



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AR8  
Title : Calcium pump crystal structure with bound AlF<sub>4</sub>, TNP-AMP and TG  
Authors : Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.  
Deposited on : 2010-11-24  
Resolution : 2.60 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](mailto: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.

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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

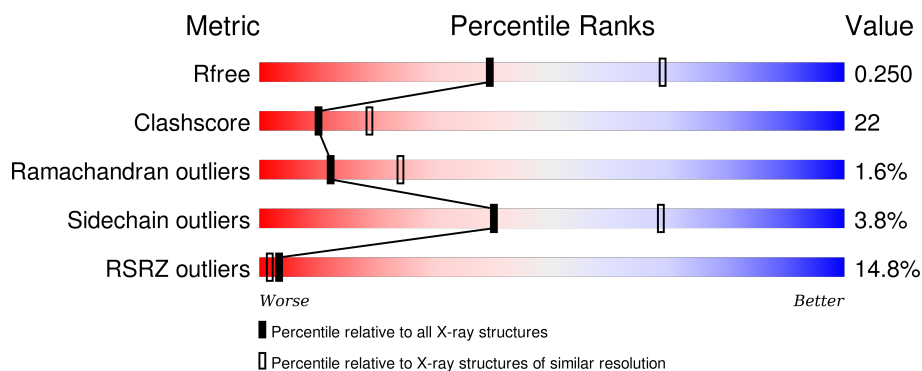
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 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>15%</div> <div>60%</div> <div>37%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7871 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	1	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

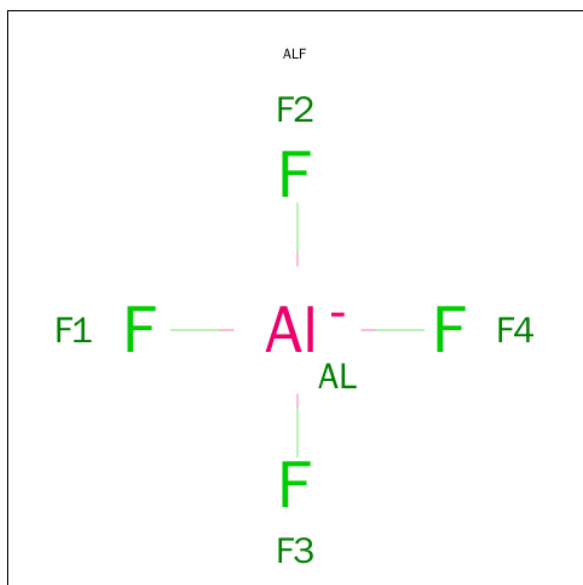
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

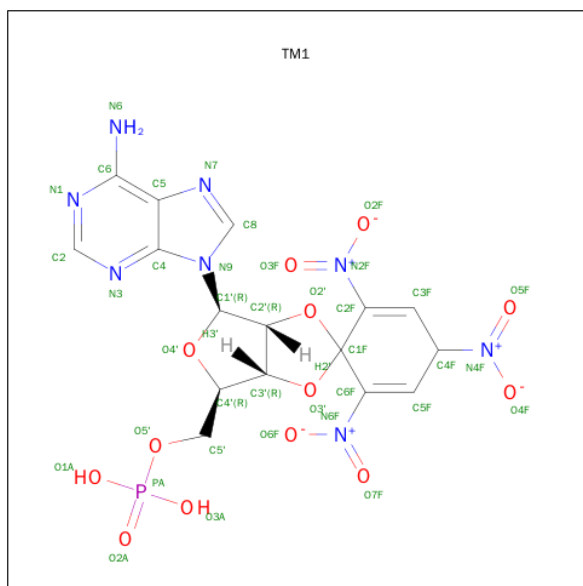
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			5	1	4		

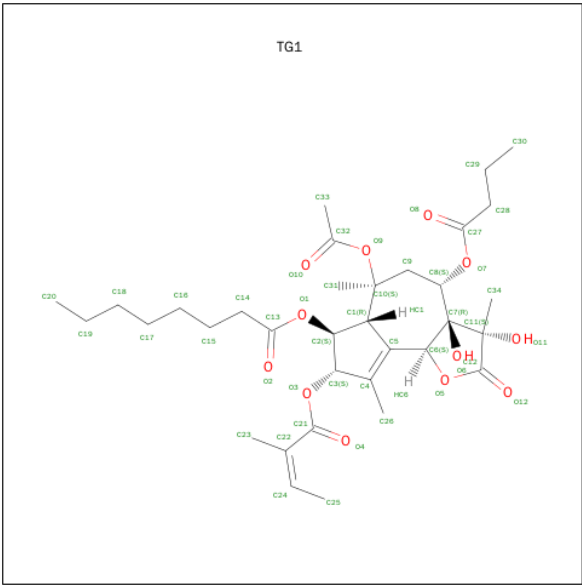
- Molecule 5 is 2',3'-O-[(1R)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE-1,1-DIYL]ADENOSINE 5'-(DIHYDROGEN PHOSPHATE) (three-letter code: TM1) (formula:  $C_{16}H_{15}N_8O_{13}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	
			38	16	8	13	1	

- Molecule 6 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<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



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

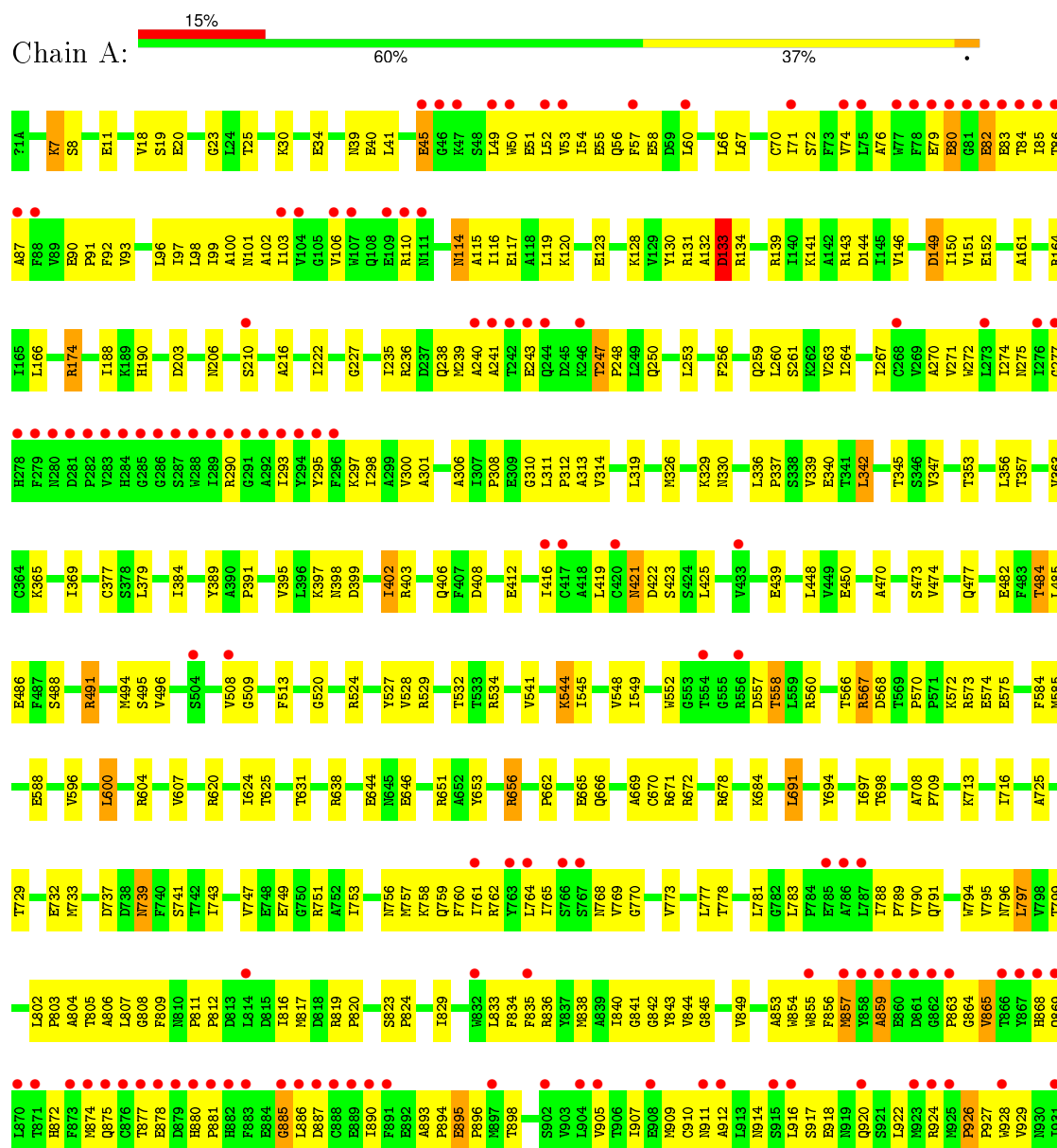
- Molecule 7 is water.

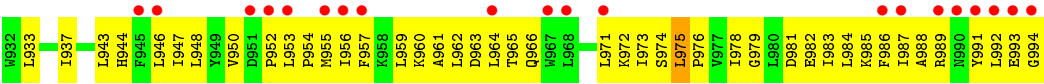
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	106	Total	O	0	0
			106	106		

### 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 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.86Å 69.87Å 141.81Å 90.00° 106.71° 90.00°	Depositor
Resolution (Å)	14.99 – 2.60 26.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (14.99-2.60) 99.9 (26.95-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.60Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.226 , 0.253 0.224 , 0.250	Depositor DCC
$R_{free}$ test set	2531 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51284 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: TM1, MG, TG1, ACE, ALF, NA

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	0.35	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 [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	342	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	1	0
5	A	38	0	12	0	0
6	A	46	0	50	3	0
7	A	106	0	0	3	0
All	All	7871	0	7827	342	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 22.

All (342) 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:836:ARG:HG3	1:A:984:LEU:HD13	1.45	0.98
1:A:421:ASN:ND2	1:A:423:SER:H	1.66	0.93
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.50	0.92
1:A:484:THR:HB	1:A:496:VAL:HG12	1.52	0.92
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.56	0.88
1:A:762:ARG:HG2	1:A:829:ILE:HD11	1.56	0.86
1:A:41:LEU:HG	1:A:236:ARG:HG3	1.59	0.85
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.62	0.82
1:A:737:ASP:OD2	1:A:739:ASN:HB2	1.79	0.81
1:A:833:LEU:HD13	1:A:836:ARG:HH21	1.45	0.81
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.63	0.79
1:A:342:LEU:HA	1:A:716:ILE:HD13	1.65	0.79
1:A:30:LYS:O	1:A:34:GLU:HG3	1.82	0.78
1:A:49:LEU:HD13	1:A:110:ARG:HD2	1.63	0.78
1:A:247:THR:HG22	1:A:250:GLN:H	1.47	0.78
1:A:86:THR:HG21	1:A:956:ILE:HA	1.66	0.77
1:A:20:GLU:HA	1:A:150:ILE:CD1	2.14	0.77
1:A:311:LEU:HD11	1:A:761:ILE:HD13	1.68	0.74
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.70	0.73
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.91	0.71
1:A:421:ASN:HD22	1:A:422:ASP:N	1.87	0.71
1:A:97:ILE:HA	1:A:100:ALA:HB3	1.72	0.71
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.72	0.71
1:A:794:TRP:HH2	1:A:943:LEU:HB3	1.55	0.71
1:A:79:GLU:HG2	1:A:87:ALA:HB2	1.71	0.71
1:A:421:ASN:HD22	1:A:423:SER:H	1.36	0.71
1:A:326:MET:HE1	1:A:339:VAL:HG22	1.74	0.70
1:A:116:ILE:H	1:A:116:ILE:HD12	1.56	0.69
1:A:981:ASP:HA	1:A:984:LEU:HD12	1.74	0.69
1:A:557:ASP:HA	1:A:638:ARG:HH12	1.57	0.69
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.76	0.68
1:A:972:LYS:HE2	1:A:972:LYS:HA	1.74	0.68
1:A:49:LEU:HA	1:A:52:LEU:HD12	1.76	0.68
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.76	0.68
1:A:52:LEU:HD13	1:A:110:ARG:HB2	1.76	0.68
1:A:271:VAL:HG12	1:A:275:ASN:ND2	2.09	0.67
1:A:342:LEU:HG	1:A:716:ILE:HG21	1.76	0.67
1:A:917:SER:OG	1:A:920:GLN:HB2	1.94	0.67
1:A:45:GLU:H	1:A:45:GLU:CD	1.97	0.66
1:A:749:GLU:O	1:A:753:ILE:HG12	1.96	0.66
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.78	0.65
1:A:486:GLU:O	1:A:491:ARG:NH2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.32	0.65
1:A:895:GLU:H	1:A:896:PRO:HD2	1.62	0.64
1:A:975:LEU:N	1:A:976:PRO:HD2	2.13	0.64
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.80	0.63
1:A:765:ILE:O	1:A:769:VAL:HG23	1.97	0.63
1:A:23:GLY:HA3	1:A:130:TYR:O	1.99	0.63
1:A:791:GLN:O	1:A:795:VAL:HG23	1.99	0.63
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.80	0.63
1:A:342:LEU:HD12	1:A:733:MET:CE	2.29	0.62
1:A:557:ASP:HA	1:A:638:ARG:HH22	1.63	0.62
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.82	0.62
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.81	0.62
1:A:791:GLN:NE2	1:A:959:LEU:HD21	2.15	0.62
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.81	0.62
1:A:85:ILE:HG23	1:A:86:THR:HG23	1.82	0.62
1:A:174:ARG:HG3	1:A:188:ILE:CD1	2.31	0.61
1:A:342:LEU:HD22	1:A:747:VAL:HG22	1.82	0.61
1:A:119:LEU:HD22	1:A:239:MET:HE3	1.82	0.61
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.30	0.61
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.82	0.61
1:A:342:LEU:HA	1:A:716:ILE:CD1	2.29	0.61
1:A:926:PRO:O	1:A:929:VAL:HG23	2.00	0.61
1:A:297:LYS:HA	1:A:300:VAL:HG22	1.82	0.61
1:A:116:ILE:HD12	1:A:116:ILE:N	2.16	0.61
1:A:8:SER:OG	1:A:11:GLU:HG3	2.01	0.61
1:A:353:THR:HA	1:A:357:THR:OG1	2.01	0.60
1:A:557:ASP:HA	1:A:638:ARG:NH1	2.16	0.60
1:A:271:VAL:HG12	1:A:275:ASN:HD21	1.66	0.60
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.83	0.60
1:A:482:GLU:CD	1:A:573:ARG:HH12	2.04	0.59
1:A:946:LEU:O	1:A:953:LEU:HD12	2.02	0.59
1:A:986:PHE:HA	1:A:989:ARG:HG2	1.84	0.59
1:A:314:VAL:HG13	1:A:805:THR:OG1	2.02	0.59
1:A:757:MET:HA	1:A:760:PHE:CE2	2.38	0.59
1:A:52:LEU:HA	1:A:55:GLU:CD	2.23	0.59
1:A:114:ASN:HD21	1:A:116:ILE:HD13	1.68	0.59
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.36	0.59
1:A:788:ILE:CG1	1:A:791:GLN:HG3	2.32	0.58
1:A:893:ALA:O	1:A:896:PRO:HD2	2.03	0.58
1:A:119:LEU:HD22	1:A:239:MET:CE	2.33	0.58
1:A:836:ARG:O	1:A:840:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:HD13	1:A:600:LEU:O	2.02	0.58
1:A:865:VAL:CG1	1:A:869:GLN:HG3	2.32	0.58
1:A:90:GLU:HB2	1:A:790:VAL:CG2	2.33	0.58
1:A:310:GLY:O	1:A:314:VAL:HG23	2.02	0.58
1:A:330:ASN:HB3	1:A:737:ASP:HB2	1.85	0.58
1:A:991:TYR:O	1:A:992:LEU:HG	2.03	0.57
1:A:101:ASN:HD21	1:A:313:ALA:HB2	1.68	0.57
1:A:725:ALA:O	1:A:729:THR:HG23	2.03	0.57
1:A:398:ASN:O	1:A:399:ASP:HB2	2.06	0.56
1:A:326:MET:CG	1:A:749:GLU:HG2	2.35	0.56
1:A:644:GLU:CD	1:A:644:GLU:H	2.08	0.56
1:A:100:ALA:O	1:A:103:ILE:HG22	2.05	0.56
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.20	0.56
1:A:395:VAL:O	1:A:402:ILE:HD13	2.05	0.56
1:A:114:ASN:OD1	1:A:117:GLU:HG2	2.06	0.56
1:A:116:ILE:O	1:A:120:LYS:HG3	2.06	0.56
1:A:978:ILE:O	1:A:982:GLU:HB2	2.06	0.56
1:A:898:THR:HG21	1:A:960:LYS:O	2.06	0.56
1:A:326:MET:HE1	1:A:339:VAL:CG2	2.35	0.56
1:A:508:VAL:HG12	1:A:509:GLY:N	2.21	0.56
1:A:549:ILE:CD1	1:A:596:VAL:HG21	2.31	0.56
1:A:86:THR:HG22	1:A:956:ILE:HG22	1.87	0.56
1:A:557:ASP:CA	1:A:638:ARG:HH22	2.19	0.56
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.86	0.56
1:A:757:MET:O	1:A:761:ILE:HG12	2.06	0.56
1:A:41:LEU:HB2	1:A:123:GLU:OE1	2.07	0.55
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.88	0.55
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.87	0.55
1:A:783:LEU:H	1:A:783:LEU:HD12	1.71	0.55
1:A:560:ARG:HD3	7:A:9001:HOH:O	2.05	0.55
1:A:79:GLU:HG2	1:A:87:ALA:CB	2.37	0.55
1:A:974:SER:C	1:A:976:PRO:HD2	2.26	0.55
1:A:308:PRO:HA	1:A:768:ASN:HD21	1.70	0.55
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.88	0.55
1:A:557:ASP:CB	1:A:638:ARG:HH22	2.19	0.55
1:A:778:THR:HG23	1:A:849:VAL:HG22	1.89	0.55
1:A:70:CYS:O	1:A:74:VAL:HG23	2.06	0.55
1:A:855:TRP:CD1	1:A:895:GLU:HB3	2.42	0.54
1:A:403:ARG:HB2	1:A:406:GLN:HG2	1.89	0.54
1:A:874:MET:O	1:A:874:MET:HG2	2.07	0.54
1:A:20:GLU:HA	1:A:150:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HG22	1:A:239:MET:CE	2.37	0.54
1:A:869:GLN:HA	1:A:872:HIS:ND1	2.22	0.54
1:A:527:TYR:CG	1:A:534:ARG:HD3	2.42	0.54
1:A:236:ARG:HD3	1:A:236:ARG:C	2.28	0.54
1:A:485:LEU:HD22	1:A:584:PHE:CE2	2.42	0.54
1:A:819:ARG:CG	1:A:820:PRO:HD2	2.38	0.54
1:A:52:LEU:HB3	1:A:106:VAL:HG13	1.90	0.54
1:A:963:ASP:H	1:A:966:GLN:HE21	1.54	0.54
1:A:66:LEU:HA	1:A:98:LEU:HD11	1.90	0.53
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.56	0.53
1:A:993:GLU:HG2	1:A:994:GLY:N	2.23	0.53
1:A:49:LEU:HB2	1:A:110:ARG:NH1	2.23	0.53
1:A:944:HIS:O	1:A:947:ILE:HG22	2.09	0.53
1:A:247:THR:HG23	1:A:248:PRO:HD2	1.90	0.53
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.43	0.53
1:A:20:GLU:HA	1:A:150:ILE:HD13	1.90	0.53
1:A:174:ARG:HD3	1:A:216:ALA:HB3	1.90	0.53
1:A:905:VAL:O	1:A:909:MET:HG2	2.09	0.53
1:A:805:THR:O	1:A:805:THR:HG22	2.08	0.52
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.90	0.52
1:A:646:GLU:OE2	1:A:651:ARG:NH1	2.39	0.52
1:A:795:VAL:HA	1:A:799:THR:OG1	2.09	0.52
1:A:887:ASP:HB3	1:A:890:ILE:HG13	1.92	0.52
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.91	0.52
1:A:85:ILE:HD11	1:A:955:MET:SD	2.48	0.52
1:A:781:LEU:HD23	1:A:783:LEU:HD13	1.92	0.52
1:A:844:VAL:CG2	1:A:907:ILE:HG21	2.37	0.52
1:A:856:PHE:CE1	1:A:896:PRO:HB3	2.45	0.52
1:A:857:MET:HG2	1:A:865:VAL:O	2.09	0.52
1:A:865:VAL:HG12	1:A:869:GLN:HG3	1.92	0.52
1:A:80:GLU:O	1:A:84:THR:HB	2.10	0.52
1:A:308:PRO:HG3	1:A:765:ILE:CD1	2.40	0.52
1:A:877:THR:HA	1:A:880:HIS:CE1	2.45	0.52
1:A:770:GLY:HA2	1:A:841:GLY:O	2.10	0.51
1:A:574:GLU:CD	1:A:574:GLU:H	2.14	0.51
1:A:508:VAL:HG12	1:A:509:GLY:H	1.74	0.51
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.93	0.51
1:A:922:LEU:O	1:A:927:PRO:HD3	2.09	0.51
1:A:146:VAL:O	1:A:149:ASP:HB2	2.10	0.51
1:A:494:MET:HG2	1:A:495:SER:N	2.26	0.51
1:A:57:PHE:HZ	1:A:99:ILE:HG12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:HA	1:A:295:TYR:OH	2.11	0.51
1:A:804:ALA:C	1:A:806:ALA:H	2.13	0.51
1:A:545:ILE:O	1:A:549:ILE:HG12	2.11	0.51
1:A:253:LEU:HD23	6:A:1003:TG1:H301	1.93	0.51
1:A:875:GLN:HG2	1:A:878:GLU:OE2	2.11	0.51
1:A:60:LEU:HD21	1:A:261:SER:HB2	1.93	0.51
1:A:916:LEU:HD21	1:A:933:LEU:HD22	1.93	0.51
1:A:947:ILE:O	1:A:947:ILE:HG12	2.10	0.50
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.42	0.50
1:A:796:ASN:O	1:A:797:LEU:HG	2.12	0.50
1:A:377:CYS:O	1:A:544:LYS:HG3	2.11	0.50
1:A:907:ILE:O	1:A:910:CYS:HB2	2.11	0.50
1:A:697:ILE:HD13	1:A:824:PRO:HG3	1.92	0.50
1:A:98:LEU:O	1:A:98:LEU:HD23	2.10	0.50
1:A:342:LEU:HD12	1:A:733:MET:SD	2.52	0.50
1:A:247:THR:HB	1:A:250:GLN:HG3	1.94	0.50
1:A:557:ASP:OD1	1:A:558:THR:N	2.45	0.50
1:A:672:ARG:NH2	7:A:4055:HOH:O	2.41	0.50
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.93	0.50
1:A:72:SER:O	1:A:76:ALA:HB2	2.12	0.50
1:A:235:ILE:HG22	1:A:239:MET:HE1	1.93	0.50
1:A:836:ARG:HD2	1:A:981:ASP:OD1	2.11	0.50
1:A:40:GLU:O	1:A:227:GLY:HA2	2.12	0.50
1:A:854:TRP:O	1:A:859:ALA:HB2	2.12	0.49
1:A:962:LEU:HD22	1:A:966:GLN:OE1	2.12	0.49
1:A:947:ILE:HD11	1:A:957:PHE:CD2	2.47	0.49
1:A:92:PHE:O	1:A:96:LEU:HB2	2.11	0.49
1:A:421:ASN:C	1:A:421:ASN:HD22	2.15	0.49
1:A:924:ARG:O	1:A:926:PRO:HD3	2.13	0.49
1:A:301:ALA:HA	1:A:789:PRO:HB3	1.94	0.49
1:A:644:GLU:CD	1:A:644:GLU:N	2.66	0.49
1:A:203:ASP:OD1	1:A:678:ARG:NH1	2.46	0.49
1:A:979:GLY:O	1:A:983:ILE:HG12	2.13	0.49
1:A:875:GLN:HA	1:A:878:GLU:HG2	1.95	0.48
1:A:128:LYS:HG2	1:A:139:ARG:HG2	1.95	0.48
1:A:947:ILE:HD11	1:A:957:PHE:CG	2.48	0.48
1:A:347:VAL:HG13	1:A:620:ARG:HG3	1.96	0.48
1:A:807:LEU:C	1:A:809:PHE:H	2.17	0.48
1:A:954:PRO:HB2	1:A:959:LEU:O	2.12	0.48
1:A:520:GLY:O	1:A:524:ARG:HG3	2.14	0.48
1:A:836:ARG:NH1	1:A:985:LYS:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:O	1:A:55:GLU:HG2	2.13	0.48
1:A:114:ASN:CB	1:A:117:GLU:HG2	2.43	0.48
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.44	0.48
1:A:311:LEU:N	1:A:312:PRO:CD	2.77	0.48
1:A:101:ASN:ND2	1:A:313:ALA:HB2	2.28	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.14	0.47
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.96	0.47
1:A:485:LEU:HD22	1:A:584:PHE:CD2	2.49	0.47
1:A:653:TYR:OH	1:A:672:ARG:NH1	2.47	0.47
1:A:950:VAL:O	1:A:954:PRO:HD2	2.14	0.47
1:A:527:TYR:HB3	1:A:534:ARG:CG	2.43	0.47
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.95	0.47
1:A:880:HIS:N	1:A:881:PRO:CD	2.78	0.47
1:A:473:SER:O	1:A:477:GLN:HG2	2.13	0.47
1:A:769:VAL:HA	6:A:1003:TG1:H231	1.96	0.47
1:A:114:ASN:HD22	1:A:115:ALA:N	2.12	0.47
1:A:116:ILE:CD1	1:A:116:ILE:H	2.26	0.47
1:A:971:LEU:O	1:A:975:LEU:HB2	2.15	0.47
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.97	0.47
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.97	0.47
1:A:885:GLY:C	1:A:886:LEU:HD12	2.36	0.47
1:A:773:VAL:CB	1:A:845:GLY:HA3	2.44	0.46
1:A:795:VAL:O	1:A:799:THR:HB	2.16	0.46
1:A:267:ILE:O	1:A:271:VAL:HG23	2.15	0.46
1:A:527:TYR:HB3	1:A:534:ARG:HG2	1.97	0.46
1:A:293:ILE:CG2	1:A:297:LYS:HE3	2.45	0.46
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.50	0.46
1:A:917:SER:CB	1:A:920:GLN:HB2	2.46	0.46
1:A:909:MET:SD	1:A:937:ILE:HG23	2.55	0.46
1:A:247:THR:HG23	1:A:248:PRO:CD	2.45	0.46
1:A:20:GLU:HG3	1:A:166:LEU:HD13	1.98	0.46
1:A:248:PRO:HG2	1:A:340:GLU:OE2	2.16	0.46
1:A:975:LEU:N	1:A:976:PRO:CD	2.78	0.46
1:A:914:ASN:HD22	1:A:922:LEU:HD21	1.81	0.46
1:A:853:ALA:HB1	1:A:857:MET:CE	2.46	0.46
1:A:82:GLU:HG3	1:A:83:GLU:N	2.31	0.46
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.15	0.46
1:A:819:ARG:HG3	1:A:820:PRO:HD2	1.97	0.46
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.46	0.46
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.98	0.46
1:A:114:ASN:CG	1:A:117:GLU:HG2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TYR:O	1:A:298:ILE:HG12	2.15	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.15	0.45
1:A:890:ILE:HG22	1:A:890:ILE:O	2.16	0.45
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.51	0.45
1:A:863:PRO:C	1:A:865:VAL:H	2.19	0.45
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.46	0.45
1:A:18:VAL:HG22	1:A:19:SER:N	2.32	0.45
1:A:791:GLN:HE22	1:A:959:LEU:HD21	1.79	0.45
1:A:975:LEU:HD13	1:A:975:LEU:O	2.16	0.45
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.97	0.45
1:A:470:ALA:O	1:A:474:VAL:HG23	2.17	0.44
1:A:865:VAL:HG13	1:A:869:GLN:HG3	2.00	0.44
1:A:816:ILE:HG23	1:A:817:MET:HG2	1.99	0.44
1:A:759:GLN:HA	1:A:759:GLN:OE1	2.17	0.44
1:A:25:THR:HA	1:A:132:ALA:HB3	1.98	0.44
1:A:264:ILE:HD11	1:A:306:ALA:HB2	1.98	0.44
1:A:345:THR:HA	1:A:697:ILE:HG22	1.99	0.44
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.99	0.44
1:A:981:ASP:OD2	1:A:985:LYS:HE3	2.18	0.44
1:A:131:ARG:HH11	1:A:131:ARG:HG3	1.82	0.44
1:A:761:ILE:O	1:A:765:ILE:HG12	2.17	0.44
1:A:758:LYS:O	1:A:762:ARG:HD2	2.17	0.44
1:A:600:LEU:HD13	1:A:600:LEU:C	2.38	0.44
1:A:7:LYS:N	1:A:7:LYS:HD2	2.32	0.44
1:A:971:LEU:O	1:A:972:LYS:HE2	2.17	0.43
1:A:290:ARG:HA	1:A:293:ILE:HD11	2.00	0.43
1:A:99:ILE:HA	1:A:102:ALA:HB3	2.00	0.43
1:A:666:GLN:O	1:A:669:ALA:HB3	2.18	0.43
1:A:788:ILE:HG13	1:A:791:GLN:HG3	1.98	0.43
1:A:788:ILE:HG12	1:A:791:GLN:HG3	1.99	0.43
1:A:491:ARG:HG3	1:A:585:MET:HB2	1.99	0.43
1:A:948:LEU:HB3	1:A:961:ALA:HB2	2.00	0.43
1:A:656:ARG:CA	1:A:656:ARG:HE	2.30	0.43
1:A:773:VAL:HG21	1:A:842:GLY:HA2	2.01	0.43
1:A:484:THR:HG22	7:A:4106:HOH:O	2.18	0.43
1:A:912:ALA:HB1	1:A:933:LEU:HD11	2.00	0.43
1:A:983:ILE:O	1:A:987:ILE:HG12	2.19	0.43
1:A:259:GLN:O	1:A:263:VAL:HG23	2.19	0.43
1:A:963:ASP:H	1:A:966:GLN:NE2	2.15	0.43
1:A:834:PHE:O	1:A:838:MET:HB2	2.18	0.43
1:A:256:PHE:HB2	6:A:1003:TG1:H291	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:PRO:HG2	1:A:665:GLU:HG3	2.00	0.43
1:A:166:LEU:HD11	1:A:222:ILE:HB	2.00	0.43
1:A:557:ASP:HA	1:A:638:ARG:CZ	2.48	0.43
1:A:397:LYS:O	1:A:398:ASN:HB2	2.19	0.43
1:A:963:ASP:C	1:A:965:THR:H	2.22	0.43
1:A:161:ALA:HA	1:A:210:SER:HB2	2.01	0.43
1:A:329:LYS:O	1:A:330:ASN:HB2	2.19	0.42
1:A:823:SER:HA	1:A:824:PRO:HD3	1.92	0.42
1:A:671:ARG:HD3	1:A:694:TYR:CE2	2.55	0.42
1:A:72:SER:O	1:A:91:PRO:HG3	2.19	0.42
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.43	0.42
1:A:93:VAL:HA	1:A:96:LEU:HB2	2.00	0.42
1:A:49:LEU:O	1:A:53:VAL:HG23	2.20	0.42
1:A:347:VAL:HG22	1:A:620:ARG:HG2	2.01	0.42
1:A:151:VAL:CG1	1:A:152:GLU:N	2.83	0.42
1:A:982:GLU:HA	1:A:982:GLU:OE1	2.20	0.42
1:A:898:THR:O	1:A:898:THR:HG22	2.19	0.42
1:A:544:LYS:O	1:A:544:LYS:HD3	2.19	0.42
1:A:39:ASN:O	1:A:143:ARG:HA	2.19	0.42
1:A:55:GLU:HA	1:A:58:GLU:HG3	2.00	0.42
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.54	0.42
1:A:926:PRO:C	1:A:928:TRP:H	2.23	0.42
1:A:973:ILE:HG22	1:A:973:ILE:O	2.19	0.42
1:A:408:ASP:OD1	1:A:532:THR:HG23	2.20	0.42
1:A:52:LEU:O	1:A:56:GLN:HG2	2.20	0.42
1:A:811:PRO:HA	1:A:812:PRO:HD2	1.96	0.41
1:A:342:LEU:CD2	1:A:747:VAL:HG22	2.47	0.41
1:A:247:THR:HB	1:A:250:GLN:CG	2.50	0.41
1:A:868:HIS:O	1:A:868:HIS:ND1	2.53	0.41
1:A:190:HIS:O	1:A:206:ASN:HA	2.20	0.41
1:A:739:ASN:OD1	1:A:741:SER:OG	2.39	0.41
1:A:256:PHE:CZ	1:A:765:ILE:HD12	2.56	0.41
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.50	0.41
1:A:708:ALA:HB3	1:A:709:PRO:HD3	2.02	0.41
1:A:764:LEU:CD1	1:A:804:ALA:HB2	2.50	0.41
1:A:835:PHE:O	1:A:838:MET:HB3	2.20	0.41
1:A:894:PRO:HB2	1:A:960:LYS:N	2.36	0.41
1:A:962:LEU:HA	1:A:966:GLN:NE2	2.35	0.41
1:A:270:ALA:O	1:A:274:ILE:HG12	2.20	0.41
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.23	0.41
1:A:863:PRO:O	1:A:865:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:THR:HA	4:A:998:ALF:F4	2.11	0.41
1:A:308:PRO:HG3	1:A:765:ILE:HD13	2.03	0.41
1:A:488:SER:HB3	1:A:491:ARG:HH21	1.85	0.41
1:A:756:ASN:HD22	1:A:808:GLY:C	2.24	0.41
1:A:235:ILE:HG22	1:A:239:MET:HE2	2.04	0.40
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.56	0.40
1:A:67:LEU:O	1:A:71:ILE:HG13	2.21	0.40
1:A:567:ARG:CD	1:A:570:PRO:HA	2.45	0.40
1:A:141:LYS:O	1:A:144:ASP:HB2	2.21	0.40
1:A:120:LYS:HB3	1:A:120:LYS:HE2	1.88	0.40
1:A:575:GLU:HG2	1:A:575:GLU:H	1.66	0.40
1:A:131:ARG:C	1:A:133:ASP:N	2.74	0.40
1:A:259:GLN:HA	1:A:259:GLN:OE1	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	877 (88%)	100 (10%)	16 (2%)	12	24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ALA
1	A	857	MET
1	A	964	LEU
1	A	859	ALA
1	A	865	VAL
1	A	918	GLU
1	A	133	ASP
1	A	241	ALA

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Mol	Chain	Res	Type
1	A	243	GLU
1	A	558	THR
1	A	895	GLU
1	A	277	GLY
1	A	797	LEU
1	A	864	GLY
1	A	926	PRO
1	A	885	GLY

### 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%)	808 (96%)	32 (4%)	40	68

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

Mol	Chain	Res	Type
1	A	7	LYS
1	A	45	GLU
1	A	80	GLU
1	A	82	GLU
1	A	114	ASN
1	A	133	ASP
1	A	134	ARG
1	A	149	ASP
1	A	164	ARG
1	A	174	ARG
1	A	238	GLN
1	A	247	THR
1	A	319	LEU
1	A	342	LEU
1	A	356	LEU
1	A	384	ILE
1	A	402	ILE
1	A	421	ASN

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Mol	Chain	Res	Type
1	A	439	GLU
1	A	484	THR
1	A	491	ARG
1	A	544	LYS
1	A	567	ARG
1	A	600	LEU
1	A	631	THR
1	A	656	ARG
1	A	691	LEU
1	A	713	LYS
1	A	732	GLU
1	A	739	ASN
1	A	911	ASN
1	A	975	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	101	ASN
1	A	114	ASN
1	A	177	GLN
1	A	238	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	421	ASN
1	A	510	ASN
1	A	612	GLN
1	A	756	ASN
1	A	768	ASN
1	A	875	GLN
1	A	911	ASN
1	A	914	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	TM1	A	1002	-	26,42,42	2.09	10 (38%)	25,66,66	3.95	7 (28%)
6	TG1	A	1003	-	43,48,48	1.88	10 (23%)	42,72,72	1.85	9 (21%)
4	ALF	A	998	-	0,4,4	0.00	-	0,6,6	0.00	-

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	TM1	A	1002	-	-	0/12/68/68	0/5/5/5
6	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
4	ALF	A	998	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	TM1	C3'-C4'	-2.80	1.44	1.52
5	A	1002	TM1	C4F-C3F	-2.72	1.38	1.49
5	A	1002	TM1	O7F-N6F	-2.67	1.17	1.22
5	A	1002	TM1	C5-N7	-2.06	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	TG1	C34-C11	2.14	1.56	1.53
6	A	1003	TG1	O3-C3	2.27	1.49	1.44
6	A	1003	TG1	C9-C8	2.55	1.55	1.52
6	A	1003	TG1	C1-C5	2.62	1.55	1.51
6	A	1003	TG1	C7-C6	2.71	1.58	1.54
5	A	1002	TM1	O2'-C1F	2.98	1.51	1.42
5	A	1002	TM1	C2-N1	2.98	1.39	1.33
6	A	1003	TG1	O6-C7	2.99	1.48	1.43
6	A	1003	TG1	C1-C2	2.99	1.59	1.54
5	A	1002	TM1	O3'-C1F	3.02	1.51	1.42
6	A	1003	TG1	C11-C7	3.23	1.59	1.55
5	A	1002	TM1	C2-N3	3.51	1.38	1.32
5	A	1002	TM1	C5'-C4'	3.55	1.63	1.51
5	A	1002	TM1	C4-N3	3.88	1.41	1.35
6	A	1003	TG1	O4-C21	5.47	1.33	1.21
6	A	1003	TG1	C7-C8	6.17	1.61	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	TM1	N3-C2-N1	-10.20	121.09	128.89
6	A	1003	TG1	O12-C12-C11	-4.39	124.22	128.26
5	A	1002	TM1	O4'-C1'-C2'	-4.25	98.91	106.60
6	A	1003	TG1	O5-C6-C7	-2.87	101.54	104.08
6	A	1003	TG1	C23-C22-C21	-2.65	109.16	116.04
6	A	1003	TG1	C2-O1-C13	2.35	121.91	117.75
6	A	1003	TG1	O5-C12-O12	2.42	125.15	121.62
6	A	1003	TG1	C3-O3-C21	2.50	119.91	116.30
5	A	1002	TM1	O3'-C3'-C2'	2.62	107.74	103.64
6	A	1003	TG1	C24-C22-C21	3.07	133.78	120.67
6	A	1003	TG1	O3-C21-O4	3.30	129.88	123.30
5	A	1002	TM1	C2'-C3'-C4'	3.34	112.07	103.69
6	A	1003	TG1	C10-O9-C32	6.12	134.47	121.90
5	A	1002	TM1	O2'-C2'-C3'	6.44	113.73	103.64
5	A	1002	TM1	O3'-C1F-O2'	8.22	114.64	106.15
5	A	1002	TM1	C4'-O4'-C1'	10.75	121.53	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1003	TG1	3	0
4	A	998	ALF	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/995 (99%)	0.72	147 (14%) 3 2	37, 71, 174, 196	1 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	16.2
1	A	279	PHE	9.4
1	A	284	HIS	9.3
1	A	282	PRO	9.2
1	A	890	ILE	9.0
1	A	289	ILE	8.3
1	A	80	GLU	7.9
1	A	883	PHE	7.6
1	A	77	TRP	7.3
1	A	876	CYS	7.1
1	A	286	GLY	7.1
1	A	280	ASN	7.0
1	A	285	GLY	6.9
1	A	991	TYR	6.9
1	A	281	ASP	6.9
1	A	283	VAL	6.8
1	A	994	GLY	6.8
1	A	287	SER	6.7
1	A	878	GLU	6.7
1	A	868	HIS	6.6
1	A	278	HIS	6.6
1	A	241	ALA	6.5
1	A	75	LEU	6.5
1	A	859	ALA	6.4
1	A	277	GLY	6.4
1	A	78	PHE	6.3
1	A	84	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	882	HIS	6.2
1	A	879	ASP	6.1
1	A	85	ILE	6.1
1	A	242	THR	5.7
1	A	867	TYR	5.5
1	A	993	GLU	5.5
1	A	47	LYS	5.5
1	A	886	LEU	5.4
1	A	924	ARG	5.4
1	A	82	GLU	5.4
1	A	891	PHE	5.4
1	A	288	TRP	5.3
1	A	881	PRO	5.1
1	A	967	TRP	5.1
1	A	857	MET	5.0
1	A	107	TRP	4.9
1	A	291	GLY	4.9
1	A	46	GLY	4.8
1	A	874	MET	4.7
1	A	49	LEU	4.6
1	A	923	MET	4.6
1	A	106	VAL	4.5
1	A	110	ARG	4.5
1	A	956	ILE	4.4
1	A	290	ARG	4.4
1	A	888	CYS	4.4
1	A	889	GLU	4.4
1	A	992	LEU	4.3
1	A	87	ALA	4.3
1	A	103	ILE	4.3
1	A	887	ASP	4.3
1	A	873	PHE	4.1
1	A	293	ILE	4.0
1	A	858	TYR	4.0
1	A	273	LEU	3.9
1	A	855	TRP	3.9
1	A	875	GLN	3.9
1	A	877	THR	3.9
1	A	111	ASN	3.8
1	A	109	GLU	3.8
1	A	83	GLU	3.8
1	A	786	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	915	SER	3.7
1	A	45	GLU	3.6
1	A	911	ASN	3.6
1	A	964	LEU	3.6
1	A	74	VAL	3.5
1	A	957	PHE	3.5
1	A	814	LEU	3.5
1	A	928	TRP	3.4
1	A	835	PHE	3.4
1	A	276	ILE	3.4
1	A	955	MET	3.4
1	A	951	ASP	3.3
1	A	866	THR	3.2
1	A	953	LEU	3.2
1	A	763	TYR	3.2
1	A	556	ARG	3.1
1	A	925	MET	3.1
1	A	79	GLU	3.1
1	A	912	ALA	3.0
1	A	104	VAL	3.0
1	A	433	VAL	3.0
1	A	968	LEU	3.0
1	A	905	VAL	3.0
1	A	766	SER	3.0
1	A	863	PRO	2.9
1	A	885	GLY	2.8
1	A	871	THR	2.8
1	A	861	ASP	2.8
1	A	987	ILE	2.8
1	A	869	GLN	2.7
1	A	71	ILE	2.7
1	A	246	LYS	2.7
1	A	880	HIS	2.7
1	A	53	VAL	2.7
1	A	60	LEU	2.7
1	A	88	PHE	2.7
1	A	897	MET	2.7
1	A	417	CYS	2.6
1	A	902	SER	2.6
1	A	504	SER	2.6
1	A	785	GLU	2.6
1	A	52	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	767	SER	2.5
1	A	862	GLY	2.5
1	A	832	TRP	2.5
1	A	870	LEU	2.4
1	A	50	TRP	2.4
1	A	764	LEU	2.4
1	A	989	ARG	2.4
1	A	210	SER	2.4
1	A	904	LEU	2.4
1	A	508	VAL	2.4
1	A	986	PHE	2.4
1	A	554	THR	2.4
1	A	787	LEU	2.4
1	A	268	CYS	2.4
1	A	946	LEU	2.3
1	A	57	PHE	2.3
1	A	294	TYR	2.3
1	A	86	THR	2.3
1	A	416	ILE	2.3
1	A	945	PHE	2.3
1	A	240	ALA	2.3
1	A	990	ASN	2.2
1	A	243	GLU	2.2
1	A	916	LEU	2.2
1	A	420	CYS	2.2
1	A	295	TYR	2.2
1	A	244	GLN	2.1
1	A	971	LEU	2.1
1	A	952	PRO	2.1
1	A	292	ALA	2.1
1	A	920	GLN	2.1
1	A	761	ILE	2.1
1	A	908	GLU	2.1
1	A	296	PHE	2.1
1	A	860	GLU	2.1
1	A	931	ILE	2.1

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

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	TM1	A	1002	38/38	0.78	0.30	1.91	146,151,157,159	0
6	TG1	A	1003	46/46	0.86	0.29	1.48	143,145,149,150	0
4	ALF	A	998	5/5	0.99	0.21	0.19	34,34,36,37	0
3	MG	A	995	1/1	0.99	0.16	-0.76	37,37,37,37	0
2	NA	A	1000	1/1	0.97	0.08	-2.49	57,57,57,57	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.