



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:04 pm GMT

PDB ID : 3AR3
Title : Calcium pump crystal structure with bound ADP and TG
Authors : Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on : 2010-11-24
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

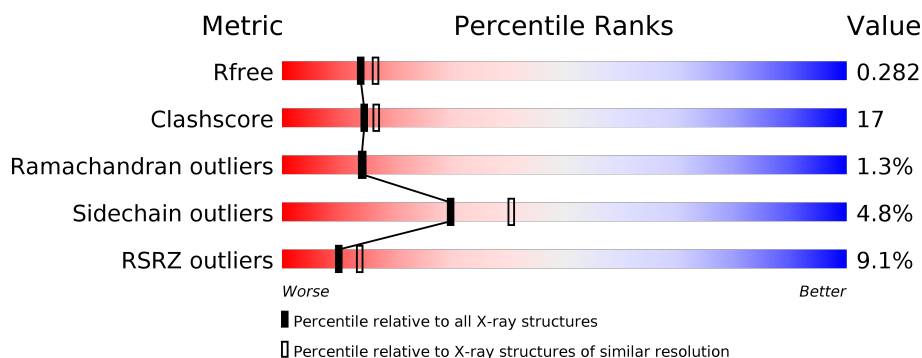
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 $\leq 5\%$. 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	<div> <div>9%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7964 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

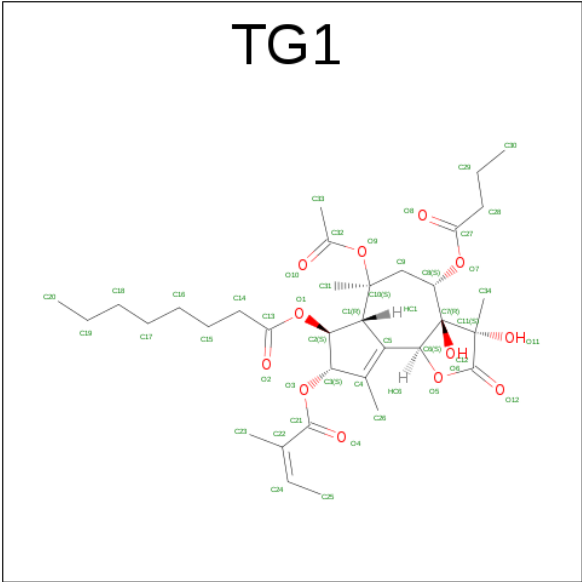
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

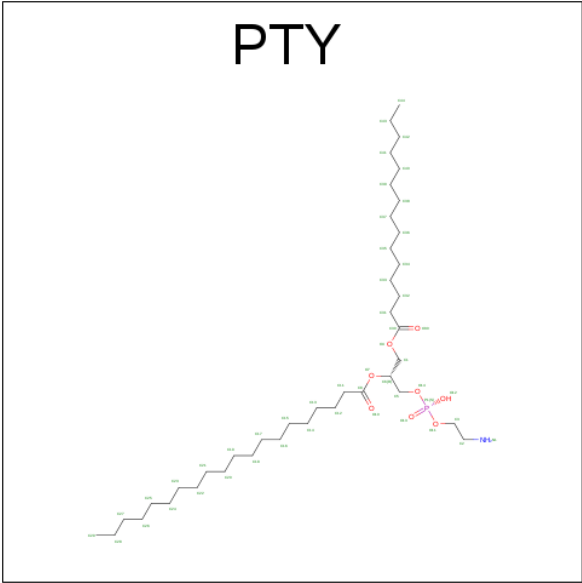
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- 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-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: C₃₄H₅₀O₁₂).



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

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



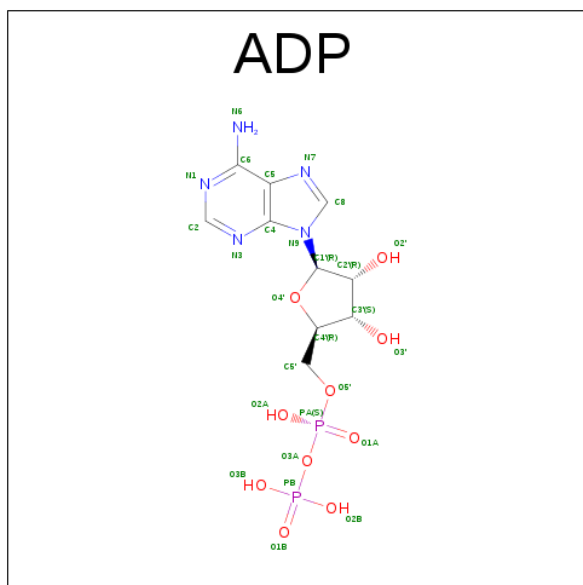
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
5	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

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

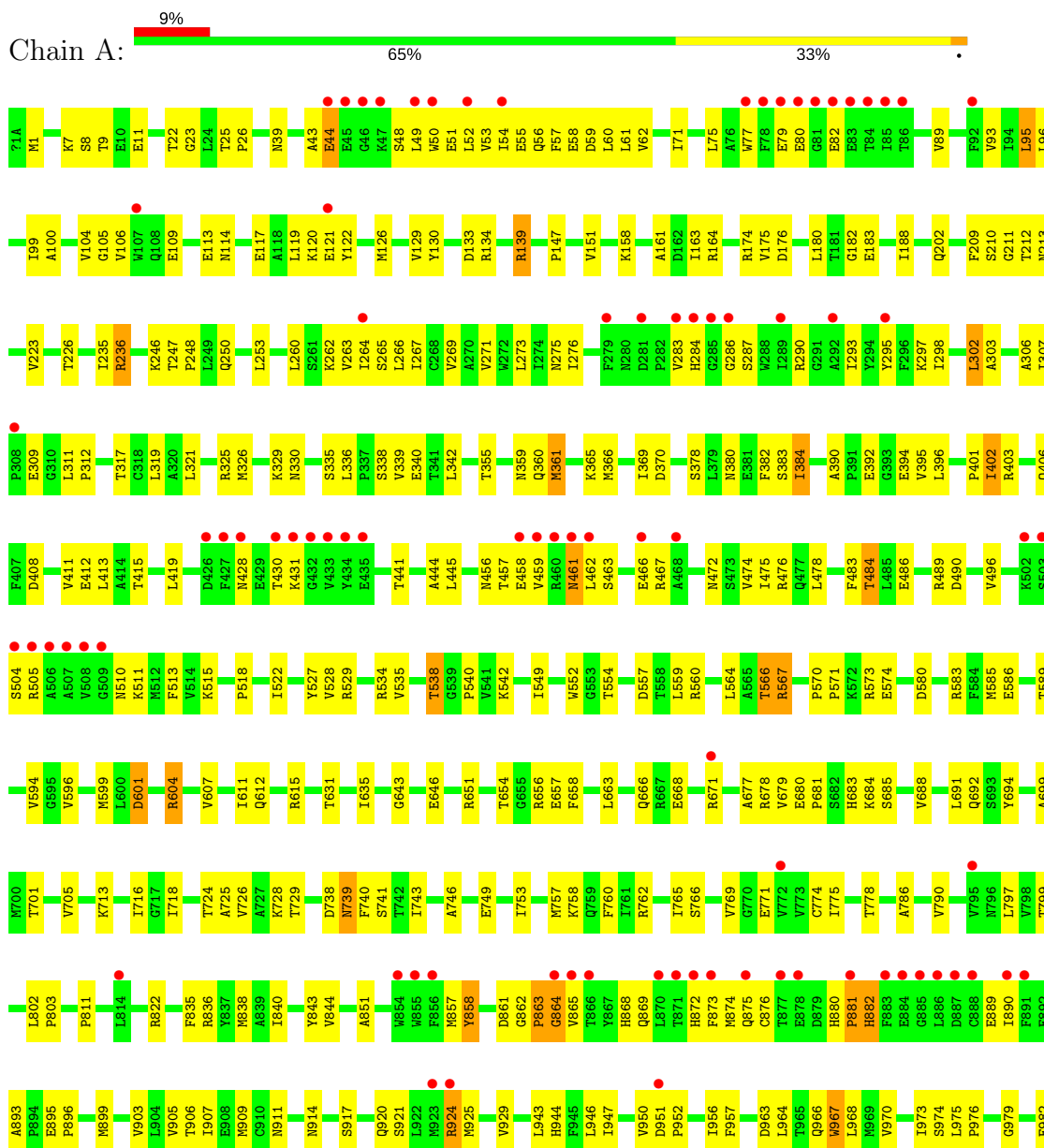
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

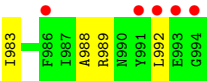


3 Residue-property plots

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.31Å 71.31Å 590.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.96 – 2.30 48.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (14.96-2.30) 99.6 (48.26-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.283 0.238 , 0.282	Depositor DCC
R_{free} test set	3484 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7964	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, ACE, ADP, 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	0.39	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(°)	Ideal(°)
1	A	601	ASP	N-CA-C	-5.16	97.08	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	269	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	46	0	50	1	0
5	A	57	0	33	1	0
6	A	27	0	12	2	0
7	A	157	0	0	10	0
All	All	7964	0	7860	269	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 17.

All (269) 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:663:LEU:HD12	1:A:663:LEU:H	1.35	0.91
1:A:484:THR:HB	1:A:496:VAL:HG12	1.63	0.79
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.65	0.78
1:A:869:GLN:HB2	1:A:872:HIS:HB2	1.65	0.78
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.67	0.77
1:A:583:ARG:O	1:A:586:GLU:HG2	1.85	0.76
1:A:474:VAL:O	1:A:478:LEU:HD12	1.87	0.75
1:A:739:ASN:HD22	1:A:740:PHE:N	1.84	0.75
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.70	0.73
1:A:395:VAL:O	1:A:396:LEU:HD23	1.89	0.72
1:A:262:LYS:O	1:A:266:LEU:HD23	1.90	0.72
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.54	0.72
1:A:89:VAL:O	1:A:93:VAL:HG23	1.89	0.72
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.90	0.71
1:A:394:GLU:HG3	1:A:396:LEU:HD21	1.72	0.71
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.71	0.71
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.73	0.71
1:A:963:ASP:H	1:A:966:GLN:NE2	1.89	0.71
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.73	0.70
1:A:515:LYS:HE3	6:A:1002:ADP:N1	2.06	0.70
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.72	0.70
1:A:202:GLN:NE2	1:A:489:ARG:HD3	2.07	0.70
1:A:865:VAL:HB	1:A:868:HIS:CB	2.22	0.70
1:A:335:SER:HB3	1:A:338:SER:OG	1.92	0.70
1:A:749:GLU:O	1:A:753:ILE:HG12	1.93	0.69
1:A:880:HIS:N	1:A:881:PRO:HD2	2.09	0.68
1:A:269:VAL:O	1:A:273:LEU:HG	1.92	0.68
1:A:403:ARG:HB3	1:A:406:GLN:OE1	1.93	0.68
1:A:899:MET:O	1:A:903:VAL:HG23	1.94	0.68
1:A:880:HIS:H	1:A:881:PRO:HD2	1.59	0.67
1:A:402:ILE:HD13	1:A:402:ILE:H	1.59	0.67
1:A:56:GLN:OE1	1:A:105:GLY:HA3	1.93	0.67
1:A:869:GLN:CB	1:A:872:HIS:HB2	2.25	0.66
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.09	0.66
1:A:312:PRO:HG2	7:A:2316:HOH:O	1.95	0.65
1:A:325:ARG:HD2	1:A:749:GLU:OE2	1.96	0.64
1:A:758:LYS:O	1:A:762:ARG:HG3	1.96	0.64
1:A:317:THR:O	1:A:321:LEU:HG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:C	1:A:384:ILE:HD13	2.18	0.64
1:A:8:SER:OG	1:A:11:GLU:HG3	1.99	0.63
1:A:133:ASP:O	1:A:134:ARG:HG3	1.98	0.63
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.81	0.63
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.80	0.63
1:A:654:THR:OG1	1:A:657:GLU:HG3	1.98	0.62
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.29	0.62
1:A:459:VAL:HB	1:A:467:ARG:NE	2.14	0.62
1:A:188:ILE:H	1:A:188:ILE:HD12	1.64	0.62
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.81	0.62
1:A:311:LEU:N	1:A:312:PRO:HD2	2.15	0.62
1:A:95:LEU:HD22	1:A:99:ILE:HD11	1.82	0.62
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.82	0.61
1:A:964:LEU:O	1:A:968:LEU:HD13	2.00	0.61
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.66	0.61
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.83	0.60
1:A:44:GLU:HB3	1:A:117:GLU:OE2	2.01	0.60
1:A:462:LEU:HB3	1:A:466:GLU:HB2	1.83	0.60
1:A:739:ASN:C	1:A:739:ASN:HD22	2.05	0.60
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.84	0.60
1:A:366:MET:HA	1:A:596:VAL:O	2.01	0.59
1:A:863:PRO:CG	1:A:890:ILE:HD13	2.31	0.59
1:A:567:ARG:CD	1:A:570:PRO:HA	2.32	0.59
1:A:428:ASN:OD1	1:A:430:THR:HB	2.01	0.59
1:A:963:ASP:H	1:A:966:GLN:HE21	1.49	0.59
1:A:554:THR:HG21	7:A:2640:HOH:O	2.02	0.59
1:A:48:SER:OG	1:A:51:GLU:HG3	2.00	0.59
1:A:209:PHE:O	1:A:212:THR:HB	2.02	0.58
1:A:688:VAL:O	1:A:692:GLN:HG3	2.03	0.58
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.86	0.58
1:A:39:ASN:OD1	1:A:226:THR:HB	2.04	0.58
1:A:836:ARG:O	1:A:840:ILE:HG12	2.04	0.58
1:A:188:ILE:HD12	1:A:188:ILE:N	2.19	0.57
1:A:75:LEU:C	1:A:77:TRP:H	2.08	0.57
1:A:979:GLY:O	1:A:983:ILE:HG13	2.05	0.57
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.86	0.57
1:A:295:TYR:O	1:A:298:ILE:HG12	2.02	0.57
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.85	0.56
1:A:868:HIS:ND1	1:A:869:GLN:N	2.53	0.56
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.05	0.56
1:A:472:ASN:HB3	1:A:476:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.83	0.56
1:A:396:LEU:HD22	1:A:401:PRO:HG3	1.88	0.56
1:A:43:ALA:HA	1:A:120:LYS:HZ1	1.70	0.56
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.88	0.56
1:A:336:LEU:O	1:A:339:VAL:HG22	2.06	0.56
1:A:52:LEU:HG	1:A:106:VAL:HG22	1.87	0.56
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.36	0.56
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.88	0.56
1:A:267:ILE:O	1:A:271:VAL:HG23	2.06	0.55
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.07	0.55
1:A:895:GLU:N	1:A:896:PRO:HD2	2.21	0.55
1:A:114:ASN:HD21	1:A:117:GLU:HG2	1.71	0.55
1:A:290:ARG:NH2	1:A:875:GLN:HG2	2.22	0.55
1:A:774:CYS:O	1:A:778:THR:HG22	2.07	0.55
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.88	0.55
1:A:585:MET:O	1:A:589:THR:HG23	2.06	0.54
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.08	0.54
1:A:273:LEU:HA	1:A:276:ILE:HG13	1.90	0.54
1:A:668:GLU:O	1:A:671:ARG:HG2	2.07	0.54
1:A:248:PRO:HB2	1:A:340:GLU:OE2	2.07	0.53
1:A:50:TRP:O	1:A:54:ILE:HG12	2.08	0.53
1:A:873:PHE:O	1:A:874:MET:HG3	2.07	0.53
1:A:472:ASN:HB3	1:A:476:ARG:HH12	1.74	0.53
1:A:863:PRO:HG2	1:A:890:ILE:HD13	1.89	0.53
1:A:247:THR:H	1:A:250:GLN:NE2	2.07	0.53
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.38	0.53
1:A:236:ARG:HD3	1:A:236:ARG:C	2.30	0.52
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.44	0.52
1:A:790:VAL:HG12	1:A:957:PHE:CE1	2.45	0.52
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.39	0.52
1:A:380:ASN:HD22	1:A:382:PHE:HZ	1.56	0.52
1:A:607:VAL:O	1:A:611:ILE:HG12	2.09	0.52
1:A:718:ILE:HD13	1:A:743:ILE:HG12	1.91	0.52
1:A:298:ILE:O	1:A:302:LEU:HB2	2.10	0.52
1:A:678:ARG:HH11	1:A:678:ARG:HG3	1.74	0.52
1:A:680:GLU:HG2	1:A:683:HIS:CE1	2.45	0.52
1:A:881:PRO:HG2	1:A:882:HIS:H	1.74	0.52
1:A:212:THR:CG2	1:A:213:ASN:N	2.73	0.51
1:A:534:ARG:HG2	1:A:535:VAL:N	2.25	0.51
1:A:484:THR:HG23	7:A:2685:HOH:O	2.10	0.51
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:TYR:HD1	1:A:858:TYR:H	1.58	0.51
1:A:402:ILE:N	1:A:402:ILE:HD13	2.25	0.51
1:A:895:GLU:CD	1:A:895:GLU:H	2.14	0.51
1:A:212:THR:HG22	1:A:213:ASN:N	2.25	0.50
1:A:303:ALA:O	1:A:307:ILE:HG12	2.11	0.50
1:A:739:ASN:ND2	1:A:741:SER:H	2.10	0.50
1:A:863:PRO:O	1:A:865:VAL:HG22	2.12	0.50
1:A:59:ASP:O	1:A:62:VAL:HG22	2.11	0.50
1:A:671:ARG:HD2	1:A:694:TYR:OH	2.11	0.50
1:A:293:ILE:O	1:A:297:LYS:HB2	2.12	0.50
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.94	0.50
1:A:396:LEU:HB2	7:A:2660:HOH:O	2.10	0.50
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.93	0.49
1:A:49:LEU:O	1:A:53:VAL:HG23	2.12	0.49
1:A:975:LEU:N	1:A:976:PRO:HD2	2.28	0.49
1:A:757:MET:HA	1:A:760:PHE:CE2	2.47	0.49
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.94	0.49
1:A:246:LYS:HB3	1:A:250:GLN:HE21	1.78	0.49
1:A:771:GLU:O	1:A:775:ILE:HG12	2.13	0.49
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.77	0.49
1:A:263:VAL:HG11	4:A:1003:TG1:O4	2.12	0.49
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.28	0.49
1:A:880:HIS:N	1:A:881:PRO:CD	2.76	0.49
1:A:325:ARG:HH12	1:A:753:ILE:CD1	2.25	0.49
1:A:287:SER:HB3	1:A:290:ARG:HG3	1.94	0.48
1:A:554:THR:CG2	1:A:554:THR:O	2.61	0.48
1:A:566:THR:HG22	1:A:594:VAL:CG2	2.43	0.48
1:A:554:THR:O	1:A:554:THR:HG22	2.13	0.48
1:A:713:LYS:HE3	7:A:2204:HOH:O	2.12	0.48
1:A:235:ILE:HD13	1:A:705:VAL:HG23	1.95	0.48
1:A:604:ARG:CG	1:A:604:ARG:HH11	2.23	0.48
1:A:126:MET:HE2	1:A:139:ARG:HD3	1.96	0.48
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.47	0.48
1:A:415:THR:HA	1:A:475:ILE:HG21	1.94	0.48
1:A:71:ILE:O	1:A:75:LEU:HD13	2.13	0.48
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.96	0.48
1:A:370:ASP:HB3	1:A:378:SER:OG	2.13	0.48
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.49	0.47
1:A:276:ILE:HG22	1:A:276:ILE:O	2.15	0.47
1:A:654:THR:HA	1:A:677:ALA:O	2.14	0.47
1:A:180:LEU:HD23	1:A:705:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:HH12	1:A:753:ILE:HD11	1.80	0.47
1:A:790:VAL:HG23	7:A:2337:HOH:O	2.14	0.47
1:A:857:MET:O	1:A:864:GLY:HA2	2.14	0.47
1:A:262:LYS:NZ	1:A:266:LEU:HD21	2.30	0.47
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.96	0.47
1:A:1:MET:CE	1:A:7:LYS:HG3	2.45	0.46
1:A:361:MET:HG2	1:A:441:THR:HA	1.96	0.46
1:A:176:ASP:O	1:A:212:THR:HG23	2.15	0.46
1:A:55:GLU:C	1:A:57:PHE:H	2.18	0.46
1:A:663:LEU:CD1	1:A:663:LEU:H	2.14	0.46
1:A:396:LEU:HD23	1:A:401:PRO:HA	1.98	0.46
1:A:952:PRO:O	1:A:956:ILE:HG13	2.16	0.46
1:A:970:VAL:O	1:A:973:ILE:HG22	2.16	0.46
1:A:858:TYR:CD1	1:A:858:TYR:N	2.81	0.46
1:A:538:THR:HB	1:A:540:PRO:HD2	1.98	0.46
1:A:811:PRO:HG3	1:A:929:VAL:CG1	2.46	0.46
1:A:161:ALA:HA	1:A:210:SER:HB2	1.98	0.46
1:A:126:MET:CE	1:A:139:ARG:HD3	2.45	0.45
1:A:59:ASP:HB3	1:A:62:VAL:CG2	2.43	0.45
1:A:701:THR:HA	1:A:718:ILE:O	2.16	0.45
1:A:25:THR:HB	1:A:26:PRO:HD2	1.99	0.45
1:A:611:ILE:O	1:A:615:ARG:HG3	2.15	0.45
1:A:989:ARG:NH2	5:A:1012:PTY:HC51	2.32	0.45
1:A:567:ARG:CZ	1:A:571:PRO:HD3	2.45	0.45
1:A:863:PRO:O	1:A:865:VAL:N	2.50	0.45
1:A:161:ALA:CA	1:A:210:SER:HB2	2.46	0.45
1:A:260:LEU:O	1:A:264:ILE:HG13	2.16	0.45
1:A:390:ALA:C	1:A:392:GLU:H	2.20	0.45
1:A:129:VAL:CG1	1:A:151:VAL:HG12	2.42	0.44
1:A:309:GLU:HB2	1:A:797:LEU:HD11	1.99	0.44
1:A:342:LEU:HA	1:A:716:ILE:CD1	2.47	0.44
1:A:724:THR:O	1:A:728:LYS:HG3	2.17	0.44
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.99	0.44
1:A:329:LYS:O	1:A:330:ASN:HB2	2.18	0.44
1:A:862:GLY:O	1:A:864:GLY:N	2.50	0.44
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.52	0.44
1:A:604:ARG:CG	1:A:604:ARG:NH1	2.78	0.44
1:A:943:LEU:O	1:A:946:LEU:HB3	2.17	0.44
1:A:174:ARG:NH2	1:A:188:ILE:HD11	2.32	0.44
1:A:361:MET:HG3	1:A:599:MET:SD	2.57	0.44
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:THR:HG22	1:A:458:GLU:N	2.32	0.44
1:A:518:PRO:HB3	1:A:549:ILE:HD13	2.00	0.44
1:A:725:ALA:O	1:A:729:THR:HG23	2.18	0.44
1:A:950:VAL:O	1:A:952:PRO:HD2	2.18	0.44
1:A:55:GLU:O	1:A:58:GLU:HG2	2.18	0.44
1:A:342:LEU:HA	1:A:716:ILE:HD13	2.00	0.44
1:A:52:LEU:CD2	1:A:106:VAL:HG13	2.47	0.43
1:A:786:ALA:HB2	7:A:2613:HOH:O	2.17	0.43
1:A:684:LYS:HB2	7:A:2631:HOH:O	2.19	0.43
1:A:100:ALA:O	1:A:104:VAL:HG23	2.18	0.43
1:A:355:THR:HG22	1:A:740:PHE:HB2	2.01	0.43
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.49	0.43
1:A:335:SER:O	1:A:338:SER:HB2	2.19	0.43
1:A:906:THR:HB	1:A:974:SER:OG	2.19	0.43
1:A:23:GLY:HA3	1:A:130:TYR:O	2.18	0.43
1:A:122:TYR:O	1:A:211:GLY:HA2	2.18	0.43
1:A:699:ALA:HA	1:A:716:ILE:O	2.19	0.43
1:A:917:SER:OG	1:A:920:GLN:HB2	2.19	0.43
1:A:359:ASN:N	1:A:601:ASP:OD1	2.50	0.43
1:A:967:TRP:O	1:A:970:VAL:HB	2.18	0.43
1:A:510:ASN:O	1:A:511:LYS:HD3	2.19	0.42
1:A:643:GLY:H	1:A:646:GLU:HG2	1.85	0.42
1:A:459:VAL:C	1:A:461:ASN:H	2.22	0.42
1:A:873:PHE:HE2	1:A:876:CYS:HA	1.84	0.42
1:A:873:PHE:HD2	1:A:876:CYS:H	1.68	0.42
1:A:95:LEU:HD22	1:A:99:ILE:CD1	2.47	0.42
1:A:96:LEU:C	1:A:96:LEU:HD23	2.40	0.42
1:A:835:PHE:O	1:A:838:MET:HB3	2.19	0.42
1:A:944:HIS:O	1:A:947:ILE:HG12	2.19	0.42
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.50	0.42
1:A:974:SER:C	1:A:976:PRO:HD2	2.40	0.42
1:A:326:MET:CG	1:A:749:GLU:HG2	2.49	0.42
1:A:865:VAL:HB	1:A:868:HIS:CG	2.55	0.42
1:A:59:ASP:OD1	1:A:61:LEU:N	2.52	0.42
1:A:631:THR:O	1:A:635:ILE:HG13	2.20	0.42
1:A:658:PHE:CZ	1:A:666:GLN:HB3	2.55	0.42
1:A:182:GLY:HA2	7:A:2302:HOH:O	2.20	0.42
1:A:260:LEU:CD2	1:A:307:ILE:HD13	2.49	0.42
1:A:441:THR:O	1:A:445:LEU:HD13	2.19	0.42
1:A:678:ARG:NH1	1:A:678:ARG:HG3	2.35	0.42
1:A:950:VAL:HG12	1:A:950:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASP:O	1:A:411:VAL:N	2.52	0.41
1:A:765:ILE:O	1:A:769:VAL:HG23	2.19	0.41
1:A:413:LEU:HD22	1:A:564:LEU:HD12	2.02	0.41
1:A:851:ALA:HB2	1:A:903:VAL:HG21	2.01	0.41
1:A:873:PHE:CE2	1:A:876:CYS:HA	2.55	0.41
1:A:114:ASN:ND2	1:A:117:GLU:HG2	2.32	0.41
1:A:175:VAL:HG11	1:A:212:THR:HG21	2.02	0.41
1:A:265:SER:O	1:A:269:VAL:HG23	2.19	0.41
1:A:309:GLU:CB	1:A:797:LEU:HD11	2.50	0.41
1:A:147:PRO:HA	1:A:223:VAL:HG12	2.02	0.41
1:A:921:SER:HB3	1:A:982:GLU:OE1	2.20	0.41
1:A:459:VAL:HB	1:A:467:ARG:CD	2.50	0.41
1:A:79:GLU:HG2	1:A:80:GLU:N	2.36	0.41
1:A:905:VAL:O	1:A:909:MET:HG2	2.21	0.41
1:A:360:GLN:HB2	7:A:2128:HOH:O	2.20	0.41
1:A:515:LYS:HE3	6:A:1002:ADP:C2	2.56	0.41
1:A:483:PHE:HE1	1:A:573:ARG:HD3	1.86	0.41
1:A:924:ARG:HA	1:A:924:ARG:HE	1.85	0.40
1:A:262:LYS:HA	1:A:262:LYS:HD2	1.90	0.40
1:A:762:ARG:O	1:A:766:SER:HB2	2.21	0.40
1:A:925:MET:HG3	1:A:929:VAL:HG21	2.02	0.40
1:A:75:LEU:C	1:A:77:TRP:N	2.74	0.40
1:A:119:LEU:C	1:A:121:GLU:H	2.25	0.40
1:A:273:LEU:HA	1:A:276:ILE:CD1	2.52	0.40
1:A:566:THR:HG22	1:A:594:VAL:HG23	2.04	0.40
1:A:283:VAL:HG13	1:A:284:HIS:N	2.36	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%)	921 (93%)	59 (6%)	13 (1%)	14	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	951	ASP
1	A	183	GLU
1	A	286	GLY
1	A	505	ARG
1	A	858	TYR
1	A	861	ASP
1	A	864	GLY
1	A	889	GLU
1	A	463	SER
1	A	456	ASN
1	A	504	SER
1	A	863	PRO
1	A	881	PRO

5.3.2 Protein sidechains ⓘ

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%)	800 (95%)	40 (5%)	30	40

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	22	THR
1	A	44	GLU
1	A	60	LEU
1	A	82	GLU
1	A	95	LEU
1	A	113	GLU
1	A	139	ARG

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Mol	Chain	Res	Type
1	A	158	LYS
1	A	164	ARG
1	A	236	ARG
1	A	253	LEU
1	A	275	ASN
1	A	302	LEU
1	A	319	LEU
1	A	361	MET
1	A	384	ILE
1	A	402	ILE
1	A	431	LYS
1	A	461	ASN
1	A	484	THR
1	A	490	ASP
1	A	538	THR
1	A	560	ARG
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	580	ASP
1	A	604	ARG
1	A	612	GLN
1	A	656	ARG
1	A	679	VAL
1	A	685	SER
1	A	691	LEU
1	A	738	ASP
1	A	739	ASN
1	A	822	ARG
1	A	882	HIS
1	A	924	ARG
1	A	967	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	250	GLN
1	A	259	GLN
1	A	275	ASN
1	A	359	ASN
1	A	461	ASN

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Mol	Chain	Res	Type
1	A	510	ASN
1	A	739	ASN
1	A	869	GLN
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 ⓘ

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 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	$\# Z > 2$
6	ADP	A	1002	3	25,29,29	1.39	4 (16%)	24,45,45	2.83	6 (25%)
4	TG1	A	1003	-	43,48,48	1.66	9 (20%)	47,72,72	1.59	10 (21%)
5	PTY	A	1011	-	18,18,49	1.52	5 (27%)	20,23,54	1.59	3 (15%)
5	PTY	A	1012	-	18,18,49	1.66	3 (16%)	20,23,54	1.61	5 (25%)
5	PTY	A	1013	-	18,18,49	1.37	3 (16%)	20,23,54	1.28	2 (10%)

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
6	ADP	A	1002	3	-	0/12/32/32	0/3/3/3
4	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
5	PTY	A	1011	-	-	0/20/20/53	0/0/0/0
5	PTY	A	1012	-	-	0/20/20/53	0/0/0/0
5	PTY	A	1013	-	-	0/20/20/53	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	ADP	C2'-C1'	-2.98	1.48	1.53
6	A	1002	ADP	C5-N7	-2.06	1.32	1.39
4	A	1003	TG1	C31-C10	2.06	1.57	1.52
5	A	1011	PTY	O4-C1	2.16	1.49	1.45
5	A	1011	PTY	C2-C3	2.23	1.59	1.50
4	A	1003	TG1	C9-C8	2.23	1.54	1.52
5	A	1012	PTY	O4-C1	2.34	1.50	1.45
6	A	1002	ADP	C4-N3	2.34	1.39	1.35
4	A	1003	TG1	C2-C3	2.36	1.57	1.53
5	A	1011	PTY	P1-O13	2.47	1.60	1.50
4	A	1003	TG1	O7-C27	2.53	1.41	1.34
4	A	1003	TG1	C11-C7	2.53	1.58	1.55
5	A	1013	PTY	C5-C6	2.57	1.58	1.50
5	A	1011	PTY	C5-C6	2.58	1.58	1.50
5	A	1013	PTY	C1-C6	2.59	1.58	1.50
5	A	1012	PTY	C5-C6	2.61	1.58	1.50
5	A	1013	PTY	P1-O13	2.67	1.60	1.50
4	A	1003	TG1	C9-C10	2.70	1.59	1.54
4	A	1003	TG1	C34-C11	2.76	1.57	1.53
6	A	1002	ADP	C2-N3	2.94	1.37	1.32
5	A	1011	PTY	C1-C6	3.22	1.59	1.50
4	A	1003	TG1	C7-C8	4.14	1.58	1.53
4	A	1003	TG1	O4-C21	4.61	1.31	1.21
5	A	1012	PTY	C1-C6	4.63	1.63	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	ADP	N3-C2-N1	-12.21	118.22	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TG1	O12-C12-C11	-4.04	124.43	128.28
6	A	1002	ADP	C4-C5-N7	-2.88	106.63	109.41
5	A	1012	PTY	O12-P1-O13	-2.88	97.39	112.28
4	A	1003	TG1	C23-C22-C21	-2.36	109.91	116.01
6	A	1002	ADP	C4'-O4'-C1'	-2.32	107.30	109.77
4	A	1003	TG1	O4-C21-C22	-2.14	118.11	125.09
4	A	1003	TG1	O11-C11-C12	-2.06	99.86	105.94
5	A	1011	PTY	O12-P1-O14	-2.04	98.53	108.14
5	A	1012	PTY	O14-P1-O13	2.08	117.63	109.25
5	A	1013	PTY	O4-C1-C6	2.12	113.98	108.66
5	A	1012	PTY	O7-C6-C1	2.22	116.49	108.44
4	A	1003	TG1	O7-C8-C9	2.24	112.11	107.30
6	A	1002	ADP	C1'-N9-C4	2.34	130.69	126.64
5	A	1012	PTY	O7-C8-C11	2.35	115.52	111.10
6	A	1002	ADP	C2'-C3'-C4'	2.44	107.38	102.62
6	A	1002	ADP	O2'-C2'-C1'	2.46	119.32	111.61
4	A	1003	TG1	C24-C22-C21	2.65	132.11	120.74
5	A	1011	PTY	O4-C1-C6	2.65	115.33	108.66
4	A	1003	TG1	O3-C21-O4	2.73	128.78	123.31
4	A	1003	TG1	O5-C12-O12	2.82	125.52	121.63
4	A	1003	TG1	C7-C6-C5	2.93	122.49	114.92
5	A	1013	PTY	O7-C8-C11	3.65	117.96	111.10
5	A	1012	PTY	O4-C1-C6	3.66	117.86	108.66
5	A	1011	PTY	O7-C8-C11	4.38	119.32	111.10
4	A	1003	TG1	C10-O9-C32	5.22	135.01	121.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	ADP	2	0
4	A	1003	TG1	1	0
5	A	1012	PTY	1	0

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, 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%)	0.50	90 (9%) 10 14	33, 62, 117, 159	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	ARG	10.2
1	A	508	VAL	10.0
1	A	885	GLY	9.9
1	A	886	LEU	9.8
1	A	506	ALA	9.8
1	A	503	SER	9.2
1	A	504	SER	8.9
1	A	883	PHE	8.6
1	A	85	ILE	8.5
1	A	81	GLY	7.8
1	A	84	THR	7.8
1	A	80	GLU	7.7
1	A	884	GLU	6.4
1	A	507	ALA	6.4
1	A	82	GLU	6.3
1	A	78	PHE	6.1
1	A	992	LEU	6.0
1	A	283	VAL	5.9
1	A	459	VAL	5.6
1	A	993	GLU	5.3
1	A	881	PRO	5.3
1	A	46	GLY	5.2
1	A	285	GLY	5.1
1	A	86	THR	5.1
1	A	433	VAL	4.9
1	A	289	ILE	4.8
1	A	872	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	427	PHE	4.3
1	A	887	ASP	4.2
1	A	430	THR	4.2
1	A	434	TYR	4.1
1	A	502	LYS	4.0
1	A	462	LEU	3.9
1	A	279	PHE	3.9
1	A	866	THR	3.9
1	A	428	ASN	3.9
1	A	286	GLY	3.8
1	A	45	GLU	3.8
1	A	50	TRP	3.8
1	A	77	TRP	3.7
1	A	107	TRP	3.7
1	A	877	THR	3.7
1	A	431	LYS	3.6
1	A	875	GLN	3.5
1	A	44	GLU	3.4
1	A	79	GLU	3.4
1	A	83	GLU	3.4
1	A	856	PHE	3.4
1	A	994	GLY	3.4
1	A	49	LEU	3.3
1	A	92	PHE	3.3
1	A	432	GLY	3.2
1	A	991	TYR	3.1
1	A	460	ARG	3.1
1	A	284	HIS	3.1
1	A	871	THR	3.0
1	A	878	GLU	2.9
1	A	54	ILE	2.9
1	A	873	PHE	2.9
1	A	435	GLU	2.8
1	A	865	VAL	2.7
1	A	864	GLY	2.7
1	A	47	LYS	2.6
1	A	52	LEU	2.6
1	A	426	ASP	2.5
1	A	890	ILE	2.5
1	A	461	ASN	2.4
1	A	951	ASP	2.4
1	A	854	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	509	GLY	2.3
1	A	468	ALA	2.3
1	A	924	ARG	2.3
1	A	292	ALA	2.3
1	A	986	PHE	2.3
1	A	121	GLU	2.3
1	A	281	ASP	2.2
1	A	795	VAL	2.2
1	A	888	CYS	2.2
1	A	458	GLU	2.1
1	A	466	GLU	2.1
1	A	264	ILE	2.1
1	A	295	TYR	2.1
1	A	308	PRO	2.1
1	A	855	TRP	2.1
1	A	891	PHE	2.1
1	A	870	LEU	2.1
1	A	814	LEU	2.0
1	A	923	MET	2.0
1	A	772	VAL	2.0
1	A	671	ARG	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(\AA^2)	Q<0.9
4	TG1	A	1003	46/46	0.91	0.22	1.63	66,75,93,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PTY	A	1013	19/50	0.74	0.26	1.08	108,121,124,125	0
5	PTY	A	1011	19/50	0.89	0.18	0.88	108,111,113,113	0
5	PTY	A	1012	19/50	0.82	0.24	0.48	110,114,118,118	0
6	ADP	A	1002	27/27	0.93	0.15	0.08	70,79,94,96	0
2	NA	A	1000	1/1	0.94	0.11	-1.21	56,56,56,56	0
3	MG	A	997	1/1	0.92	0.18	-	90,90,90,90	0
3	MG	A	1001	1/1	0.73	0.30	-	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.