Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID	:	3AR6
Title	:	Calcium pump crystal structure with bound TNP-ADP and TG in the absence of calcium
Authors	:	Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on	:	2010-11-24
Resolution	:	2.20 Å(reported)

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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.
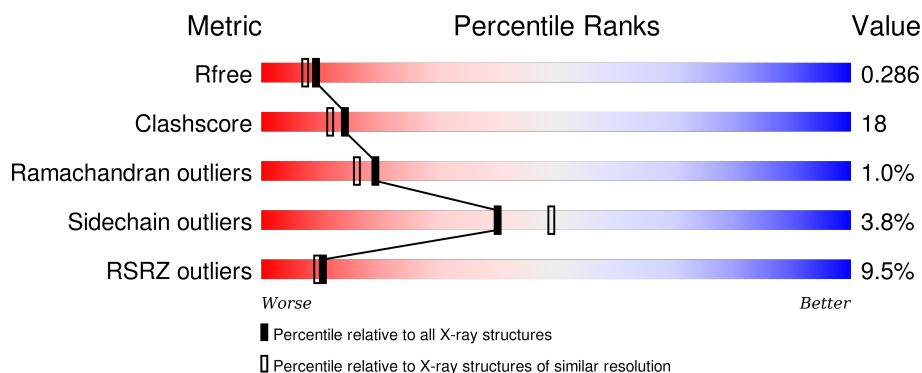
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	995	

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	12D	A	1002	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 (i)

There are 7 unique types of molecules in this entry. The entry contains 8093 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
			Total	C	N	O	S			
1	A	995	7674	4878	1287	1452	57	0	0	0

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

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

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

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

- Molecule 4 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-DECAHYD RO-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: $C_{34}H_{50}O_{12}$).
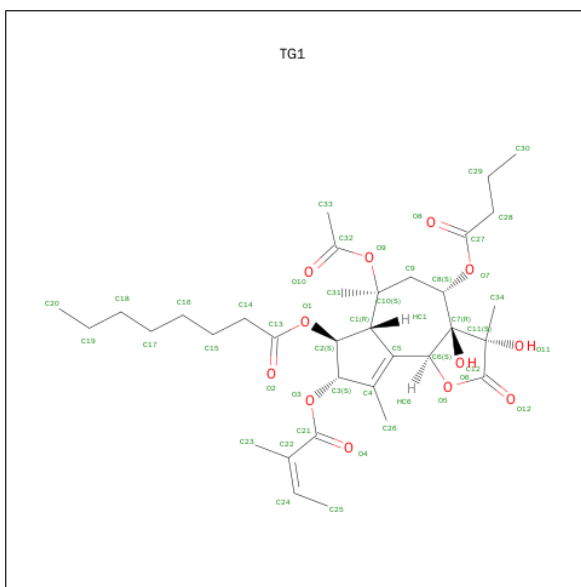
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 46	C 34	O 12	0	0

- Molecule 5 is 2',3'-O-[(1R,6R)-2,4,6-TRINITROCYCLOHEXA-2,4-DIENE-1,1-DIYL]ADENOSINE 5'-(TRIHYDROGEN DIPHOSPHATE) (three-letter code: 12D) (formula: $C_{16}H_{16}N_8O_{16}P_2$).
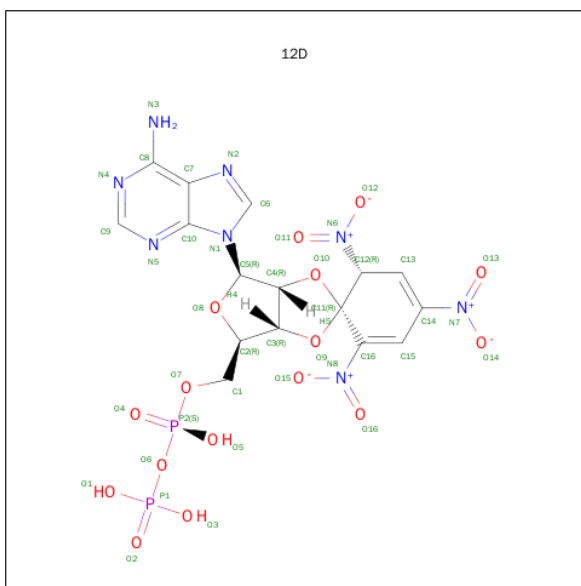
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 42	C 16	N 8	O 16	P 2	0	0

- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:

$C_{40}H_{80}NO_8P$).
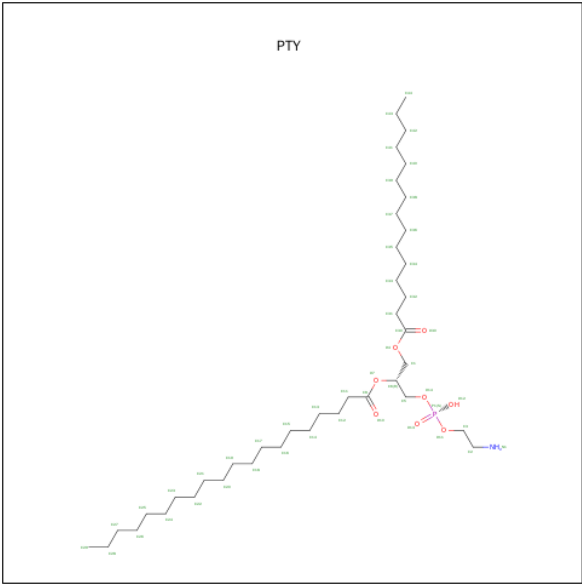
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	272	Total	O	0	0
			272	272		

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
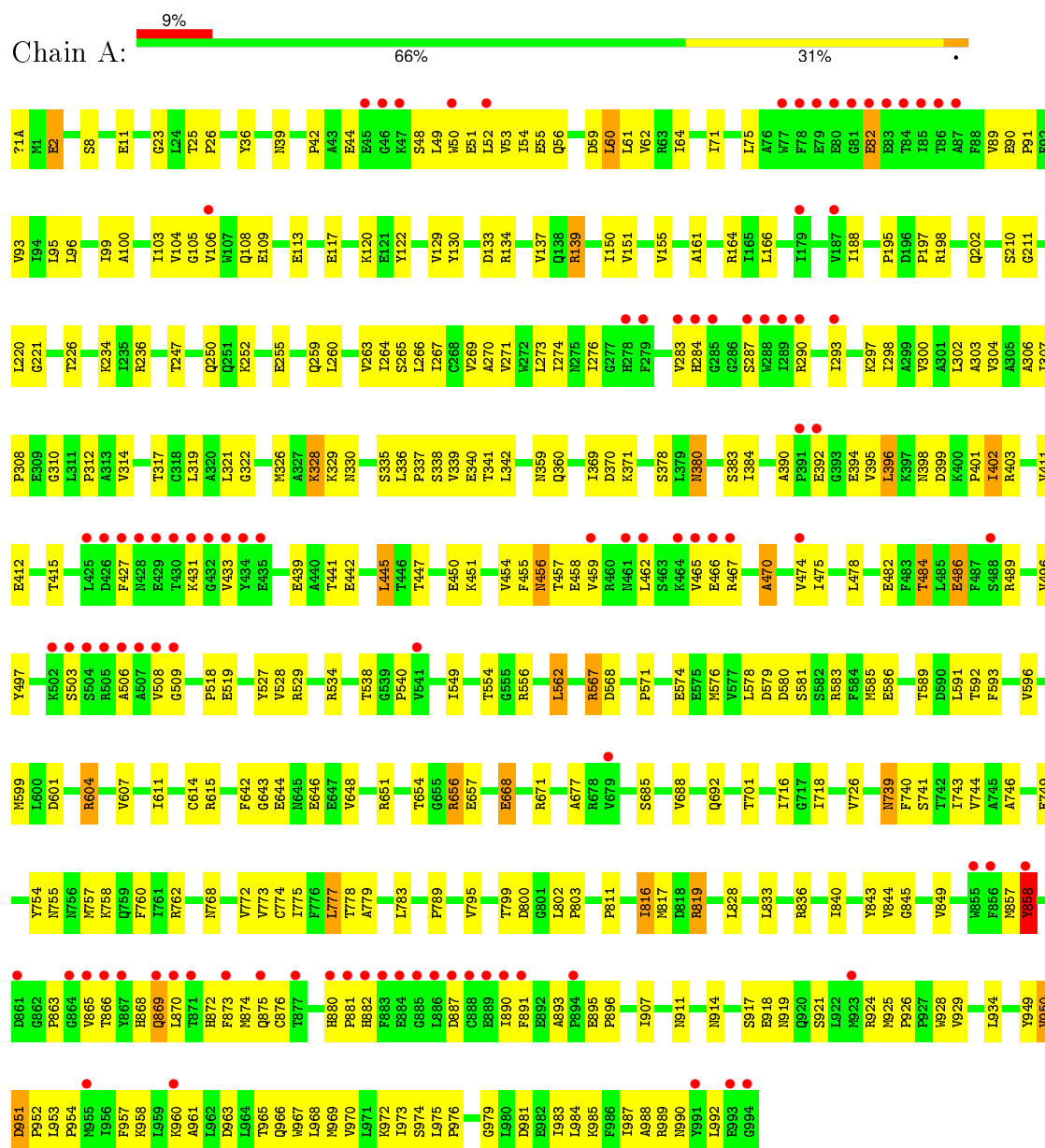
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.62Å 71.62Å 588.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 49.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.20) 99.3 (49.03-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.287 0.249 , 0.286	Depositor DCC
R_{free} test set	3941 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 79508 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8093	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TG1, 12D, ACE, NA, PTY

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	0.36	0/7813	0.60	1/10594 (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	601	ASP	N-CA-C	-5.26	96.79	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	285	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	46	0	50	3	0
5	A	42	0	12	0	0
6	A	57	0	33	2	0
7	A	272	0	0	11	0
All	All	8093	0	7860	285	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 (285) 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:988:ALA:HA	1:A:992:LEU:HD12	1.49	0.94
1:A:819:ARG:HB3	1:A:819:ARG:HH11	1.33	0.94
1:A:963:ASP:HB3	1:A:966:GLN:HG3	1.47	0.94
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.52	0.91
1:A:290:ARG:HH22	1:A:875:GLN:HA	1.44	0.83
1:A:963:ASP:H	1:A:966:GLN:HE21	1.27	0.82
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.63	0.78
1:A:287:SER:HB3	1:A:290:ARG:HB2	1.64	0.78
1:A:819:ARG:HB3	1:A:819:ARG:NH1	2.00	0.76
1:A:188:ILE:HD12	1:A:486:GLU:HG2	1.69	0.74
1:A:739:ASN:HD22	1:A:740:PHE:N	1.86	0.73
1:A:508:VAL:HG12	1:A:509:GLY:H	1.54	0.73
1:A:963:ASP:N	1:A:966:GLN:HE21	1.87	0.73
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.72	0.72
1:A:758:LYS:O	1:A:762:ARG:HG3	1.90	0.71
1:A:836:ARG:O	1:A:840:ILE:HG12	1.91	0.71
1:A:328:LYS:NZ	1:A:328:LYS:HA	2.05	0.71
1:A:326:MET:HE1	1:A:339:VAL:HG12	1.72	0.70
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.73	0.69
1:A:643:GLY:H	1:A:646:GLU:HG2	1.55	0.69
1:A:402:ILE:HD13	1:A:402:ILE:H	1.58	0.69
1:A:921:SER:H	1:A:989:ARG:HH12	1.41	0.68
1:A:395:VAL:O	1:A:396:LEU:HD23	1.94	0.68
1:A:921:SER:H	1:A:989:ARG:NH1	1.91	0.68
1:A:484:THR:HB	1:A:496:VAL:HG12	1.74	0.68
1:A:571:PRO:HG2	1:A:576:MET:SD	2.34	0.68
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.30	0.66
1:A:924:ARG:HA	1:A:924:ARG:HE	1.60	0.66
1:A:328:LYS:HZ3	1:A:328:LYS:HA	1.59	0.65
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.78	0.65
1:A:104:VAL:HG12	1:A:108:GLN:HE21	1.60	0.65
1:A:857:MET:HB3	1:A:866:THR:HA	1.79	0.65
1:A:370:ASP:HB3	1:A:378:SER:OG	1.97	0.65
1:A:2:GLU:CD	1:A:2:GLU:H	2.00	0.64
1:A:133:ASP:O	1:A:134:ARG:HG3	1.97	0.64
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.80	0.64
1:A:863:PRO:HG2	1:A:890:ILE:HD12	1.80	0.63
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.80	0.63
1:A:48:SER:OG	1:A:51:GLU:HG3	1.99	0.63
1:A:75:LEU:HD21	1:A:297:LYS:HG3	1.81	0.62
1:A:688:VAL:O	1:A:692:GLN:HG3	1.99	0.62
1:A:462:LEU:HD22	1:A:466:GLU:OE1	2.00	0.62
1:A:567:ARG:HG2	1:A:591:LEU:HD23	1.80	0.62
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.30	0.62
1:A:50:TRP:O	1:A:54:ILE:HG12	1.99	0.62
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.34	0.62
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.99	0.62
1:A:427:PHE:HB3	1:A:465:VAL:HG22	1.82	0.61
1:A:23:GLY:HA3	1:A:130:TYR:O	2.00	0.61
1:A:611:ILE:O	1:A:615:ARG:HG3	2.00	0.61
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.29	0.61
1:A:643:GLY:N	1:A:646:GLU:HG2	2.15	0.61
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.83	0.61
1:A:303:ALA:O	1:A:307:ILE:HG12	2.01	0.61
1:A:990:ASN:HD21	6:A:1012:PTY:HC31	1.66	0.61
1:A:90:GLU:OE1	1:A:789:PRO:HG2	2.02	0.60
1:A:873:PHE:HD2	1:A:876:CYS:H	1.49	0.60
1:A:383:SER:O	1:A:384:ILE:HD13	2.02	0.60
1:A:778:THR:HG21	7:A:2181:HOH:O	2.01	0.60
1:A:271:VAL:HG11	1:A:298:ILE:HD11	1.84	0.59
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.84	0.59
1:A:273:LEU:HA	1:A:276:ILE:HD11	1.84	0.59
1:A:384:ILE:HD12	1:A:395:VAL:HG22	1.83	0.59
1:A:580:ASP:OD2	1:A:583:ARG:HG3	2.03	0.59
1:A:335:SER:HB3	1:A:338:SER:OG	2.04	0.58
1:A:300:VAL:O	1:A:304:VAL:HG23	2.03	0.58
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.84	0.58
1:A:441:THR:HG23	1:A:599:MET:SD	2.43	0.58
1:A:604:ARG:CB	1:A:607:VAL:HG13	2.34	0.58
1:A:757:MET:HA	1:A:760:PHE:CE2	2.39	0.58
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.34	0.57
1:A:51:GLU:O	1:A:55:GLU:HG3	2.04	0.57
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.66	0.57
1:A:974:SER:C	1:A:976:PRO:HD2	2.25	0.57
1:A:960:LYS:HD3	1:A:961:ALA:O	2.04	0.57
1:A:188:ILE:HD12	1:A:486:GLU:CG	2.34	0.56
1:A:166:LEU:H	1:A:221:GLY:HA2	1.71	0.56
1:A:574:GLU:CD	1:A:574:GLU:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:HIS:N	1:A:881:PRO:HD2	2.21	0.55
1:A:8:SER:OG	1:A:11:GLU:HG3	2.07	0.55
1:A:604:ARG:HB2	1:A:607:VAL:HG13	1.88	0.55
1:A:312:PRO:HG2	7:A:2023:HOH:O	2.06	0.55
1:A:503:SER:HB3	1:A:506:ALA:HB2	1.89	0.55
1:A:267:ILE:O	1:A:271:VAL:HG23	2.06	0.55
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.06	0.55
1:A:247:THR:H	1:A:250:GLN:NE2	2.05	0.55
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.10	0.54
1:A:49:LEU:O	1:A:53:VAL:HG23	2.07	0.54
1:A:403:ARG:HD3	1:A:456:ASN:HD21	1.71	0.54
1:A:150:ILE:CG2	1:A:220:LEU:HD11	2.38	0.54
1:A:322:GLY:O	1:A:326:MET:HG3	2.08	0.54
1:A:873:PHE:HE2	1:A:876:CYS:HA	1.73	0.54
1:A:538:THR:HG22	1:A:540:PRO:HD2	1.89	0.54
1:A:100:ALA:O	1:A:104:VAL:HG23	2.08	0.53
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.41	0.53
1:A:75:LEU:HD11	1:A:293:ILE:HG23	1.89	0.53
1:A:95:LEU:HD23	1:A:95:LEU:O	2.09	0.53
1:A:967:TRP:O	1:A:970:VAL:HB	2.09	0.53
1:A:120:LYS:HE3	7:A:2270:HOH:O	2.08	0.53
1:A:874:MET:HG2	1:A:891:PHE:CD2	2.44	0.53
1:A:963:ASP:H	1:A:966:GLN:NE2	2.00	0.53
1:A:755:ASN:ND2	1:A:816:ILE:HD11	2.24	0.53
1:A:921:SER:N	1:A:989:ARG:HH12	2.07	0.53
1:A:895:GLU:N	1:A:896:PRO:HD2	2.24	0.53
1:A:150:ILE:HG23	1:A:220:LEU:HD11	1.91	0.52
1:A:921:SER:CB	1:A:989:ARG:HH12	2.23	0.52
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.45	0.52
1:A:534:ARG:HH21	1:A:568:ASP:CB	2.22	0.52
1:A:918:GLU:C	1:A:919:ASN:HD22	2.13	0.52
1:A:819:ARG:NH1	1:A:819:ARG:CB	2.71	0.52
1:A:643:GLY:H	1:A:646:GLU:CG	2.23	0.52
1:A:122:TYR:O	1:A:211:GLY:HA2	2.09	0.52
1:A:654:THR:HA	1:A:677:ALA:O	2.11	0.52
1:A:339:VAL:HG23	1:A:340:GLU:N	2.25	0.51
1:A:921:SER:HB2	1:A:989:ARG:HH12	1.75	0.51
1:A:271:VAL:HG11	1:A:298:ILE:CD1	2.40	0.51
1:A:963:ASP:OD2	1:A:965:THR:HB	2.11	0.51
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.10	0.51
1:A:139:ARG:HG3	1:A:139:ARG:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD22	1:A:336:LEU:H	1.76	0.51
1:A:604:ARG:HG3	7:A:2122:HOH:O	2.10	0.51
1:A:273:LEU:HA	1:A:276:ILE:CG1	2.41	0.51
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.92	0.51
1:A:668:GLU:O	1:A:671:ARG:HG2	2.11	0.50
1:A:161:ALA:HA	1:A:210:SER:HB2	1.93	0.50
1:A:60:LEU:O	1:A:64:ILE:HG12	2.11	0.50
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.93	0.50
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.93	0.50
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.11	0.50
1:A:981:ASP:OD2	1:A:985:LYS:HE3	2.12	0.50
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.94	0.50
1:A:236:ARG:HD3	1:A:236:ARG:C	2.32	0.50
1:A:924:ARG:O	1:A:926:PRO:HD3	2.11	0.50
1:A:298:ILE:O	1:A:302:LEU:HB2	2.11	0.49
1:A:607:VAL:O	1:A:611:ILE:HG12	2.12	0.49
1:A:668:GLU:HA	1:A:671:ARG:HD2	1.93	0.49
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.93	0.49
1:A:454:VAL:HG22	7:A:2139:HOH:O	2.12	0.49
1:A:554:THR:HG23	7:A:2398:HOH:O	2.12	0.49
1:A:762:ARG:HD3	1:A:828:LEU:O	2.12	0.49
1:A:442:GLU:O	1:A:445:LEU:HB2	2.12	0.49
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.95	0.49
1:A:529:ARG:NH2	1:A:568:ASP:OD2	2.43	0.49
1:A:881:PRO:HG2	1:A:882:HIS:H	1.76	0.49
1:A:963:ASP:HB3	1:A:966:GLN:CG	2.33	0.49
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.95	0.49
1:A:202:GLN:NE2	1:A:489:ARG:NH1	2.61	0.49
1:A:104:VAL:HG12	1:A:108:GLN:NE2	2.28	0.48
1:A:772:VAL:HG12	4:A:1003:TG1:H202	1.95	0.48
1:A:302:LEU:HD13	1:A:302:LEU:O	2.13	0.48
1:A:342:LEU:HD13	1:A:716:ILE:HG21	1.94	0.48
1:A:583:ARG:O	1:A:586:GLU:HB3	2.13	0.48
1:A:924:ARG:NE	1:A:924:ARG:HA	2.26	0.48
1:A:949:TYR:O	1:A:951:ASP:N	2.46	0.48
1:A:969:MET:O	1:A:973:ILE:HG13	2.13	0.48
1:A:527:TYR:O	1:A:592:THR:HA	2.14	0.48
1:A:762:ARG:HD2	1:A:833:LEU:HD21	1.94	0.48
1:A:95:LEU:O	1:A:99:ILE:HG13	2.14	0.48
1:A:858:TYR:CD1	1:A:858:TYR:N	2.78	0.48
1:A:151:VAL:O	1:A:220:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ILE:O	1:A:844:VAL:HG23	2.13	0.48
1:A:274:ILE:HG22	1:A:274:ILE:O	2.13	0.48
1:A:973:ILE:O	1:A:976:PRO:HG2	2.14	0.48
1:A:975:LEU:N	1:A:976:PRO:HD2	2.28	0.47
1:A:195:PRO:O	1:A:197:PRO:HD3	2.14	0.47
1:A:979:GLY:O	1:A:983:ILE:HG13	2.14	0.47
1:A:777:LEU:HB3	1:A:849:VAL:HG21	1.97	0.47
1:A:604:ARG:O	1:A:607:VAL:HG22	2.15	0.47
1:A:450:GLU:OE2	1:A:450:GLU:HA	2.15	0.47
1:A:455:PHE:O	1:A:456:ASN:C	2.53	0.47
1:A:865:VAL:HB	1:A:868:HIS:CB	2.45	0.47
1:A:273:LEU:HA	1:A:276:ILE:CD1	2.45	0.47
1:A:508:VAL:HG12	1:A:509:GLY:N	2.28	0.46
1:A:44:GLU:OE1	1:A:117:GLU:HG3	2.14	0.46
1:A:887:ASP:OD1	1:A:890:ILE:HG23	2.15	0.46
1:A:755:ASN:HD22	1:A:816:ILE:HD11	1.81	0.46
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.15	0.46
1:A:604:ARG:HB3	1:A:607:VAL:HG13	1.98	0.46
1:A:310:GLY:O	1:A:314:VAL:HG23	2.15	0.46
1:A:775:ILE:HA	1:A:778:THR:HG22	1.98	0.46
1:A:161:ALA:CA	1:A:210:SER:HB2	2.46	0.46
1:A:474:VAL:O	1:A:478:LEU:HD13	2.16	0.46
1:A:394:GLU:HG3	1:A:396:LEU:HD21	1.97	0.46
1:A:783:LEU:HD23	1:A:870:LEU:HB2	1.98	0.46
1:A:585:MET:O	1:A:589:THR:HG23	2.16	0.46
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.16	0.45
1:A:921:SER:HB2	1:A:989:ARG:HH22	1.80	0.45
1:A:458:GLU:HG2	7:A:2390:HOH:O	2.16	0.45
1:A:642:PHE:CG	1:A:648:VAL:HG11	2.51	0.45
1:A:270:ALA:O	1:A:274:ILE:HG13	2.16	0.45
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.51	0.45
1:A:774:CYS:O	1:A:778:THR:HG22	2.16	0.45
1:A:263:VAL:HG11	4:A:1003:TG1:O4	2.17	0.45
1:A:394:GLU:HB2	7:A:2273:HOH:O	2.16	0.45
1:A:398:ASN:O	1:A:399:ASP:HB2	2.17	0.45
1:A:593:PHE:HZ	1:A:596:VAL:HG23	1.82	0.45
1:A:302:LEU:HD13	1:A:302:LEU:C	2.37	0.45
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.32	0.45
1:A:739:ASN:ND2	1:A:741:SER:H	2.14	0.45
1:A:104:VAL:O	1:A:108:GLN:HG3	2.17	0.45
1:A:983:ILE:O	1:A:987:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:GLU:HG3	1:A:960:LYS:HD2	1.99	0.45
1:A:614:CYS:SG	1:A:744:VAL:HG22	2.57	0.45
1:A:336:LEU:O	1:A:339:VAL:HG22	2.17	0.44
1:A:739:ASN:C	1:A:739:ASN:HD22	2.20	0.44
1:A:25:THR:HB	1:A:26:PRO:HD2	2.00	0.44
1:A:968:LEU:O	1:A:972:LYS:HB2	2.17	0.44
1:A:390:ALA:C	1:A:392:GLU:H	2.21	0.44
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.48	0.44
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.99	0.44
1:A:342:LEU:HD21	1:A:746:ALA:HB1	2.00	0.44
1:A:800:ASP:C	1:A:803:PRO:HD2	2.38	0.44
1:A:259:GLN:O	1:A:263:VAL:HG23	2.17	0.43
1:A:283:VAL:HG13	1:A:284:HIS:N	2.33	0.43
1:A:89:VAL:O	1:A:93:VAL:HG23	2.18	0.43
1:A:957:PHE:O	1:A:958:LYS:HB2	2.18	0.43
1:A:415:THR:HA	1:A:475:ILE:HG21	2.00	0.43
1:A:252:LYS:HD3	1:A:828:LEU:CD1	2.49	0.43
1:A:527:TYR:HB2	1:A:592:THR:OG1	2.17	0.43
1:A:96:LEU:C	1:A:96:LEU:HD23	2.38	0.43
1:A:656:ARG:HG2	1:A:656:ARG:NH1	2.33	0.43
1:A:800:ASP:O	1:A:803:PRO:HD2	2.19	0.43
1:A:71:ILE:O	1:A:75:LEU:HB2	2.19	0.43
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.84	0.43
1:A:701:THR:HA	1:A:718:ILE:O	2.18	0.43
1:A:326:MET:HE1	1:A:339:VAL:CG1	2.43	0.43
1:A:137:VAL:O	1:A:137:VAL:HG13	2.19	0.43
1:A:1(A):ACE:H3	1:A:36:TYR:CE1	2.54	0.43
1:A:556:ARG:HH12	1:A:644:GLU:CG	2.32	0.43
1:A:604:ARG:HB2	1:A:607:VAL:CG1	2.48	0.42
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.84	0.42
1:A:844:VAL:HG22	1:A:907:ILE:HG21	2.01	0.42
1:A:234:LYS:NZ	7:A:2298:HOH:O	2.52	0.42
1:A:265:SER:O	1:A:269:VAL:HG23	2.20	0.42
1:A:534:ARG:NH2	1:A:568:ASP:HB2	2.34	0.42
1:A:754:TYR:HA	1:A:757:MET:HE2	2.01	0.42
1:A:953:LEU:N	1:A:954:PRO:HD2	2.34	0.42
1:A:304:VAL:HG21	1:A:789:PRO:HB3	2.01	0.42
1:A:202:GLN:OE1	1:A:489:ARG:NH1	2.53	0.42
1:A:836:ARG:HG2	1:A:984:LEU:HB3	2.01	0.42
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.84	0.42
1:A:155:VAL:O	1:A:155:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:THR:O	1:A:321:LEU:HG	2.19	0.42
1:A:917:SER:HB2	1:A:925:MET:SD	2.60	0.42
1:A:845:GLY:O	1:A:849:VAL:HG23	2.20	0.42
1:A:329:LYS:O	1:A:330:ASN:HB2	2.20	0.42
1:A:462:LEU:HB3	1:A:466:GLU:HB2	2.02	0.42
1:A:411:VAL:HG22	1:A:454:VAL:HB	2.00	0.42
1:A:457:THR:HG22	1:A:458:GLU:N	2.34	0.42
1:A:82:GLU:OE1	1:A:82:GLU:N	2.52	0.42
1:A:402:ILE:N	1:A:402:ILE:HD13	2.31	0.42
1:A:760:PHE:C	1:A:760:PHE:CD1	2.93	0.42
1:A:482:GLU:HG3	1:A:497:TYR:HD1	1.85	0.42
1:A:380:ASN:HD22	1:A:380:ASN:C	2.23	0.42
1:A:740:PHE:O	1:A:743:ILE:HB	2.20	0.41
1:A:579:ASP:HB2	7:A:2049:HOH:O	2.20	0.41
1:A:260:LEU:HD13	4:A:1003:TG1:H252	2.02	0.41
1:A:439:GLU:HG3	1:A:441:THR:H	1.84	0.41
1:A:893:ALA:O	1:A:896:PRO:HD2	2.19	0.41
1:A:290:ARG:HH11	1:A:290:ARG:HB3	1.85	0.41
1:A:395:VAL:O	1:A:401:PRO:HA	2.20	0.41
1:A:880:HIS:N	1:A:881:PRO:CD	2.83	0.41
1:A:39:ASN:OD1	1:A:226:THR:HB	2.21	0.41
1:A:273:LEU:CD2	1:A:276:ILE:HD11	2.51	0.41
1:A:656:ARG:HA	1:A:656:ARG:NE	2.36	0.41
1:A:562:LEU:HD12	1:A:562:LEU:HA	1.87	0.41
1:A:104:VAL:HG21	6:A:1011:PTY:HC11	2.02	0.41
1:A:252:LYS:O	1:A:255:GLU:HG2	2.21	0.41
1:A:777:LEU:C	1:A:779:ALA:H	2.25	0.41
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.51	0.41
1:A:273:LEU:HA	1:A:276:ILE:HG13	2.03	0.41
1:A:816:ILE:HG22	1:A:817:MET:N	2.35	0.41
1:A:198:ARG:NH1	1:A:198:ARG:HG3	2.36	0.41
1:A:459:VAL:HG12	1:A:470:ALA:HB1	2.03	0.41
1:A:921:SER:N	1:A:989:ARG:NH1	2.62	0.40
1:A:99:ILE:O	1:A:103:ILE:HG13	2.21	0.40
1:A:811:PRO:HG3	1:A:929:VAL:CG1	2.51	0.40
1:A:773:VAL:O	1:A:777:LEU:HB2	2.21	0.40
1:A:554:THR:O	1:A:554:THR:HG22	2.22	0.40
1:A:2:GLU:CD	1:A:2:GLU:N	2.71	0.40
1:A:868:HIS:O	1:A:868:HIS:ND1	2.54	0.40
1:A:795:VAL:HA	1:A:799:THR:HB	2.04	0.40
1:A:447:THR:HG22	1:A:451:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLN:HB2	7:A:2143:HOH:O	2.20	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%)	927 (93%)	56 (6%)	10 (1%)	19 16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ASN
1	A	951	ASP
1	A	858	TYR
1	A	869	GLN
1	A	950	VAL
1	A	470	ALA
1	A	82	GLU
1	A	581	SER
1	A	578	LEU
1	A	433	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	840/840 (100%)	808 (96%)	32 (4%)	40 49

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	60	LEU
1	A	109	GLU
1	A	113	GLU
1	A	139	ARG
1	A	164	ARG
1	A	266	LEU
1	A	319	LEU
1	A	328	LYS
1	A	341	THR
1	A	359	ASN
1	A	371	LYS
1	A	380	ASN
1	A	396	LEU
1	A	402	ILE
1	A	431	LYS
1	A	445	LEU
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	519	GLU
1	A	562	LEU
1	A	567	ARG
1	A	604	ARG
1	A	656	ARG
1	A	668	GLU
1	A	685	SER
1	A	739	ASN
1	A	777	LEU
1	A	816	ILE
1	A	819	ARG
1	A	858	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	380	ASN
1	A	398	ASN
1	A	456	ASN
1	A	461	ASN
1	A	510	ASN
1	A	612	GLN
1	A	628	ASN
1	A	739	ASN
1	A	755	ASN
1	A	875	GLN
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN
1	A	990	ASN

5.3.3   RNA (i)

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 7 ligands modelled in this entry, 2 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
5	12D	A	1002	-	30,46,46	2.35	10 (33%)	36,73,73	3.55	12 (33%)
4	TG1	A	1003	-	43,48,48	1.86	9 (20%)	42,72,72	1.68	10 (23%)
6	PTY	A	1011	-	17,18,49	1.48	3 (17%)	18,23,54	1.38	3 (16%)
6	PTY	A	1012	-	17,18,49	1.34	3 (17%)	18,23,54	1.21	2 (11%)
6	PTY	A	1013	-	17,18,49	1.19	2 (11%)	18,23,54	1.44	1 (5%)

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	12D	A	1002	-	2/2/13/15	0/18/74/74	0/5/5/5
4	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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	12D	P1-O1	-2.34	1.46	1.54
5	A	1002	12D	P1-O3	-2.12	1.47	1.54
5	A	1002	12D	C3-C2	-2.05	1.46	1.52
4	A	1003	TG1	C34-C11	2.00	1.56	1.53
6	A	1013	PTY	P1-O13	2.20	1.59	1.51
4	A	1003	TG1	C11-C7	2.24	1.58	1.55
6	A	1013	PTY	C5-C6	2.31	1.57	1.50
6	A	1011	PTY	C5-C6	2.44	1.57	1.50
6	A	1012	PTY	P1-O13	2.51	1.60	1.51
6	A	1012	PTY	C5-C6	2.55	1.57	1.50
4	A	1003	TG1	C31-C10	2.61	1.58	1.52
5	A	1002	12D	P1-O2	2.63	1.59	1.51
6	A	1011	PTY	P1-O13	2.66	1.60	1.51
4	A	1003	TG1	C9-C8	2.70	1.55	1.52
5	A	1002	12D	C9-N5	2.96	1.37	1.32
4	A	1003	TG1	C21-C22	3.04	1.61	1.50
4	A	1003	TG1	C1-C5	3.14	1.56	1.51
6	A	1012	PTY	C1-C6	3.16	1.59	1.50
4	A	1003	TG1	C2-C3	3.32	1.59	1.53
5	A	1002	12D	C10-N5	3.33	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	12D	C9-N4	3.35	1.40	1.33
6	A	1011	PTY	C1-C6	3.69	1.61	1.50
5	A	1002	12D	O10-C11	5.12	1.49	1.42
4	A	1003	TG1	C7-C8	5.31	1.60	1.53
5	A	1002	12D	C13-C14	5.63	1.42	1.33
4	A	1003	TG1	O4-C21	5.93	1.34	1.21
5	A	1002	12D	O9-C11	6.29	1.51	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	12D	N5-C9-N4	-10.58	120.79	128.89
5	A	1002	12D	C11-O10-C4	-4.24	98.93	106.92
5	A	1002	12D	O8-C5-C4	-3.80	99.72	106.60
4	A	1003	TG1	O12-C12-C11	-3.18	125.33	128.26
4	A	1003	TG1	O11-C11-C12	-3.09	96.58	106.08
4	A	1003	TG1	O5-C6-C7	-3.03	101.40	104.08
5	A	1002	12D	O10-C11-C16	-3.00	101.62	109.55
5	A	1002	12D	C15-C14-C13	-2.92	116.88	122.40
4	A	1003	TG1	C23-C22-C24	-2.29	115.02	123.55
6	A	1011	PTY	O11-P1-O13	-2.01	101.80	109.62
4	A	1003	TG1	C31-C10-C9	2.01	114.53	110.32
5	A	1002	12D	O9-C11-C16	2.05	114.98	109.55
5	A	1002	12D	C4-C3-C2	2.09	108.94	103.69
6	A	1012	PTY	O7-C8-C11	2.19	115.22	111.10
5	A	1002	12D	O6-P2-O7	2.28	108.98	102.94
5	A	1002	12D	O10-C4-C5	2.31	116.54	109.55
4	A	1003	TG1	C34-C11-C12	2.34	117.28	112.49
4	A	1003	TG1	O5-C12-O12	2.35	125.05	121.62
6	A	1012	PTY	O4-C1-C6	2.62	115.73	108.69
6	A	1011	PTY	O4-C1-C6	2.88	116.45	108.69
4	A	1003	TG1	C24-C22-C21	3.07	133.80	120.67
4	A	1003	TG1	O7-C8-C9	3.17	112.82	107.03
6	A	1011	PTY	O7-C8-C11	3.41	117.54	111.10
6	A	1013	PTY	O7-C8-C11	3.66	118.00	111.10
4	A	1003	TG1	C10-O9-C32	5.61	133.41	121.90
5	A	1002	12D	O10-C4-C3	6.90	114.45	103.64
5	A	1002	12D	C11-C12-N6	9.83	126.84	108.10
5	A	1002	12D	C2-O8-C5	10.16	120.89	109.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1002	12D	C11
5	A	1002	12D	C12

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	TG1	3	0
6	A	1011	PTY	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	0.55	94 (9%)	10	9	30, 56, 118, 145	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	ARG	13.1
1	A	85	ILE	11.6
1	A	883	PHE	11.6
1	A	886	LEU	9.8
1	A	433	VAL	9.5
1	A	77	TRP	9.0
1	A	504	SER	8.9
1	A	86	THR	8.8
1	A	506	ALA	8.8
1	A	78	PHE	8.3
1	A	459	VAL	7.8
1	A	885	GLY	7.7
1	A	508	VAL	7.3
1	A	430	THR	7.2
1	A	507	ALA	7.1
1	A	427	PHE	7.0
1	A	431	LYS	6.7
1	A	80	GLU	6.4
1	A	866	THR	6.4
1	A	426	ASP	6.4
1	A	428	ASN	6.3
1	A	503	SER	6.1
1	A	881	PRO	5.9
1	A	84	THR	5.9
1	A	884	GLU	5.4
1	A	870	LEU	5.4
1	A	464	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	993	GLU	5.0
1	A	434	TYR	4.9
1	A	887	ASP	4.9
1	A	435	GLU	4.9
1	A	432	GLY	4.8
1	A	890	ILE	4.6
1	A	81	GLY	4.6
1	A	873	PHE	4.5
1	A	287	SER	4.4
1	A	856	PHE	4.3
1	A	465	VAL	4.3
1	A	467	ARG	4.2
1	A	875	GLN	4.0
1	A	502	LYS	3.9
1	A	82	GLU	3.9
1	A	880	HIS	3.8
1	A	425	LEU	3.7
1	A	429	GLU	3.7
1	A	289	ILE	3.7
1	A	466	GLU	3.6
1	A	509	GLY	3.6
1	A	877	THR	3.6
1	A	861	ASP	3.6
1	A	888	CYS	3.5
1	A	865	VAL	3.4
1	A	889	GLU	3.4
1	A	79	GLU	3.3
1	A	994	GLY	3.2
1	A	283	VAL	3.0
1	A	462	LEU	3.0
1	A	284	HIS	2.9
1	A	858	TYR	2.9
1	A	46	GLY	2.8
1	A	882	HIS	2.8
1	A	474	VAL	2.8
1	A	290	ARG	2.8
1	A	894	PRO	2.8
1	A	106	VAL	2.7
1	A	864	GLY	2.7
1	A	50	TRP	2.6
1	A	187	VAL	2.6
1	A	288	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	855	TRP	2.6
1	A	871	THR	2.6
1	A	923	MET	2.6
1	A	679	VAL	2.5
1	A	891	PHE	2.5
1	A	179	ILE	2.4
1	A	960	LYS	2.4
1	A	52	LEU	2.4
1	A	278	HIS	2.4
1	A	45	GLU	2.4
1	A	83	GLU	2.3
1	A	955	MET	2.3
1	A	869	GLN	2.2
1	A	867	TYR	2.2
1	A	991	TYR	2.2
1	A	87	ALA	2.2
1	A	279	PHE	2.1
1	A	47	LYS	2.1
1	A	392	GLU	2.1
1	A	285	GLY	2.1
1	A	461	ASN	2.1
1	A	391	PRO	2.1
1	A	488	SER	2.1
1	A	293	ILE	2.0
1	A	541	VAL	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, 95th 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
6	PTY	A	1012	19/50	0.70	0.37	4.03	113,120,123,125	0
6	PTY	A	1011	19/50	0.79	0.21	2.39	108,110,113,114	0
5	12D	A	1002	42/42	0.95	0.20	0.77	48,59,72,76	0
6	PTY	A	1013	19/50	0.76	0.18	0.23	85,92,97,97	0
4	TG1	A	1003	46/46	0.94	0.14	-0.16	53,60,73,76	0
2	NA	A	1000	1/1	0.96	0.13	-1.30	52,52,52,52	0
3	MG	A	998	1/1	0.90	0.22	-	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.