85	0.75
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.68	0.74
1:A:924:ARG:HA	1:A:924:ARG:HE	1.53	0.74
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.88	0.73
1:A:583:ARG:HD2	7:A:2218:HOH:O	1.88	0.72
1:A:179:ILE:O	1:A:705:VAL:HG22	1.90	0.72
1:A:89:VAL:O	1:A:93:VAL:HG23	1.89	0.71
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.21	0.71
1:A:56:GLN:OE1	1:A:105:GLY:HA3	1.90	0.71
1:A:55:GLU:HA	1:A:58:GLU:HG3	1.73	0.70
1:A:680:GLU:HB2	1:A:683:HIS:CD2	2.26	0.70
1:A:397:LYS:HB2	1:A:402:ILE:HG21	1.74	0.69
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.75	0.69
1:A:836:ARG:O	1:A:840:ILE:HG12	1.93	0.68
1:A:680:GLU:H	1:A:683:HIS:CD2	2.10	0.68
1:A:312:PRO:HG2	7:A:2357:HOH:O	1.93	0.68
1:A:554:THR:HG21	7:A:2365:HOH:O	1.92	0.68
1:A:680:GLU:H	1:A:683:HIS:HD2	1.41	0.67
1:A:583:ARG:O	1:A:586:GLU:HG2	1.95	0.67
1:A:149:ASP:HB2	7:A:2356:HOH:O	1.94	0.67
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.77	0.67
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.77	0.66
1:A:663:LEU:HD12	1:A:663:LEU:H	1.59	0.66
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.77	0.66
1:A:758:LYS:O	1:A:762:ARG:HG3	1.96	0.66
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.78	0.65
1:A:174:ARG:NH2	1:A:188:ILE:HD11	2.12	0.65
1:A:968:LEU:O	1:A:972:LYS:HG3	1.97	0.65
1:A:606:GLU:OE1	1:A:606:GLU:N	2.28	0.64
1:A:397:LYS:HB2	1:A:402:ILE:CG2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:CZ	1:A:188:ILE:HD11	2.28	0.64
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.79	0.64
1:A:290:ARG:HH22	1:A:875:GLN:HB3	1.63	0.63
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.98	0.63
1:A:857:MET:O	1:A:864:GLY:HA2	1.98	0.63
1:A:49:LEU:O	1:A:53:VAL:HG23	1.98	0.62
1:A:515:LYS:HE3	2:A:1002:ATP:N1	2.15	0.62
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.82	0.62
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.81	0.62
1:A:262:LYS:O	1:A:266:LEU:HD23	1.99	0.62
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.81	0.61
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.81	0.61
1:A:366:MET:CE	1:A:384:ILE:HD11	2.30	0.61
1:A:176:ASP:O	1:A:212:THR:HG23	1.99	0.61
1:A:395:VAL:O	1:A:396:LEU:HD23	2.00	0.61
1:A:328:LYS:HZ3	1:A:328:LYS:HA	1.65	0.60
1:A:403:ARG:HG2	7:A:2133:HOH:O	2.01	0.60
1:A:402:ILE:HD13	1:A:402:ILE:H	1.65	0.60
1:A:459:VAL:HB	1:A:467:ARG:NE	2.16	0.59
1:A:472:ASN:HB3	1:A:476:ARG:HH12	1.68	0.59
1:A:567:ARG:CD	1:A:570:PRO:HA	2.32	0.59
1:A:873:PHE:CE1	1:A:881:PRO:HG3	2.37	0.59
1:A:529:ARG:CZ	1:A:592:THR:HG21	2.32	0.59
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.66	0.59
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.85	0.59
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.86	0.58
1:A:924:ARG:NE	1:A:924:ARG:HA	2.17	0.58
1:A:247:THR:H	1:A:250:GLN:NE2	2.02	0.58
1:A:554:THR:HG23	7:A:2155:HOH:O	2.03	0.57
1:A:325:ARG:HH12	1:A:753:ILE:HD11	1.68	0.57
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.04	0.57
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.38	0.57
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.04	0.57
1:A:880:HIS:N	1:A:881:PRO:HD2	2.19	0.57
1:A:668:GLU:OE1	1:A:671:ARG:HD3	2.03	0.57
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.33	0.57
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.20	0.56
1:A:328:LYS:HZ2	1:A:328:LYS:HA	1.66	0.56
1:A:383:SER:O	1:A:384:ILE:HD13	2.05	0.56
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.20	0.56
1:A:262:LYS:NZ	1:A:266:LEU:HD21	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:CD1	1:A:109:GLU:HG3	2.34	0.55
1:A:881:PRO:HG2	1:A:882:HIS:H	1.71	0.55
1:A:346:SER:OG	1:A:696:GLU:OE2	2.23	0.55
1:A:48:SER:OG	1:A:51:GLU:HG3	2.05	0.55
1:A:769:VAL:HA	5:A:1003:TG1:H231	1.88	0.55
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.88	0.55
1:A:481:LYS:HD3	1:A:484:THR:HG22	1.89	0.55
1:A:663:LEU:N	1:A:663:LEU:HD12	2.22	0.55
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.89	0.55
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.42	0.55
1:A:339:VAL:HG23	1:A:340:GLU:N	2.22	0.55
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.36	0.54
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.90	0.54
1:A:865:VAL:HB	1:A:868:HIS:CB	2.37	0.54
1:A:484:THR:HB	1:A:496:VAL:HG12	1.90	0.54
1:A:384:ILE:HD12	1:A:395:VAL:HG22	1.90	0.54
1:A:390:ALA:C	1:A:392:GLU:H	2.11	0.54
1:A:921:SER:HB3	1:A:982:GLU:OE1	2.08	0.54
1:A:668:GLU:O	1:A:671:ARG:HG2	2.08	0.54
1:A:739:ASN:C	1:A:739:ASN:HD22	2.12	0.53
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.90	0.53
1:A:411:VAL:HG22	1:A:454:VAL:HB	1.90	0.53
1:A:604:ARG:HG3	7:A:2033:HOH:O	2.07	0.53
1:A:459:VAL:HB	1:A:467:ARG:CD	2.39	0.53
1:A:60:LEU:HD12	1:A:258:GLU:OE1	2.08	0.53
1:A:289:ILE:O	1:A:293:ILE:HG13	2.08	0.53
1:A:899:MET:O	1:A:903:VAL:HG23	2.08	0.53
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.38	0.53
1:A:184:SER:HB2	7:A:2194:HOH:O	2.08	0.53
1:A:663:LEU:CD1	1:A:663:LEU:H	2.21	0.52
1:A:762:ARG:HD3	1:A:828:LEU:O	2.09	0.52
1:A:325:ARG:HH12	1:A:753:ILE:CD1	2.23	0.52
1:A:8:SER:OG	1:A:11:GLU:HG3	2.09	0.52
1:A:38:HIS:HE1	7:A:2386:HOH:O	1.93	0.52
1:A:311:LEU:N	1:A:312:PRO:HD2	2.24	0.52
1:A:472:ASN:HB3	1:A:476:ARG:NH1	2.24	0.52
1:A:654:THR:HA	1:A:677:ALA:O	2.08	0.52
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.91	0.52
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.91	0.52
1:A:195:PRO:HA	7:A:2369:HOH:O	2.07	0.52
1:A:534:ARG:HG2	1:A:535:VAL:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.09	0.52
1:A:298:ILE:O	1:A:302:LEU:HB2	2.10	0.51
1:A:974:SER:C	1:A:976:PRO:HD2	2.31	0.51
1:A:749:GLU:O	1:A:753:ILE:HG12	2.11	0.51
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.93	0.51
1:A:975:LEU:N	1:A:976:PRO:HD2	2.26	0.51
1:A:212:THR:HG22	1:A:213:ASN:N	2.25	0.51
1:A:379:LEU:HD11	1:A:544:LYS:HD2	1.93	0.51
1:A:757:MET:HA	1:A:760:PHE:CE2	2.45	0.51
1:A:122:TYR:O	1:A:211:GLY:HA2	2.10	0.50
1:A:964:LEU:O	1:A:968:LEU:HD13	2.11	0.50
1:A:262:LYS:HZ3	1:A:266:LEU:HD21	1.76	0.50
1:A:771:GLU:O	1:A:775:ILE:HG12	2.12	0.50
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.23	0.50
1:A:263:VAL:HG11	5:A:1003:TG1:O4	2.12	0.50
1:A:895:GLU:N	1:A:896:PRO:HD2	2.26	0.50
1:A:82:GLU:C	1:A:84:THR:H	2.14	0.50
1:A:236:ARG:HD3	1:A:236:ARG:C	2.31	0.50
1:A:303:ALA:O	1:A:307:ILE:HG12	2.11	0.50
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.76	0.50
1:A:361:MET:HG2	1:A:599:MET:SD	2.52	0.50
1:A:381:GLU:HG2	7:A:2371:HOH:O	2.12	0.50
1:A:450:GLU:OE2	1:A:450:GLU:HA	2.11	0.50
1:A:273:LEU:HA	1:A:276:ILE:HG13	1.94	0.49
1:A:943:LEU:O	1:A:946:LEU:HB3	2.12	0.49
1:A:428:ASN:OD1	1:A:430:THR:HB	2.12	0.49
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.93	0.49
1:A:847:ALA:CA	1:A:973:ILE:HD11	2.37	0.49
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.90	0.49
1:A:212:THR:CG2	1:A:213:ASN:N	2.76	0.49
1:A:242:THR:O	1:A:712:LYS:NZ	2.45	0.49
1:A:571:PRO:HG2	1:A:576:MET:SD	2.53	0.49
1:A:680:GLU:N	1:A:683:HIS:CD2	2.80	0.49
1:A:198:ARG:HD3	1:A:198:ARG:O	2.13	0.49
1:A:701:THR:HA	1:A:718:ILE:O	2.13	0.49
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.94	0.49
1:A:366:MET:HE2	1:A:384:ILE:HD11	1.94	0.48
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.77	0.48
1:A:659:ASP:OD1	1:A:683:HIS:HE1	1.96	0.48
1:A:739:ASN:ND2	1:A:741:SER:H	2.10	0.48
1:A:869:GLN:HB2	1:A:872:HIS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:O	1:A:797:LEU:HD13	2.13	0.48
1:A:202:GLN:OE1	1:A:489:ARG:HD3	2.14	0.48
1:A:688:VAL:O	1:A:692:GLN:HG3	2.12	0.48
1:A:905:VAL:O	1:A:909:MET:HG2	2.13	0.48
1:A:473:SER:O	1:A:477:GLN:HG2	2.14	0.48
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.95	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.14	0.48
1:A:577:VAL:HG23	1:A:583:ARG:NH1	2.29	0.48
1:A:754:TYR:HD1	1:A:757:MET:HE3	1.79	0.48
1:A:328:LYS:CE	1:A:328:LYS:HA	2.43	0.48
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.44	0.48
1:A:60:LEU:O	1:A:64:ILE:HG12	2.14	0.47
1:A:573:ARG:HG3	7:A:2137:HOH:O	2.14	0.47
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.96	0.47
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.95	0.47
1:A:952:PRO:O	1:A:956:ILE:HG13	2.14	0.47
1:A:403:ARG:HB3	1:A:406:GLN:HG3	1.96	0.47
1:A:366:MET:HE1	1:A:384:ILE:HD11	1.96	0.47
1:A:656:ARG:NH1	1:A:656:ARG:HG2	2.29	0.47
1:A:573:ARG:HG2	1:A:573:ARG:HH11	1.80	0.47
1:A:680:GLU:N	1:A:683:HIS:HD2	2.11	0.47
1:A:880:HIS:H	1:A:881:PRO:HD2	1.78	0.47
1:A:882:HIS:NE2	1:A:885:GLY:HA3	2.30	0.47
1:A:278:HIS:HA	1:A:281:ASP:OD2	2.14	0.47
1:A:260:LEU:CD2	1:A:307:ILE:HD13	2.44	0.47
1:A:534:ARG:NH2	1:A:568:ASP:HB2	2.30	0.47
1:A:863:PRO:C	1:A:865:VAL:H	2.18	0.46
1:A:515:LYS:HE3	2:A:1002:ATP:C2	2.50	0.46
1:A:725:ALA:O	1:A:729:THR:HG23	2.15	0.46
1:A:402:ILE:N	1:A:402:ILE:HD13	2.30	0.46
1:A:366:MET:HA	1:A:596:VAL:O	2.16	0.46
1:A:1:MET:CE	1:A:7:LYS:HG3	2.44	0.46
1:A:71:ILE:O	1:A:75:LEU:HD13	2.16	0.46
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.98	0.46
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.44	0.46
1:A:273:LEU:HA	1:A:276:ILE:HD11	1.98	0.46
1:A:534:ARG:HH21	1:A:568:ASP:CB	2.28	0.46
1:A:858:TYR:CD1	1:A:858:TYR:N	2.84	0.46
1:A:442:GLU:OE2	1:A:515:LYS:NZ	2.49	0.46
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.50	0.46
1:A:95:LEU:HD22	1:A:99:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:SER:HB3	1:A:697:ILE:H	1.80	0.45
1:A:295:TYR:O	1:A:298:ILE:HG12	2.17	0.45
1:A:890:ILE:C	1:A:890:ILE:HD12	2.37	0.45
1:A:574:GLU:CD	1:A:574:GLU:H	2.19	0.45
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.46	0.45
1:A:274:ILE:HG22	1:A:274:ILE:O	2.14	0.45
1:A:895:GLU:CD	1:A:895:GLU:H	2.19	0.45
1:A:149:ASP:CB	7:A:2356:HOH:O	2.60	0.45
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.80	0.45
1:A:534:ARG:HH21	1:A:568:ASP:HB2	1.82	0.44
1:A:516:GLY:HA2	2:A:1002:ATP:N3	2.33	0.44
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.32	0.44
1:A:124:PRO:HB3	1:A:158:LYS:HB3	1.99	0.44
1:A:420:CYS:SG	1:A:515:LYS:HE2	2.58	0.44
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.99	0.44
1:A:209:PHE:O	1:A:212:THR:HB	2.18	0.44
1:A:114:ASN:OD1	1:A:117:GLU:HG2	2.17	0.44
1:A:611:ILE:O	1:A:615:ARG:HG3	2.18	0.44
1:A:967:TRP:O	1:A:970:VAL:HB	2.17	0.44
1:A:604:ARG:NH1	1:A:604:ARG:CG	2.79	0.43
1:A:52:LEU:CD2	1:A:106:VAL:HG13	2.49	0.43
1:A:688:VAL:HG11	1:A:713:LYS:HG2	2.01	0.43
1:A:2:GLU:HG3	7:A:2291:HOH:O	2.19	0.43
1:A:380:ASN:HD22	1:A:382:PHE:HZ	1.66	0.43
1:A:325:ARG:HD2	1:A:749:GLU:OE2	2.19	0.43
1:A:855:TRP:HA	1:A:859:ALA:CB	2.49	0.43
1:A:126:MET:CE	1:A:139:ARG:HD3	2.49	0.43
1:A:788:ILE:HD13	1:A:958:LYS:HD2	2.01	0.43
1:A:628:ASN:ND2	1:A:631:THR:H	2.17	0.43
1:A:96:LEU:HD23	1:A:96:LEU:C	2.39	0.43
1:A:67:LEU:O	1:A:67:LEU:HD12	2.19	0.43
1:A:795:VAL:HA	1:A:799:THR:HB	2.01	0.43
1:A:369:ILE:HG13	1:A:528:VAL:HG11	1.99	0.43
1:A:133:ASP:O	1:A:134:ARG:HG3	2.19	0.42
1:A:75:LEU:C	1:A:77:TRP:H	2.22	0.42
1:A:388:THR:OG1	1:A:389:TYR:N	2.52	0.42
1:A:273:LEU:HA	1:A:276:ILE:CG1	2.48	0.42
1:A:922:LEU:HD22	1:A:927:PRO:HG3	2.02	0.42
1:A:6:SER:HA	1:A:194:VAL:O	2.20	0.42
1:A:990:ASN:HD21	6:A:1012:PTY:C2	2.32	0.42
1:A:724:THR:O	1:A:728:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:120:LYS:HZ1	1.85	0.42
1:A:100:ALA:O	1:A:104:VAL:HG23	2.20	0.42
1:A:558:THR:HG22	1:A:634:ALA:HB1	2.01	0.42
1:A:988:ALA:O	1:A:992:LEU:HB2	2.19	0.42
1:A:273:LEU:HA	1:A:276:ILE:CD1	2.50	0.42
1:A:326:MET:HG2	1:A:749:GLU:HG2	2.01	0.42
1:A:360:GLN:HB2	7:A:2237:HOH:O	2.20	0.42
1:A:607:VAL:O	1:A:611:ILE:HG12	2.19	0.41
1:A:708:ALA:HB3	1:A:709:PRO:HD3	2.02	0.41
1:A:917:SER:OG	1:A:920:GLN:HB2	2.20	0.41
1:A:800:ASP:C	1:A:803:PRO:HD2	2.41	0.41
1:A:950:VAL:O	1:A:954:PRO:HD2	2.20	0.41
1:A:459:VAL:C	1:A:461:ASN:H	2.23	0.41
1:A:434:TYR:HE1	1:A:464:LYS:HE3	1.86	0.41
1:A:415:THR:HA	1:A:475:ILE:HG21	2.01	0.41
1:A:790:VAL:HG12	1:A:957:PHE:CD1	2.56	0.41
1:A:950:VAL:O	1:A:952:PRO:HD2	2.20	0.41
1:A:554:THR:HG22	1:A:554:THR:O	2.20	0.41
1:A:573:ARG:NH1	1:A:573:ARG:HG2	2.36	0.41
1:A:269:VAL:O	1:A:273:LEU:HG	2.20	0.41
1:A:175:VAL:HG12	1:A:177:GLN:HG3	2.02	0.41
1:A:336:LEU:O	1:A:339:VAL:HG22	2.21	0.41
1:A:290:ARG:NH2	1:A:875:GLN:HB3	2.33	0.41
1:A:361:MET:CG	1:A:599:MET:SD	3.08	0.40
1:A:382:PHE:CD1	1:A:382:PHE:N	2.89	0.40
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.51	0.40
1:A:529:ARG:HH21	1:A:534:ARG:HB2	1.86	0.40
1:A:406:GLN:HG2	7:A:2224:HOH:O	2.22	0.40
1:A:41:LEU:HD13	1:A:236:ARG:HG3	2.04	0.40
1:A:774:CYS:O	1:A:778:THR:HG22	2.21	0.40
1:A:518:PRO:HB3	1:A:549:ILE:HD13	2.02	0.40
1:A:717:GLY:O	1:A:731:SER:HB2	2.22	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	993/995 (100%)	932 (94%)	54 (5%)	7 (1%)	26 18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	951	ASP
1	A	858	TYR
1	A	869	GLN
1	A	505	ARG
1	A	430	THR
1	A	863	PRO
1	A	391	PRO

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	840/840 (100%)	811 (96%)	29 (4%)	43 41

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	44	GLU
1	A	60	LEU
1	A	82	GLU
1	A	113	GLU
1	A	189	LYS
1	A	198	ARG
1	A	236	ARG
1	A	253	LEU
1	A	319	LEU

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Mol	Chain	Res	Type
1	A	328	LYS
1	A	394	GLU
1	A	402	ILE
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	490	ASP
1	A	529	ARG
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	604	ARG
1	A	656	ARG
1	A	691	LEU
1	A	739	ASN
1	A	789	PRO
1	A	822	ARG
1	A	873	PHE
1	A	876	CYS

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	111	ASN
1	A	138	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	461	ASN
1	A	472	ASN
1	A	510	ASN
1	A	628	ASN
1	A	683	HIS
1	A	739	ASN
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
2	ATP	A	1002	3	24,33,33	1.37	2 (8%)	31,52,52	1.67	5 (16%)
5	TG1	A	1003	-	43,48,48	1.66	12 (27%)	42,72,72	1.76	10 (23%)
6	PTY	A	1011	-	17,18,49	1.28	3 (17%)	18,23,54	1.19	2 (11%)
6	PTY	A	1012	-	17,18,49	1.33	3 (17%)	18,23,54	1.49	4 (22%)
6	PTY	A	1013	-	17,18,49	1.27	3 (17%)	18,23,54	1.28	2 (11%)

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
2	ATP	A	1002	3	-	0/18/38/38	0/3/3/3
5	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
6	PTY	A	1011	-	-	0/20/20/53	0/0/0/0
6	PTY	A	1012	-	-	0/20/20/53	0/0/0/0
6	PTY	A	1013	-	-	0/20/20/53	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1012	PTY	P1-O13	2.06	1.58	1.51
5	A	1003	TG1	C31-C10	2.10	1.57	1.52
5	A	1003	TG1	O1-C13	2.15	1.40	1.34
6	A	1011	PTY	P1-O13	2.16	1.59	1.51
5	A	1003	TG1	C7-C6	2.17	1.57	1.54
5	A	1003	TG1	C2-C3	2.18	1.57	1.53
6	A	1013	PTY	P1-O13	2.20	1.59	1.51
5	A	1003	TG1	O7-C27	2.22	1.40	1.34
6	A	1011	PTY	C5-C6	2.33	1.57	1.50
6	A	1012	PTY	C5-C6	2.44	1.57	1.50
6	A	1013	PTY	C5-C6	2.53	1.57	1.50
5	A	1003	TG1	C9-C8	2.68	1.55	1.52
6	A	1013	PTY	C1-C6	2.74	1.58	1.50
5	A	1003	TG1	C1-C5	2.84	1.56	1.51
5	A	1003	TG1	C11-C7	3.01	1.59	1.55
6	A	1011	PTY	C1-C6	3.08	1.59	1.50
6	A	1012	PTY	C1-C6	3.17	1.59	1.50
5	A	1003	TG1	C1-C2	3.27	1.60	1.54
5	A	1003	TG1	C34-C11	3.32	1.58	1.53
2	A	1002	ATP	C2-N1	3.41	1.40	1.33
2	A	1002	ATP	C4-N3	3.77	1.41	1.35
5	A	1003	TG1	O4-C21	3.81	1.29	1.21
5	A	1003	TG1	C7-C8	3.99	1.58	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	ATP	N3-C2-N1	-5.26	124.86	128.89
5	A	1003	TG1	O12-C12-C11	-4.06	124.52	128.26
2	A	1002	ATP	PA-O3A-PB	-3.70	122.33	132.73
5	A	1003	TG1	O5-C6-C7	-3.55	100.94	104.08
2	A	1002	ATP	PB-O3B-PG	-3.40	121.28	132.67
6	A	1012	PTY	O12-P1-O13	-3.17	95.33	112.53
5	A	1003	TG1	C23-C22-C21	-2.20	110.33	116.04
5	A	1003	TG1	O4-C21-C22	-2.12	118.23	125.17
5	A	1003	TG1	C26-C4-C3	-2.04	118.86	121.51
6	A	1012	PTY	O14-P1-O13	2.02	117.46	109.62
6	A	1013	PTY	O4-C1-C6	2.17	114.52	108.69
2	A	1002	ATP	C4-C5-N7	2.27	111.57	109.48
5	A	1003	TG1	C24-C22-C21	2.38	130.85	120.67
6	A	1012	PTY	O4-C1-C6	2.43	115.23	108.69
6	A	1011	PTY	O4-C1-C6	2.47	115.34	108.69
5	A	1003	TG1	O5-C12-O12	2.53	125.31	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1003	TG1	O3-C21-O4	2.64	128.56	123.30
5	A	1003	TG1	O7-C8-C9	2.90	112.32	107.03
6	A	1012	PTY	O7-C8-C11	2.91	116.60	111.10
6	A	1011	PTY	O7-C8-C11	3.20	117.14	111.10
2	A	1002	ATP	C2'-C1'-N9	3.26	119.28	114.29
6	A	1013	PTY	O7-C8-C11	3.57	117.83	111.10
5	A	1003	TG1	C10-O9-C32	6.32	134.87	121.90

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
2	A	1002	ATP	3	0
5	A	1003	TG1	2	0
6	A	1012	PTY	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	994/995 (99%)	0.79	104 (10%)	8	13	28, 55, 107, 152	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	14.9
1	A	883	PHE	12.6
1	A	886	LEU	12.4
1	A	506	ALA	12.1
1	A	507	ALA	11.7
1	A	508	VAL	11.0
1	A	81	GLY	10.1
1	A	80	GLU	9.8
1	A	504	SER	9.3
1	A	84	THR	9.2
1	A	994	GLY	8.6
1	A	78	PHE	8.5
1	A	993	GLU	8.2
1	A	885	GLY	8.2
1	A	505	ARG	8.1
1	A	82	GLU	7.7
1	A	503	SER	7.1
1	A	877	THR	6.9
1	A	866	THR	6.7
1	A	289	ILE	6.0
1	A	462	LEU	6.0
1	A	46	GLY	5.9
1	A	992	LEU	5.9
1	A	86	THR	5.7
1	A	890	ILE	5.6
1	A	884	GLU	5.6
1	A	873	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	864	GLY	5.3
1	A	875	GLN	5.1
1	A	856	PHE	4.9
1	A	433	VAL	4.9
1	A	865	VAL	4.8
1	A	77	TRP	4.8
1	A	887	ASP	4.7
1	A	464	LYS	4.6
1	A	459	VAL	4.6
1	A	76	ALA	4.6
1	A	286	GLY	4.5
1	A	285	GLY	4.5
1	A	79	GLU	4.3
1	A	461	ASN	4.3
1	A	881	PRO	4.2
1	A	870	LEU	4.2
1	A	891	PHE	4.1
1	A	293	ILE	4.1
1	A	295	TYR	4.0
1	A	52	LEU	4.0
1	A	888	CYS	4.0
1	A	92	PHE	3.9
1	A	855	TRP	3.8
1	A	430	THR	3.8
1	A	960	LYS	3.7
1	A	951	ASP	3.7
1	A	434	TYR	3.6
1	A	955	MET	3.5
1	A	861	ASP	3.5
1	A	432	GLY	3.5
1	A	83	GLU	3.4
1	A	894	PRO	3.4
1	A	468	ALA	3.4
1	A	991	TYR	3.3
1	A	431	LYS	3.3
1	A	427	PHE	3.3
1	A	959	LEU	3.2
1	A	402	ILE	3.1
1	A	867	TYR	3.1
1	A	435	GLU	3.1
1	A	859	ALA	3.1
1	A	428	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	874	MET	3.0
1	A	466	GLU	2.9
1	A	857	MET	2.9
1	A	880	HIS	2.8
1	A	871	THR	2.8
1	A	876	CYS	2.8
1	A	973	ILE	2.7
1	A	478	LEU	2.7
1	A	671	ARG	2.6
1	A	279	PHE	2.6
1	A	986	PHE	2.6
1	A	882	HIS	2.6
1	A	276	ILE	2.5
1	A	878	GLU	2.5
1	A	281	ASP	2.5
1	A	778	THR	2.5
1	A	869	GLN	2.5
1	A	45	GLU	2.4
1	A	50	TRP	2.5
1	A	88	PHE	2.4
1	A	187	VAL	2.4
1	A	892	GLU	2.4
1	A	283	VAL	2.3
1	A	460	ARG	2.3
1	A	47	LYS	2.2
1	A	121	GLU	2.2
1	A	956	ILE	2.2
1	A	87	ALA	2.2
1	A	75	LEU	2.1
1	A	854	TRP	2.1
1	A	509	GLY	2.1
1	A	49	LEU	2.1
1	A	901	LEU	2.0
1	A	790	VAL	2.0
1	A	400	LYS	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
5	TG1	A	1003	46/46	0.87	0.23	5.20	61,68,84,86	0
6	PTY	A	1012	19/50	0.77	0.30	3.53	109,113,116,116	0
6	PTY	A	1011	19/50	0.83	0.19	2.10	114,115,117,117	0
6	PTY	A	1013	19/50	0.78	0.18	-0.03	99,108,108,108	0
2	ATP	A	1002	31/31	0.98	0.12	-0.55	42,52,62,64	0
3	MG	A	1001	1/1	0.85	0.11	-1.30	65,65,65,65	0
4	NA	A	1000	1/1	0.96	0.11	-1.39	43,43,43,43	0
3	MG	A	997	1/1	0.99	0.13	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.