



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:14 PM UTC

PDB ID : 2EAR / pdb\_00002ear  
Title : P21 crystal of the SR CA2+-ATPase with bound TG  
Authors : Takahashi, M.; Kondou, Y.; Toyoshima, C.  
Deposited on : 2007-02-02  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

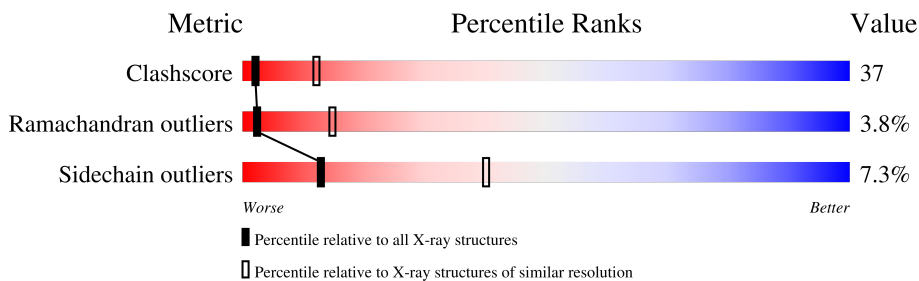
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	 43%      48%      8%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 7718 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.

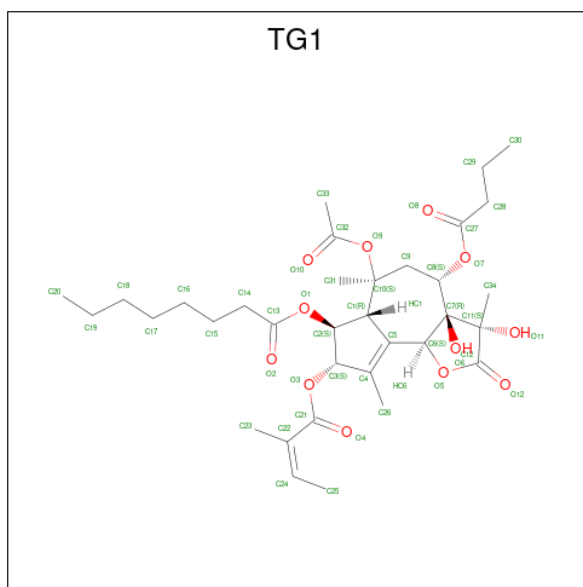
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	995	7672	4878	1287	1450	57	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 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 (CCD ID: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



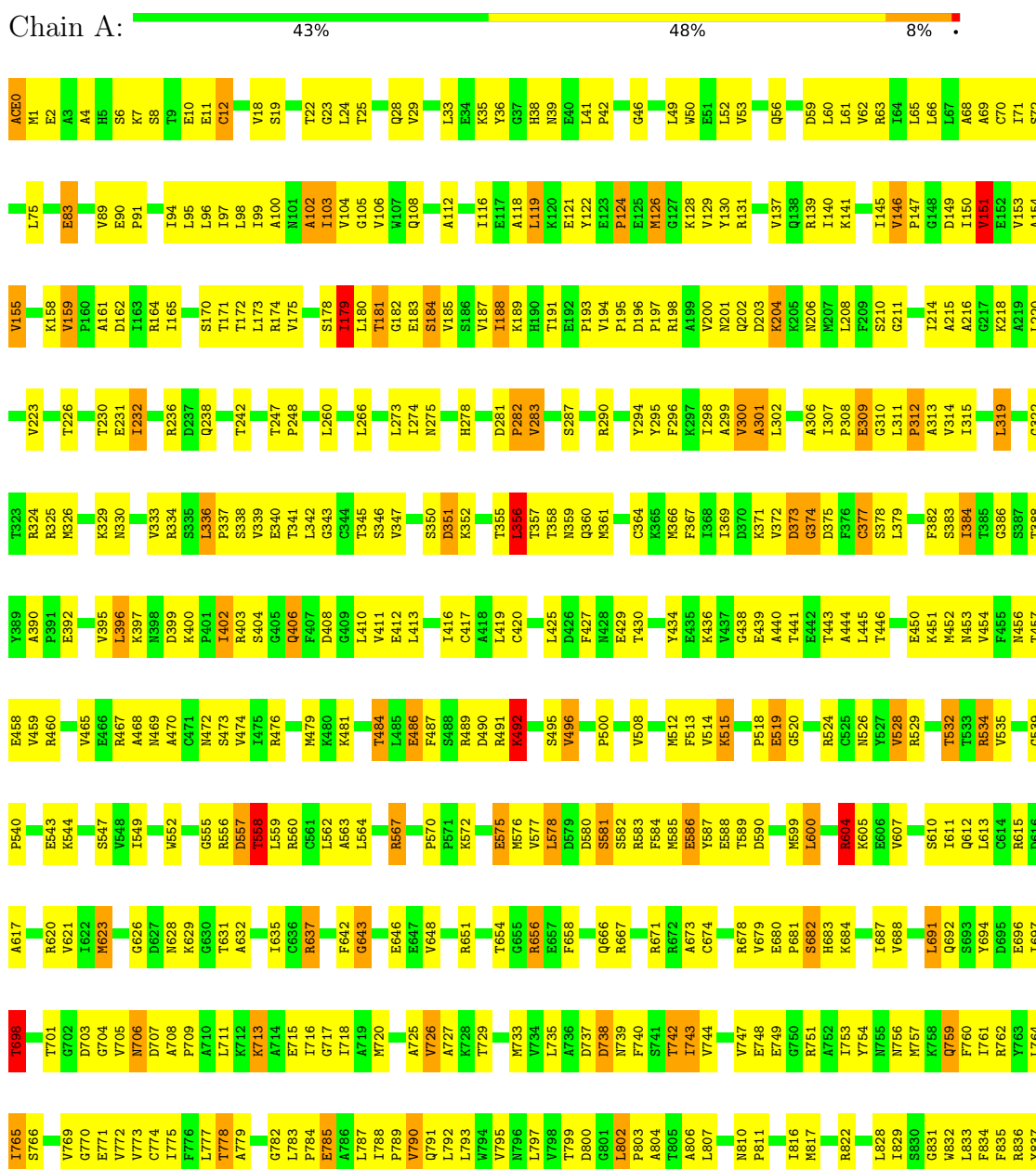
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	46	34	12	0	0

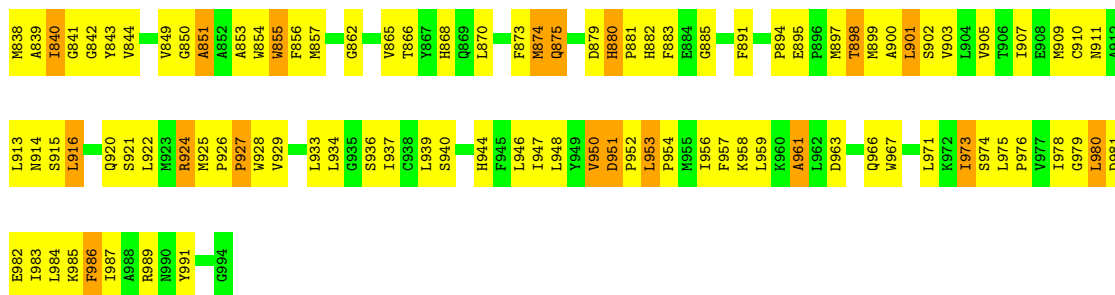
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.85Å 95.94Å 154.49Å 90.00° 94.90° 90.00°	Depositor
Resolution (Å)	14.95 – 3.10	Depositor
% Data completeness (in resolution range)	99.5 (14.95-3.10)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

## 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: ACE, TG1

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	0.62	3/7811 (0.0%)	1.02	31/10593 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	-26.21	0.81	1.33
1	A	682	SER	C-N	-5.97	1.25	1.33
1	A	855	TRP	NE1-CE2	-5.34	1.31	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	ACE	C-N-CA	11.30	155.59	121.70
1	A	146	VAL	N-CA-C	10.69	117.96	109.19
1	A	159	VAL	CA-C-N	8.62	128.33	119.19
1	A	159	VAL	C-N-CA	8.62	128.33	119.19
1	A	0	ACE	O-C-N	-7.41	100.79	123.00
1	A	356	LEU	N-CA-C	-7.18	104.67	113.50
1	A	103	ILE	N-CA-C	-7.11	104.84	111.45
1	A	916	LEU	N-CA-C	-6.91	105.79	114.56
1	A	400	LYS	CA-C-N	6.86	127.27	119.93
1	A	400	LYS	C-N-CA	6.86	127.27	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	637	ARG	N-CA-C	-6.67	104.01	111.28
1	A	980	LEU	N-CA-C	-6.32	104.31	111.07
1	A	406	GLN	N-CA-C	-6.27	105.49	113.01
1	A	967	TRP	N-CA-C	-5.75	106.26	113.28
1	A	743	ILE	N-CA-C	-5.64	104.85	111.00
1	A	874	MET	N-CA-C	-5.60	108.24	114.62
1	A	211	GLY	N-CA-C	-5.48	107.38	113.79
1	A	102	ALA	N-CA-C	-5.42	107.92	114.75
1	A	567	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	765	ILE	N-CA-C	-5.30	107.65	113.43
1	A	698	THR	N-CA-C	5.24	117.79	109.24
1	A	851	ALA	N-CA-C	-5.23	106.74	113.01
1	A	632	ALA	N-CA-C	-5.18	105.32	110.97
1	A	151	VAL	N-CA-C	5.15	116.60	109.29
1	A	924	ARG	N-CA-C	-5.11	107.21	113.50
1	A	604	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	717	GLY	N-CA-C	-5.09	105.25	112.37
1	A	532	THR	N-CA-C	-5.07	107.75	114.04
1	A	643	GLY	N-CA-C	-5.07	106.75	112.33
1	A	373	ASP	N-CA-C	5.06	116.11	108.07
1	A	351	ASP	N-CA-C	-5.01	103.91	110.53

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ALA	Mainchain
1	A	302	LEU	Mainchain
1	A	558	THR	Mainchain
1	A	600	LEU	Mainchain
1	A	70	CYS	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7672	0	7765	578	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	46	0	50	1	0
All	All	7718	0	7815	578	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 37.

All (578) 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:0:ACE:CH3	1:A:1:MET:N	2.14	1.11
1:A:558:THR:HG21	1:A:635:ILE:HG12	1.20	1.11
1:A:232:ILE:HD12	1:A:232:ILE:H	1.11	1.08
1:A:0:ACE:C	1:A:1:MET:CA	2.27	1.06
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.41	1.02
1:A:322:GLY:HA2	1:A:325:ARG:HH12	1.27	1.00
1:A:322:GLY:HA2	1:A:325:ARG:NH1	1.78	0.97
1:A:604:ARG:HB3	1:A:607:VAL:HG13	1.48	0.95
1:A:29:VAL:HG21	1:A:131:ARG:NH1	1.82	0.95
1:A:526:ASN:ND2	1:A:590:ASP:HA	1.84	0.92
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.35	0.92
1:A:351:ASP:H	1:A:701:THR:HG21	1.32	0.92
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.55	0.88
1:A:345:THR:HA	1:A:697:ILE:HG22	1.56	0.88
1:A:898:THR:HA	1:A:959:LEU:HD22	1.56	0.88
1:A:671:ARG:HB3	1:A:694:TYR:CE1	2.08	0.88
1:A:416:ILE:HG23	1:A:513:PHE:HB3	1.56	0.87
1:A:558:THR:HG21	1:A:635:ILE:CG1	2.04	0.86
1:A:898:THR:HB	1:A:959:LEU:HA	1.59	0.84
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.59	0.84
1:A:41:LEU:HD21	1:A:119:LEU:HD12	1.60	0.83
1:A:558:THR:CG2	1:A:635:ILE:HG12	2.06	0.83
1:A:715:GLU:C	1:A:716:ILE:HD12	2.04	0.83
1:A:828:LEU:HD13	2:A:1003:TG1:H291	1.60	0.82
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.61	0.82
1:A:950:VAL:O	1:A:954:PRO:HD2	1.78	0.81
1:A:775:ILE:HA	1:A:778:THR:HG22	1.62	0.81
1:A:922:LEU:HD23	1:A:927:PRO:CG	2.12	0.80
1:A:278:HIS:ND1	1:A:282:PRO:HG2	1.95	0.79
1:A:720:MET:HE3	1:A:738:ASP:CB	2.13	0.79
1:A:201:ASN:HA	1:A:204:LYS:HE2	1.64	0.78
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.66	0.78
1:A:326:MET:HE3	1:A:333:VAL:HG21	1.65	0.77
1:A:130:TYR:HE2	1:A:137:VAL:HG23	1.49	0.77
1:A:720:MET:HE3	1:A:738:ASP:HB2	1.66	0.76
1:A:828:LEU:H	1:A:828:LEU:HD12	1.51	0.75
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.15	0.75
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.86	0.75
1:A:95:LEU:HD23	1:A:95:LEU:O	1.87	0.75
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.69	0.75
1:A:29:VAL:HG21	1:A:131:ARG:HH11	1.52	0.74
1:A:519:GLU:HG2	1:A:520:GLY:H	1.51	0.74
1:A:0:ACE:C	1:A:1:MET:H3	0.71	0.74
1:A:984:LEU:O	1:A:987:ILE:HG22	1.87	0.74
1:A:345:THR:HA	1:A:697:ILE:CG2	2.17	0.74
1:A:232:ILE:HD12	1:A:232:ILE:N	1.96	0.74
1:A:49:LEU:HG	1:A:50:TRP:H	1.52	0.74
1:A:725:ALA:O	1:A:729:THR:HG23	1.87	0.74
1:A:764:LEU:HD23	1:A:764:LEU:O	1.88	0.73
1:A:351:ASP:OD2	1:A:701:THR:HG23	1.89	0.73
1:A:857:MET:HG2	1:A:866:THR:HB	1.69	0.73
1:A:281:ASP:HB2	1:A:282:PRO:HD3	1.68	0.73
1:A:410:LEU:HD22	1:A:452:MET:HE3	1.71	0.72
1:A:425:LEU:HB3	1:A:469:ASN:HD21	1.52	0.72
1:A:326:MET:CE	1:A:333:VAL:HG21	2.19	0.72
1:A:468:ALA:C	1:A:469:ASN:HD22	1.99	0.71
1:A:287:SER:HA	1:A:290:ARG:HB3	1.72	0.71
1:A:637:ARG:HG2	1:A:637:ARG:HH11	1.55	0.71
1:A:515:LYS:O	1:A:515:LYS:HG3	1.91	0.70
1:A:922:LEU:HD23	1:A:927:PRO:HG2	1.72	0.70
1:A:586:GLU:HG3	1:A:587:TYR:H	1.57	0.70
1:A:586:GLU:O	1:A:589:THR:HG22	1.91	0.70
1:A:643:GLY:HA3	1:A:646:GLU:HG3	1.72	0.70
1:A:232:ILE:H	1:A:232:ILE:CD1	1.88	0.70
1:A:210:SER:O	1:A:232:ILE:HG12	1.92	0.70
1:A:715:GLU:HB3	1:A:716:ILE:HD12	1.74	0.69
1:A:802:LEU:HD12	1:A:936:SER:HB2	1.74	0.69
1:A:604:ARG:HB3	1:A:607:VAL:CG1	2.22	0.69
1:A:266:LEU:O	1:A:266:LEU:HD13	1.92	0.69
1:A:18:VAL:HG22	1:A:24:LEU:HD23	1.74	0.69
1:A:19:SER:HB3	1:A:22:THR:OG1	1.93	0.69
1:A:342:LEU:HD21	1:A:733:MET:CE	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD23	1:A:705:VAL:HG21	1.76	0.68
1:A:692:GLN:C	1:A:694:TYR:H	2.01	0.68
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.34	0.68
1:A:188:ILE:HD12	1:A:188:ILE:N	2.08	0.67
1:A:922:LEU:HD23	1:A:927:PRO:HG3	1.75	0.67
1:A:188:ILE:HD12	1:A:188:ILE:H	1.60	0.67
1:A:308:PRO:HG2	1:A:765:ILE:HG22	1.76	0.67
1:A:754:TYR:HD1	1:A:757:MET:HE3	1.59	0.67
1:A:880:HIS:H	1:A:881:PRO:HD2	1.59	0.66
1:A:180:LEU:HD23	1:A:705:VAL:CG2	2.25	0.66
1:A:170:SER:OG	1:A:218:LYS:N	2.28	0.66
1:A:299:ALA:C	1:A:301:ALA:H	2.04	0.66
1:A:680:GLU:HB2	1:A:683:HIS:CE1	2.31	0.66
1:A:425:LEU:HB3	1:A:469:ASN:ND2	2.11	0.66
1:A:126:MET:HE2	1:A:141:LYS:HA	1.76	0.65
1:A:238:GLN:O	1:A:242:THR:HG23	1.95	0.65
1:A:753:ILE:O	1:A:757:MET:HG3	1.97	0.65
1:A:586:GLU:HG3	1:A:587:TYR:N	2.09	0.65
1:A:322:GLY:CA	1:A:325:ARG:HH12	2.06	0.65
1:A:364:CYS:O	1:A:384:ILE:HG12	1.97	0.64
1:A:759:GLN:HA	1:A:759:GLN:OE1	1.97	0.64
1:A:948:LEU:HG	1:A:961:ALA:HA	1.80	0.64
1:A:375:ASP:O	1:A:540:PRO:HB3	1.97	0.64
1:A:351:ASP:N	1:A:701:THR:HG21	2.10	0.64
1:A:458:GLU:OE2	1:A:460:ARG:HG2	1.97	0.64
1:A:544:LYS:O	1:A:547:SER:HB3	1.98	0.64
1:A:946:LEU:O	1:A:953:LEU:HD12	1.98	0.64
1:A:743:ILE:O	1:A:747:VAL:HG23	1.98	0.64
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.62	0.64
1:A:248:PRO:HG2	1:A:340:GLU:OE1	1.98	0.63
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.79	0.63
1:A:356:LEU:HD23	1:A:623:MET:HG3	1.81	0.63
1:A:491:ARG:HH12	1:A:588:GLU:CD	2.07	0.63
1:A:496:VAL:HG13	1:A:496:VAL:O	1.99	0.63
1:A:427:PHE:HA	1:A:434:TYR:HA	1.81	0.62
1:A:903:VAL:HG13	1:A:974:SER:OG	1.99	0.62
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.82	0.62
1:A:355:THR:HG23	1:A:720:MET:HE1	1.82	0.62
1:A:642:PHE:CD1	1:A:648:VAL:HG11	2.35	0.62
1:A:35:LYS:HD3	1:A:36:TYR:CZ	2.36	0.61
1:A:757:MET:HA	1:A:760:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.81	0.61
1:A:372:VAL:HA	1:A:377:CYS:HB2	1.81	0.61
1:A:403:ARG:HB3	1:A:406:GLN:HG3	1.81	0.61
1:A:838:MET:HE3	1:A:838:MET:HA	1.82	0.61
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.82	0.61
1:A:617:ALA:HB2	1:A:817:MET:HE3	1.82	0.61
1:A:811:PRO:HG2	1:A:929:VAL:HG12	1.82	0.61
1:A:716:ILE:HD12	1:A:716:ILE:N	2.16	0.61
1:A:775:ILE:HA	1:A:778:THR:CG2	2.31	0.61
1:A:324:ARG:HG3	1:A:325:ARG:N	2.14	0.61
1:A:417:CYS:SG	1:A:564:LEU:HD21	2.41	0.61
1:A:311:LEU:C	1:A:313:ALA:H	2.09	0.61
1:A:540:PRO:O	1:A:543:GLU:HB2	2.01	0.61
1:A:338:SER:HA	1:A:341:THR:HG22	1.83	0.60
1:A:916:LEU:HB3	1:A:925:MET:HE3	1.84	0.60
1:A:833:LEU:HD12	1:A:836:ARG:HE	1.67	0.60
1:A:436:LYS:HB3	1:A:443:THR:HG21	1.84	0.60
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.84	0.60
1:A:351:ASP:H	1:A:701:THR:CG2	2.09	0.59
1:A:556:ARG:HB3	1:A:556:ARG:NH1	2.18	0.59
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.36	0.59
1:A:281:ASP:O	1:A:283:VAL:HG13	2.03	0.59
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.85	0.59
1:A:687:ILE:HG22	1:A:691:LEU:CD2	2.32	0.59
1:A:23:GLY:HA3	1:A:130:TYR:O	2.03	0.59
1:A:637:ARG:HG2	1:A:637:ARG:NH1	2.17	0.58
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.18	0.58
1:A:470:ALA:O	1:A:474:VAL:HG23	2.04	0.58
1:A:762:ARG:HD3	1:A:828:LEU:HB3	1.85	0.58
1:A:857:MET:HA	1:A:866:THR:HG22	1.84	0.58
1:A:612:GLN:O	1:A:615:ARG:HB2	2.03	0.58
1:A:178:SER:HB3	1:A:184:SER:HA	1.85	0.58
1:A:90:GLU:HB2	1:A:790:VAL:CG2	2.34	0.58
1:A:33:LEU:HD21	1:A:38:HIS:CE1	2.39	0.58
1:A:783:LEU:C	1:A:785:GLU:H	2.12	0.57
1:A:739:ASN:HB3	1:A:742:THR:HG23	1.86	0.57
1:A:560:ARG:NH1	1:A:562:LEU:HD11	2.18	0.57
1:A:756:ASN:OD1	1:A:810:ASN:HB2	2.04	0.57
1:A:383:SER:HB3	1:A:396:LEU:CD1	2.34	0.57
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.34	0.57
1:A:350:SER:HA	1:A:701:THR:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG23	1:A:28:GLN:OE1	2.04	0.57
1:A:329:LYS:O	1:A:330:ASN:HB2	2.04	0.57
1:A:419:LEU:HD11	1:A:479:MET:HB2	1.86	0.57
1:A:791:GLN:O	1:A:795:VAL:HG23	2.05	0.57
1:A:629:LYS:HB2	1:A:654:THR:HG22	1.87	0.57
1:A:832:TRP:HZ2	1:A:987:ILE:HG21	1.69	0.57
1:A:882:HIS:NE2	1:A:885:GLY:HA3	2.20	0.57
1:A:984:LEU:C	1:A:987:ILE:HG22	2.30	0.57
1:A:61:LEU:HD21	1:A:260:LEU:HD23	1.86	0.57
1:A:783:LEU:HD23	1:A:874:MET:HE2	1.87	0.57
1:A:875:GLN:NE2	1:A:875:GLN:H	2.03	0.57
1:A:926:PRO:O	1:A:929:VAL:HG23	2.05	0.57
1:A:52:LEU:HB3	1:A:106:VAL:HG23	1.86	0.56
1:A:153:VAL:HB	1:A:214:ILE:HD12	1.86	0.56
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.87	0.56
1:A:65:LEU:CD2	1:A:307:ILE:HD12	2.36	0.56
1:A:129:VAL:O	1:A:130:TYR:HD2	1.89	0.56
1:A:188:ILE:CD1	1:A:486:GLU:HG2	2.35	0.56
1:A:103:ILE:C	1:A:105:GLY:H	2.11	0.56
1:A:766:SER:HA	1:A:769:VAL:HG23	1.88	0.56
1:A:161:ALA:HA	1:A:210:SER:HB2	1.87	0.56
1:A:973:ILE:HD13	1:A:973:ILE:O	2.06	0.56
1:A:18:VAL:HG22	1:A:24:LEU:CD2	2.36	0.56
1:A:982:GLU:O	1:A:986:PHE:HB2	2.06	0.56
1:A:920:GLN:O	1:A:985:LYS:HE2	2.06	0.56
1:A:897:MET:C	1:A:899:MET:H	2.14	0.55
1:A:162:ASP:OD2	1:A:230:THR:HB	2.06	0.55
1:A:879:ASP:HB3	1:A:882:HIS:O	2.06	0.55
1:A:388:THR:HG23	1:A:390:ALA:H	1.72	0.55
1:A:605:LYS:HD2	1:A:605:LYS:H	1.71	0.55
1:A:873:PHE:HZ	1:A:881:PRO:HG3	1.72	0.55
1:A:6:SER:HA	1:A:194:VAL:O	2.06	0.55
1:A:905:VAL:O	1:A:909:MET:HG2	2.07	0.55
1:A:490:ASP:OD2	1:A:491:ARG:N	2.40	0.55
1:A:558:THR:CG2	1:A:635:ILE:CG1	2.78	0.55
1:A:844:VAL:HB	1:A:907:ILE:HD12	1.89	0.55
1:A:479:MET:HE2	1:A:500:PRO:HA	1.88	0.55
1:A:963:ASP:HB3	1:A:966:GLN:HG2	1.88	0.55
1:A:757:MET:O	1:A:761:ILE:HG13	2.06	0.54
1:A:151:VAL:HG13	1:A:223:VAL:HG23	1.89	0.54
1:A:397:LYS:N	1:A:402:ILE:HD12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASP:O	1:A:558:THR:C	2.50	0.54
1:A:804:ALA:O	1:A:807:LEU:HB2	2.08	0.54
1:A:875:GLN:H	1:A:875:GLN:HE21	1.53	0.54
1:A:775:ILE:CA	1:A:778:THR:HG22	2.37	0.54
1:A:910:CYS:HB3	1:A:978:ILE:HD11	1.90	0.54
1:A:410:LEU:HD22	1:A:452:MET:CE	2.38	0.54
1:A:210:SER:HB3	1:A:232:ILE:CD1	2.38	0.54
1:A:679:VAL:HG22	1:A:683:HIS:HB2	1.90	0.54
1:A:122:TYR:HE1	1:A:726:VAL:CG2	2.21	0.54
1:A:715:GLU:HB3	1:A:716:ILE:CD1	2.36	0.53
1:A:795:VAL:HA	1:A:799:THR:HB	1.91	0.53
1:A:839:ALA:O	1:A:841:GLY:N	2.41	0.53
1:A:926:PRO:C	1:A:928:TRP:H	2.16	0.53
1:A:24:LEU:HG	1:A:149:ASP:HA	1.89	0.53
1:A:371:LYS:HG2	1:A:378:SER:OG	2.07	0.53
1:A:450:GLU:HG3	1:A:468:ALA:O	2.09	0.53
1:A:310:GLY:O	1:A:314:VAL:HG23	2.09	0.53
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.89	0.53
1:A:979:GLY:O	1:A:983:ILE:HG12	2.09	0.53
1:A:175:VAL:HG11	1:A:208:LEU:HD22	1.91	0.53
1:A:275:ASN:N	1:A:275:ASN:HD22	2.06	0.53
1:A:735:LEU:HD22	1:A:742:THR:OG1	2.09	0.53
1:A:897:MET:O	1:A:899:MET:N	2.41	0.53
1:A:72:SER:C	1:A:91:PRO:HG3	2.34	0.53
1:A:626:GLY:O	1:A:678:ARG:HD3	2.07	0.53
1:A:481:LYS:HE3	1:A:496:VAL:HG21	1.90	0.52
1:A:126:MET:HG3	1:A:140:ILE:O	2.09	0.52
1:A:583:ARG:HH11	1:A:583:ARG:HG2	1.75	0.52
1:A:707:ASP:O	1:A:711:LEU:HG	2.10	0.52
1:A:308:PRO:C	1:A:310:GLY:H	2.18	0.52
1:A:122:TYR:HE1	1:A:726:VAL:HG21	1.75	0.52
1:A:441:THR:O	1:A:444:ALA:N	2.43	0.52
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.92	0.52
1:A:909:MET:N	1:A:909:MET:HE2	2.24	0.52
1:A:90:GLU:HB2	1:A:790:VAL:HG21	1.92	0.52
1:A:104:VAL:HG12	1:A:104:VAL:O	2.08	0.52
1:A:311:LEU:N	1:A:312:PRO:HD2	2.25	0.52
1:A:326:MET:HE1	1:A:339:VAL:HG12	1.90	0.52
1:A:386:GLY:HA3	1:A:451:LYS:NZ	2.24	0.52
1:A:441:THR:HG23	1:A:599:MET:SD	2.50	0.52
1:A:520:GLY:O	1:A:524:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:O	1:A:62:VAL:HG12	2.10	0.52
1:A:326:MET:HE3	1:A:333:VAL:CG2	2.38	0.52
1:A:901:LEU:HD23	1:A:902:SER:N	2.24	0.52
1:A:97:ILE:CD1	1:A:797:LEU:HD21	2.41	0.51
1:A:631:THR:O	1:A:635:ILE:HG13	2.11	0.51
1:A:897:MET:C	1:A:899:MET:N	2.68	0.51
1:A:429:GLU:OE1	1:A:465:VAL:HG21	2.11	0.51
1:A:658:PHE:CZ	1:A:666:GLN:HG2	2.45	0.51
1:A:761:ILE:O	1:A:765:ILE:HG12	2.10	0.51
1:A:294:TYR:O	1:A:298:ILE:HG23	2.11	0.51
1:A:703:ASP:HA	1:A:727:ALA:HB1	1.91	0.51
1:A:901:LEU:HD13	1:A:959:LEU:HD11	1.93	0.51
1:A:924:ARG:C	1:A:926:PRO:HD3	2.35	0.51
1:A:56:GLN:HA	1:A:56:GLN:NE2	2.25	0.51
1:A:129:VAL:C	1:A:130:TYR:HD2	2.19	0.51
1:A:420:CYS:SG	1:A:515:LYS:HG2	2.51	0.51
1:A:350:SER:HA	1:A:701:THR:HG21	1.92	0.51
1:A:0:ACE:H2	1:A:147:PRO:HB3	1.92	0.51
1:A:692:GLN:C	1:A:694:TYR:N	2.68	0.51
1:A:572:LYS:HB3	1:A:575:GLU:HG2	1.94	0.50
1:A:833:LEU:CD1	1:A:836:ARG:HE	2.24	0.50
1:A:367:PHE:C	1:A:367:PHE:CD2	2.90	0.50
1:A:183:GLU:O	1:A:185:VAL:N	2.44	0.50
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.92	0.50
1:A:39:ASN:OD1	1:A:226:THR:HB	2.12	0.50
1:A:556:ARG:HB3	1:A:556:ARG:HH11	1.76	0.50
1:A:680:GLU:CB	1:A:681:PRO:CD	2.85	0.50
1:A:325:ARG:HH11	1:A:325:ARG:HB3	1.77	0.50
1:A:783:LEU:N	1:A:784:PRO:CD	2.75	0.50
1:A:469:ASN:HD22	1:A:469:ASN:N	2.04	0.50
1:A:628:ASN:O	1:A:629:LYS:C	2.52	0.50
1:A:346:SER:OG	1:A:696:GLU:HG2	2.12	0.50
1:A:771:GLU:O	1:A:775:ILE:HG12	2.11	0.50
1:A:984:LEU:HA	1:A:987:ILE:HG22	1.94	0.50
1:A:179:ILE:O	1:A:705:VAL:HG22	2.12	0.50
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.93	0.50
1:A:586:GLU:C	1:A:588:GLU:H	2.19	0.50
1:A:784:PRO:O	1:A:785:GLU:C	2.54	0.50
1:A:402:ILE:HD13	1:A:402:ILE:H	1.77	0.49
1:A:678:ARG:HG3	1:A:678:ARG:NH1	2.26	0.49
1:A:642:PHE:CE2	1:A:674:CYS:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:TYR:CD1	1:A:757:MET:HE3	2.45	0.49
1:A:806:ALA:HB1	1:A:933:LEU:HA	1.94	0.49
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.36	0.49
1:A:174:ARG:O	1:A:215:ALA:N	2.44	0.49
1:A:403:ARG:NE	1:A:406:GLN:HG3	2.27	0.49
1:A:306:ALA:HB2	1:A:772:VAL:HG21	1.94	0.49
1:A:765:ILE:HD11	1:A:829:ILE:HD11	1.93	0.49
1:A:795:VAL:HG13	1:A:799:THR:HG21	1.94	0.49
1:A:10:GLU:O	1:A:11:GLU:C	2.55	0.49
1:A:308:PRO:HB3	1:A:764:LEU:HD22	1.95	0.49
1:A:519:GLU:H	1:A:519:GLU:CD	2.21	0.49
1:A:671:ARG:HB3	1:A:694:TYR:HE1	1.71	0.49
1:A:29:VAL:CG2	1:A:131:ARG:NH1	2.67	0.49
1:A:680:GLU:N	1:A:683:HIS:ND1	2.54	0.49
1:A:130:TYR:HE2	1:A:137:VAL:CG2	2.21	0.49
1:A:539:GLY:O	1:A:543:GLU:HG2	2.12	0.49
1:A:778:THR:HG23	1:A:778:THR:O	2.11	0.49
1:A:97:ILE:HD11	1:A:797:LEU:HD21	1.94	0.49
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.28	0.49
1:A:413:LEU:HD22	1:A:564:LEU:HD23	1.95	0.49
1:A:18:VAL:HG11	1:A:150:ILE:HG23	1.94	0.48
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.42	0.48
1:A:481:LYS:HE3	1:A:496:VAL:CG2	2.43	0.48
1:A:395:VAL:O	1:A:402:ILE:HD13	2.12	0.48
1:A:771:GLU:OE1	1:A:792:LEU:HD22	2.12	0.48
1:A:0:ACE:O	1:A:1:MET:CA	2.52	0.48
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.95	0.48
1:A:419:LEU:CD1	1:A:479:MET:HB2	2.43	0.48
1:A:651:ARG:O	1:A:673:ALA:HA	2.13	0.48
1:A:810:ASN:HD21	1:A:916:LEU:HD23	1.78	0.48
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.94	0.48
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.94	0.48
1:A:137:VAL:HG13	1:A:137:VAL:O	2.13	0.48
1:A:584:PHE:HA	1:A:587:TYR:HD2	1.78	0.48
1:A:684:LYS:O	1:A:688:VAL:HG23	2.14	0.48
1:A:984:LEU:HA	1:A:987:ILE:CG2	2.44	0.48
1:A:1:MET:CE	1:A:7:LYS:HG3	2.43	0.48
1:A:89:VAL:HG12	1:A:790:VAL:HG11	1.96	0.48
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.95	0.48
1:A:777:LEU:C	1:A:779:ALA:H	2.22	0.48
1:A:835:PHE:O	1:A:838:MET:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:ILE:HG13	1:A:957:PHE:HD1	1.77	0.48
1:A:956:ILE:HG13	1:A:957:PHE:CD1	2.49	0.48
1:A:986:PHE:CE2	1:A:989:ARG:CZ	2.97	0.48
1:A:469:ASN:ND2	1:A:469:ASN:N	2.59	0.47
1:A:916:LEU:HD21	1:A:933:LEU:HD22	1.96	0.47
1:A:626:GLY:O	1:A:678:ARG:CD	2.61	0.47
1:A:704:GLY:O	1:A:705:VAL:C	2.56	0.47
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.95	0.47
1:A:898:THR:HA	1:A:959:LEU:CD2	2.37	0.47
1:A:576:MET:HG2	1:A:587:TYR:CE1	2.50	0.47
1:A:615:ARG:NH1	1:A:615:ARG:HG2	2.30	0.47
1:A:411:VAL:O	1:A:412:GLU:C	2.57	0.47
1:A:839:ALA:C	1:A:841:GLY:N	2.72	0.47
1:A:862:GLY:O	1:A:865:VAL:HG22	2.15	0.47
1:A:922:LEU:N	1:A:922:LEU:HD12	2.29	0.47
1:A:35:LYS:HD3	1:A:36:TYR:CE2	2.50	0.47
1:A:390:ALA:C	1:A:392:GLU:H	2.23	0.47
1:A:419:LEU:O	1:A:496:VAL:HG21	2.14	0.47
1:A:679:VAL:HG22	1:A:683:HIS:CB	2.44	0.47
1:A:953:LEU:H	1:A:954:PRO:HD2	1.79	0.47
1:A:958:LYS:O	1:A:959:LEU:HD23	2.14	0.47
1:A:299:ALA:C	1:A:301:ALA:N	2.70	0.47
1:A:901:LEU:HD23	1:A:901:LEU:C	2.39	0.47
1:A:396:LEU:HD12	1:A:396:LEU:O	2.15	0.47
1:A:487:PHE:CE1	1:A:492:LYS:C	2.93	0.47
1:A:10:GLU:C	1:A:12:CYS:N	2.72	0.47
1:A:578:LEU:HD23	1:A:578:LEU:N	2.30	0.47
1:A:762:ARG:HD2	1:A:829:ILE:HG12	1.97	0.46
1:A:799:THR:CG2	1:A:905:VAL:HG22	2.40	0.46
1:A:901:LEU:CD2	1:A:944:HIS:HE1	2.28	0.46
1:A:69:ALA:C	1:A:71:ILE:H	2.21	0.46
1:A:367:PHE:HD1	1:A:552:TRP:CH2	2.34	0.46
1:A:373:ASP:O	1:A:374:GLY:C	2.59	0.46
1:A:671:ARG:HD2	1:A:694:TYR:OH	2.15	0.46
1:A:765:ILE:HD11	1:A:829:ILE:CD1	2.45	0.46
1:A:922:LEU:HB3	1:A:927:PRO:CG	2.45	0.46
1:A:103:ILE:C	1:A:105:GLY:N	2.73	0.46
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.97	0.46
1:A:342:LEU:HD21	1:A:733:MET:HE2	1.98	0.46
1:A:947:ILE:HA	1:A:953:LEU:HB3	1.96	0.46
1:A:456:ASN:O	1:A:457:THR:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG11	1:A:131:ARG:HH12	1.81	0.46
1:A:342:LEU:CD2	1:A:733:MET:CE	2.94	0.46
1:A:83:GLU:CD	1:A:83:GLU:H	2.24	0.46
1:A:210:SER:HB3	1:A:232:ILE:HD11	1.98	0.46
1:A:356:LEU:CD2	1:A:623:MET:HG3	2.45	0.46
1:A:487:PHE:HE1	1:A:492:LYS:C	2.24	0.46
1:A:196:ASP:OD1	1:A:198:ARG:HG2	2.16	0.46
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.45	0.46
1:A:678:ARG:HG3	1:A:678:ARG:HH11	1.81	0.46
1:A:146:VAL:O	1:A:147:PRO:C	2.59	0.45
1:A:697:ILE:HG22	1:A:697:ILE:O	2.15	0.45
1:A:65:LEU:HD21	1:A:307:ILE:HD12	1.98	0.45
1:A:306:ALA:HB2	1:A:772:VAL:CG2	2.46	0.45
1:A:434:TYR:CE2	1:A:468:ALA:HB2	2.52	0.45
1:A:175:VAL:HG22	1:A:189:LYS:HE2	1.98	0.45
1:A:373:ASP:CG	1:A:374:GLY:N	2.74	0.45
1:A:903:VAL:O	1:A:907:ILE:HG12	2.16	0.45
1:A:948:LEU:HA	1:A:954:PRO:HB3	1.98	0.45
1:A:248:PRO:HG2	1:A:340:GLU:CD	2.41	0.45
1:A:586:GLU:C	1:A:588:GLU:N	2.73	0.45
1:A:679:VAL:CG2	1:A:683:HIS:CB	2.94	0.45
1:A:766:SER:HG	1:A:837:TYR:HD1	1.63	0.45
1:A:851:ALA:HB3	1:A:900:ALA:HA	1.99	0.45
1:A:921:SER:O	1:A:925:MET:HB2	2.17	0.45
1:A:7:LYS:O	1:A:164:ARG:NH1	2.45	0.45
1:A:315:ILE:O	1:A:319:LEU:HB2	2.16	0.45
1:A:667:ARG:NH2	1:A:694:TYR:CE2	2.83	0.45
1:A:718:ILE:HA	1:A:733:MET:O	2.17	0.45
1:A:36:TYR:CE1	1:A:147:PRO:HB2	2.51	0.45
1:A:181:THR:HA	1:A:706:ASN:OD1	2.17	0.45
1:A:193:PRO:O	1:A:195:PRO:HD3	2.17	0.45
1:A:791:GLN:NE2	1:A:901:LEU:HB2	2.30	0.45
1:A:836:ARG:HA	1:A:984:LEU:HD13	1.99	0.45
1:A:273:LEU:C	1:A:273:LEU:HD23	2.42	0.45
1:A:629:LYS:HB2	1:A:654:THR:CG2	2.46	0.45
1:A:629:LYS:HD2	1:A:654:THR:HG23	1.97	0.45
1:A:766:SER:HA	1:A:769:VAL:CG2	2.47	0.45
1:A:452:MET:O	1:A:453:ASN:HB3	2.17	0.45
1:A:795:VAL:HA	1:A:799:THR:CB	2.47	0.45
1:A:927:PRO:O	1:A:934:LEU:HD21	2.16	0.45
1:A:180:LEU:HA	1:A:705:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TYR:N	1:A:295:TYR:CD1	2.85	0.45
1:A:782:GLY:C	1:A:784:PRO:HD2	2.42	0.45
1:A:611:ILE:HD12	1:A:621:VAL:HG11	1.98	0.45
1:A:839:ALA:C	1:A:841:GLY:H	2.24	0.45
1:A:844:VAL:CG1	1:A:907:ILE:HD12	2.47	0.45
1:A:905:VAL:O	1:A:905:VAL:HG12	2.16	0.45
1:A:951:ASP:HA	1:A:954:PRO:HG2	1.99	0.45
1:A:96:LEU:C	1:A:96:LEU:HD23	2.42	0.44
1:A:116:ILE:O	1:A:116:ILE:HG22	2.17	0.44
1:A:308:PRO:HB3	1:A:764:LEU:CD2	2.48	0.44
1:A:583:ARG:HG2	1:A:583:ARG:NH1	2.31	0.44
1:A:403:ARG:NH1	1:A:456:ASN:HD21	2.16	0.44
1:A:759:GLN:C	1:A:761:ILE:N	2.75	0.44
1:A:844:VAL:CB	1:A:907:ILE:HD12	2.46	0.44
1:A:10:GLU:O	1:A:12:CYS:N	2.50	0.44
1:A:159:VAL:O	1:A:210:SER:HA	2.18	0.44
1:A:402:ILE:HD13	1:A:402:ILE:N	2.31	0.44
1:A:450:GLU:O	1:A:451:LYS:C	2.61	0.44
1:A:897:MET:HE3	1:A:958:LYS:HB3	1.99	0.44
1:A:188:ILE:H	1:A:188:ILE:CD1	2.28	0.44
1:A:358:THR:OG1	1:A:360:GLN:HG2	2.17	0.44
1:A:713:LYS:HB2	1:A:713:LYS:NZ	2.33	0.44
1:A:762:ARG:O	1:A:766:SER:HB2	2.17	0.44
1:A:308:PRO:C	1:A:310:GLY:N	2.76	0.44
1:A:458:GLU:OE1	1:A:460:ARG:NE	2.51	0.44
1:A:612:GLN:O	1:A:615:ARG:N	2.46	0.44
1:A:90:GLU:CG	1:A:790:VAL:HG22	2.48	0.44
1:A:388:THR:HG23	1:A:390:ALA:N	2.31	0.44
1:A:715:GLU:CB	1:A:716:ILE:HD12	2.45	0.44
1:A:266:LEU:HD13	1:A:266:LEU:C	2.43	0.44
1:A:311:LEU:O	1:A:313:ALA:N	2.51	0.44
1:A:319:LEU:HG	1:A:339:VAL:HG21	2.00	0.44
1:A:457:THR:O	1:A:459:VAL:HG13	2.18	0.44
1:A:1:MET:HE2	1:A:4:ALA:HA	2.00	0.44
1:A:178:SER:O	1:A:179:ILE:C	2.61	0.44
1:A:53:VAL:O	1:A:56:GLN:HB3	2.18	0.43
1:A:68:ALA:HA	1:A:300:VAL:HG12	2.00	0.43
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.98	0.43
1:A:124:PRO:HD3	1:A:158:LYS:HG2	2.00	0.43
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.82	0.43
1:A:386:GLY:HA3	1:A:451:LYS:HZ3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.83	0.43
1:A:369:ILE:HD13	1:A:379:LEU:HD22	1.99	0.43
1:A:586:GLU:CG	1:A:587:TYR:N	2.81	0.43
1:A:181:THR:OG1	1:A:182:GLY:N	2.52	0.43
1:A:322:GLY:O	1:A:326:MET:HG3	2.18	0.43
1:A:436:LYS:HE3	1:A:440:ALA:HB2	1.99	0.43
1:A:581:SER:O	1:A:583:ARG:N	2.51	0.43
1:A:789:PRO:O	1:A:793:LEU:HD23	2.18	0.43
1:A:897:MET:CE	1:A:958:LYS:HB3	2.48	0.43
1:A:66:LEU:HD13	1:A:98:LEU:HD13	2.01	0.43
1:A:200:VAL:O	1:A:201:ASN:C	2.62	0.43
1:A:100:ALA:C	1:A:102:ALA:H	2.26	0.43
1:A:774:CYS:SG	1:A:787:LEU:CD1	3.06	0.43
1:A:236:ARG:HD3	1:A:236:ARG:C	2.43	0.43
1:A:473:SER:HA	1:A:476:ARG:HH11	1.84	0.43
1:A:974:SER:C	1:A:976:PRO:HD2	2.43	0.43
1:A:72:SER:OG	1:A:91:PRO:HG3	2.19	0.43
1:A:512:MET:HB2	1:A:567:ARG:CB	2.49	0.43
1:A:705:VAL:O	1:A:706:ASN:C	2.60	0.43
1:A:926:PRO:O	1:A:928:TRP:N	2.52	0.43
1:A:604:ARG:O	1:A:607:VAL:HG22	2.19	0.43
1:A:760:PHE:CD1	1:A:760:PHE:C	2.96	0.43
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.81	0.43
1:A:161:ALA:CA	1:A:210:SER:HB2	2.49	0.43
1:A:203:ASP:OD2	1:A:489:ARG:HD3	2.19	0.43
1:A:341:THR:C	1:A:343:GLY:N	2.75	0.43
1:A:939:LEU:O	1:A:939:LEU:HG	2.19	0.43
1:A:703:ASP:HA	1:A:727:ALA:CB	2.49	0.42
1:A:739:ASN:OD1	1:A:740:PHE:N	2.52	0.42
1:A:844:VAL:HG12	1:A:907:ILE:HD12	1.99	0.42
1:A:65:LEU:HD11	1:A:307:ILE:HG21	2.00	0.42
1:A:840:ILE:HG22	1:A:840:ILE:O	2.20	0.42
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.55	0.42
1:A:1:MET:HG2	1:A:4:ALA:HB2	2.02	0.42
1:A:60:LEU:O	1:A:63:ARG:N	2.50	0.42
1:A:347:VAL:HA	1:A:620:ARG:O	2.19	0.42
1:A:369:ILE:HD13	1:A:379:LEU:CD2	2.49	0.42
1:A:382:PHE:CD1	1:A:382:PHE:N	2.87	0.42
1:A:438:GLY:O	1:A:439:GLU:C	2.63	0.42
1:A:458:GLU:CD	1:A:460:ARG:HG2	2.45	0.42
1:A:512:MET:HB2	1:A:567:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:GLY:HA2	1:A:841:GLY:O	2.20	0.42
1:A:850:GLY:O	1:A:854:TRP:HB2	2.18	0.42
1:A:922:LEU:HB3	1:A:927:PRO:HD3	1.99	0.42
1:A:174:ARG:HA	1:A:187:VAL:O	2.20	0.42
1:A:352:LYS:HG2	1:A:357:THR:HG23	2.00	0.42
1:A:789:PRO:C	1:A:791:GLN:H	2.26	0.42
1:A:508:VAL:HG12	1:A:508:VAL:O	2.19	0.42
1:A:783:LEU:O	1:A:783:LEU:HG	2.19	0.42
1:A:800:ASP:C	1:A:803:PRO:HD2	2.45	0.42
1:A:683:HIS:O	1:A:687:ILE:HG13	2.19	0.42
1:A:853:ALA:C	1:A:855:TRP:H	2.28	0.42
1:A:118:ALA:O	1:A:121:GLU:HB3	2.20	0.42
1:A:130:TYR:CE2	1:A:137:VAL:HG23	2.40	0.42
1:A:178:SER:C	1:A:180:LEU:N	2.77	0.42
1:A:210:SER:O	1:A:232:ILE:CG1	2.65	0.42
1:A:311:LEU:C	1:A:313:ALA:N	2.74	0.42
1:A:737:ASP:OD1	1:A:737:ASP:N	2.50	0.42
1:A:855:TRP:C	1:A:857:MET:H	2.28	0.42
1:A:933:LEU:O	1:A:937:ILE:HG13	2.19	0.42
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.49	0.42
1:A:173:LEU:HD12	1:A:216:ALA:O	2.20	0.42
1:A:347:VAL:HB	1:A:698:THR:HG23	2.02	0.42
1:A:577:VAL:HB	1:A:580:ASP:OD2	2.20	0.42
1:A:334:ARG:NH1	1:A:729:THR:HA	2.35	0.42
1:A:612:GLN:HA	1:A:615:ARG:HD2	2.01	0.42
1:A:656:ARG:HA	1:A:656:ARG:NE	2.34	0.42
1:A:716:ILE:N	1:A:716:ILE:CD1	2.82	0.42
1:A:748:GLU:O	1:A:751:ARG:HB3	2.20	0.42
1:A:870:LEU:HD22	1:A:891:PHE:CZ	2.55	0.42
1:A:145:ILE:HG22	1:A:146:VAL:N	2.35	0.42
1:A:760:PHE:HB3	1:A:807:LEU:HB2	2.02	0.42
1:A:831:GLY:O	1:A:834:PHE:HB3	2.19	0.42
1:A:840:ILE:HD13	1:A:980:LEU:HD23	2.02	0.42
1:A:8:SER:O	1:A:12:CYS:HB2	2.20	0.41
1:A:373:ASP:O	1:A:375:ASP:N	2.53	0.41
1:A:534:ARG:HG2	1:A:535:VAL:N	2.33	0.41
1:A:572:LYS:CB	1:A:575:GLU:HG2	2.50	0.41
1:A:839:ALA:O	1:A:842:GLY:N	2.50	0.41
1:A:916:LEU:HB3	1:A:925:MET:CE	2.50	0.41
1:A:934:LEU:HD23	1:A:937:ILE:HD12	2.02	0.41
1:A:0:ACE:O	1:A:1:MET:N	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PRO:O	1:A:197:PRO:HD3	2.20	0.41
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.93	0.41
1:A:436:LYS:HE2	1:A:438:GLY:O	2.20	0.41
1:A:484:THR:HB	1:A:496:VAL:HG23	2.02	0.41
1:A:704:GLY:H	1:A:727:ALA:HB2	1.86	0.41
1:A:720:MET:HB3	1:A:738:ASP:HB3	2.03	0.41
1:A:971:LEU:C	1:A:973:ILE:H	2.28	0.41
1:A:984:LEU:CA	1:A:987:ILE:HG22	2.50	0.41
1:A:359:ASN:HD22	1:A:359:ASN:HA	1.57	0.41
1:A:470:ALA:O	1:A:473:SER:OG	2.36	0.41
1:A:473:SER:HA	1:A:476:ARG:NH1	2.35	0.41
1:A:607:VAL:O	1:A:611:ILE:HG12	2.21	0.41
1:A:762:ARG:NH1	1:A:833:LEU:CD2	2.83	0.41
1:A:783:LEU:O	1:A:785:GLU:N	2.50	0.41
1:A:106:VAL:O	1:A:106:VAL:HG22	2.21	0.41
1:A:358:THR:CB	1:A:360:GLN:HG2	2.51	0.41
1:A:557:ASP:O	1:A:559:LEU:HG	2.19	0.41
1:A:937:ILE:O	1:A:940:SER:HB3	2.21	0.41
1:A:164:ARG:O	1:A:165:ILE:C	2.64	0.41
1:A:171:THR:HG22	1:A:172:THR:HG23	2.03	0.41
1:A:230:THR:O	1:A:231:GLU:C	2.63	0.41
1:A:519:GLU:HG2	1:A:520:GLY:N	2.27	0.41
1:A:621:VAL:HG21	1:A:740:PHE:CZ	2.56	0.41
1:A:773:VAL:O	1:A:774:CYS:C	2.62	0.41
1:A:913:LEU:C	1:A:915:SER:H	2.29	0.41
1:A:683:HIS:O	1:A:684:LYS:C	2.61	0.41
1:A:94:ILE:C	1:A:96:LEU:N	2.78	0.41
1:A:179:ILE:HG23	1:A:180:LEU:N	2.36	0.41
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.36	0.41
1:A:770:GLY:O	1:A:773:VAL:N	2.54	0.41
1:A:372:VAL:O	1:A:373:ASP:HB2	2.21	0.41
1:A:708:ALA:N	1:A:709:PRO:CD	2.84	0.41
1:A:769:VAL:O	1:A:773:VAL:HG23	2.21	0.41
1:A:772:VAL:O	1:A:773:VAL:C	2.64	0.41
1:A:336:LEU:O	1:A:337:PRO:C	2.63	0.40
1:A:338:SER:O	1:A:341:THR:HG22	2.21	0.40
1:A:408:ASP:O	1:A:411:VAL:HB	2.22	0.40
1:A:119:LEU:HD22	1:A:119:LEU:HA	1.95	0.40
1:A:202:GLN:OE1	1:A:489:ARG:CZ	2.69	0.40
1:A:765:ILE:O	1:A:769:VAL:HG23	2.20	0.40
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD21	1:A:296:PHE:C	2.46	0.40
1:A:361:MET:HA	1:A:600:LEU:O	2.21	0.40
1:A:739:ASN:HB3	1:A:742:THR:CG2	2.51	0.40
1:A:926:PRO:C	1:A:928:TRP:N	2.80	0.40
1:A:99:ILE:O	1:A:103:ILE:HG13	2.21	0.40
1:A:137:VAL:O	1:A:137:VAL:HG22	2.20	0.40
1:A:308:PRO:O	1:A:310:GLY:N	2.55	0.40
1:A:788:ILE:O	1:A:791:GLN:HB3	2.21	0.40
1:A:122:TYR:CE1	1:A:726:VAL:HG21	2.53	0.40
1:A:154:ALA:O	1:A:155:VAL:C	2.65	0.40
1:A:832:TRP:CZ2	1:A:987:ILE:HG21	2.53	0.40
1:A:855:TRP:HA	1:A:855:TRP:CE3	2.57	0.40
1:A:986:PHE:CE2	1:A:989:ARG:NH2	2.89	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%)	786 (79%)	169 (17%)	38 (4%)	<b>2</b> <b>15</b>

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883	PHE
1	A	2	GLU
1	A	155	VAL
1	A	184	SER
1	A	496	VAL
1	A	582	SER
1	A	822	ARG
1	A	840	ILE

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Mol	Chain	Res	Type
1	A	856	PHE
1	A	898	THR
1	A	961	ALA
1	A	300	VAL
1	A	309	GLU
1	A	399	ASP
1	A	492	LYS
1	A	519	GLU
1	A	558	THR
1	A	581	SER
1	A	785	GLU
1	A	895	GLU
1	A	46	GLY
1	A	404	SER
1	A	927	PRO
1	A	112	ALA
1	A	282	PRO
1	A	312	PRO
1	A	374	GLY
1	A	778	THR
1	A	880	HIS
1	A	283	VAL
1	A	894	PRO
1	A	950	VAL
1	A	953	LEU
1	A	981	ASP
1	A	179	ILE
1	A	951	ASP
1	A	124	PRO
1	A	555	GLY

### 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%)	779 (93%)	61 (7%)	13 40

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

Mol	Chain	Res	Type
1	A	12	CYS
1	A	83	GLU
1	A	108	GLN
1	A	119	LEU
1	A	126	MET
1	A	128	LYS
1	A	151	VAL
1	A	179	ILE
1	A	181	THR
1	A	188	ILE
1	A	191	THR
1	A	204	LYS
1	A	220	LEU
1	A	232	ILE
1	A	247	THR
1	A	309	GLU
1	A	319	LEU
1	A	336	LEU
1	A	356	LEU
1	A	377	CYS
1	A	384	ILE
1	A	396	LEU
1	A	402	ILE
1	A	430	THR
1	A	445	LEU
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	492	LYS
1	A	515	LYS
1	A	528	VAL
1	A	532	THR
1	A	534	ARG
1	A	557	ASP
1	A	575	GLU
1	A	578	LEU
1	A	585	MET
1	A	586	GLU
1	A	604	ARG
1	A	613	LEU
1	A	623	MET
1	A	656	ARG

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Mol	Chain	Res	Type
1	A	682	SER
1	A	691	LEU
1	A	698	THR
1	A	706	ASN
1	A	713	LYS
1	A	726	VAL
1	A	738	ASP
1	A	742	THR
1	A	759	GLN
1	A	790	VAL
1	A	802	LEU
1	A	816	ILE
1	A	868	HIS
1	A	875	GLN
1	A	901	LEU
1	A	973	ILE
1	A	975	LEU
1	A	986	PHE
1	A	991	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	38	HIS
1	A	56	GLN
1	A	101	ASN
1	A	190	HIS
1	A	250	GLN
1	A	275	ASN
1	A	284	HIS
1	A	359	ASN
1	A	461	ASN
1	A	469	ASN
1	A	472	ASN
1	A	510	ASN
1	A	526	ASN
1	A	645	ASN
1	A	706	ASN
1	A	755	ASN
1	A	791	GLN
1	A	869	GLN

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Mol	Chain	Res	Type
1	A	875	GLN
1	A	914	ASN
1	A	920	GLN
1	A	944	HIS

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TG1	A	1003	-	44,48,48	2.53	13 (29%)	47,72,72	2.29	13 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TG1	A	1003	-	-	6/33/99/99	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	TG1	O4-C21	10.29	1.42	1.21
2	A	1003	TG1	C1-C2	6.62	1.65	1.54
2	A	1003	TG1	O1-C13	4.65	1.47	1.34
2	A	1003	TG1	C21-C22	3.48	1.61	1.50
2	A	1003	TG1	C9-C10	3.26	1.59	1.54
2	A	1003	TG1	C9-C8	3.17	1.56	1.52
2	A	1003	TG1	O7-C8	3.09	1.51	1.46
2	A	1003	TG1	C3-C4	2.96	1.54	1.50
2	A	1003	TG1	C1-C5	2.93	1.56	1.51
2	A	1003	TG1	O5-C6	-2.31	1.42	1.46
2	A	1003	TG1	C2-C3	2.25	1.57	1.53
2	A	1003	TG1	O3-C3	2.17	1.48	1.44
2	A	1003	TG1	O7-C27	2.09	1.40	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	TG1	C10-O9-C32	6.77	137.21	121.36
2	A	1003	TG1	O7-C8-C9	5.26	116.04	106.63
2	A	1003	TG1	O1-C2-C3	-4.96	100.81	110.18
2	A	1003	TG1	C2-O1-C13	4.70	125.23	117.59
2	A	1003	TG1	C7-C6-C5	4.54	127.34	115.41
2	A	1003	TG1	C24-C22-C21	3.99	135.78	120.79
2	A	1003	TG1	O12-C12-C11	-3.65	124.59	128.28
2	A	1003	TG1	C10-C1-C5	-3.08	110.89	115.07
2	A	1003	TG1	O11-C11-C12	-2.99	96.14	106.35
2	A	1003	TG1	O5-C12-O12	2.56	124.91	121.60
2	A	1003	TG1	C23-C22-C24	-2.41	113.89	123.12
2	A	1003	TG1	C23-C22-C21	-2.35	110.09	116.12
2	A	1003	TG1	O1-C2-C1	2.20	115.63	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

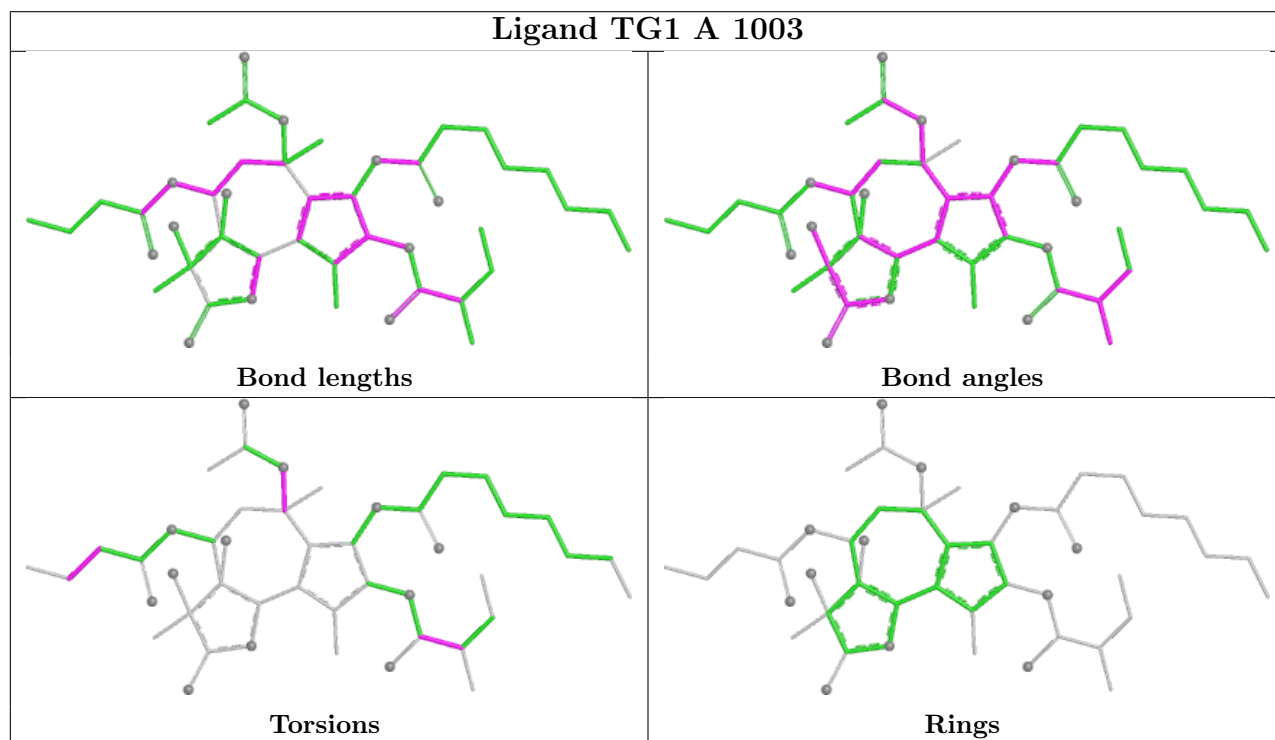
Mol	Chain	Res	Type	Atoms
2	A	1003	TG1	O3-C21-C22-C23
2	A	1003	TG1	C27-C28-C29-C30
2	A	1003	TG1	O3-C21-C22-C24
2	A	1003	TG1	O4-C21-C22-C23
2	A	1003	TG1	O4-C21-C22-C24
2	A	1003	TG1	C1-C10-O9-C32

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	TG1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	0:ACE	C	1:MET	N	0.80

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.