



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 06:00 pm GMT

PDB ID : 1WPG
Title : Crystal structure of the SR CA2+-ATPase with MGF4
Authors : Toyoshima, C.; Nomura, H.; Tsuda, T.
Deposited on : 2004-09-02
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

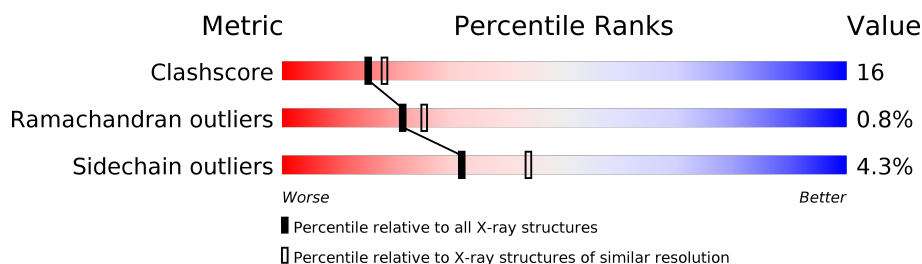
1 Overall quality at a glance

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))
Clashscore	122078	5071 (2.30-2.30)
Ramachandran outliers	120005	5021 (2.30-2.30)
Sidechain outliers	119972	5020 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	
1	B	994	
1	C	994	
1	D	994	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31698 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	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	B	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	C	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	D	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

There are 4 discrepancies between the modelled and reference sequences:

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

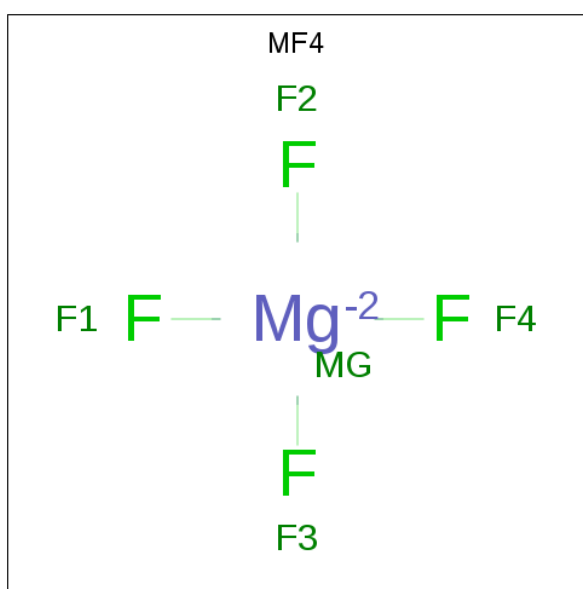
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).



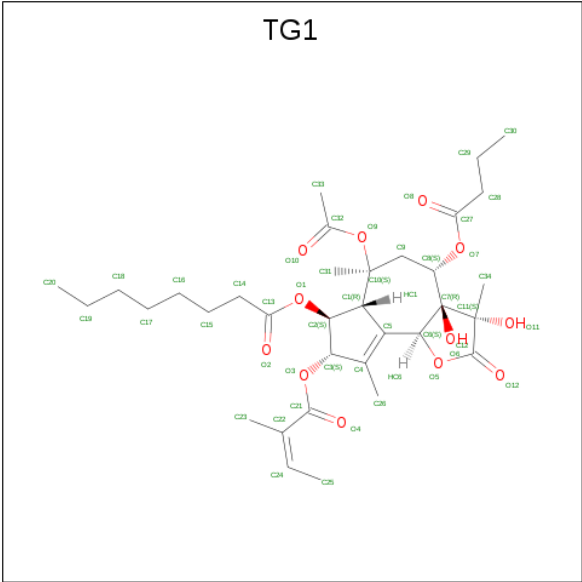
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total F Mg 5 4 1	0	0
4	B	1	Total F Mg 5 4 1	0	0
4	C	1	Total F Mg 5 4 1	0	0
4	D	1	Total F Mg 5 4 1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- 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-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
6	A	1	Total	C	O	0	0
			46	34	12		
6	B	1	Total	C	O	0	0
			46	34	12		
6	C	1	Total	C	O	0	0
			46	34	12		
6	D	1	Total	C	O	0	0
			46	34	12		

- Molecule 7 is water.

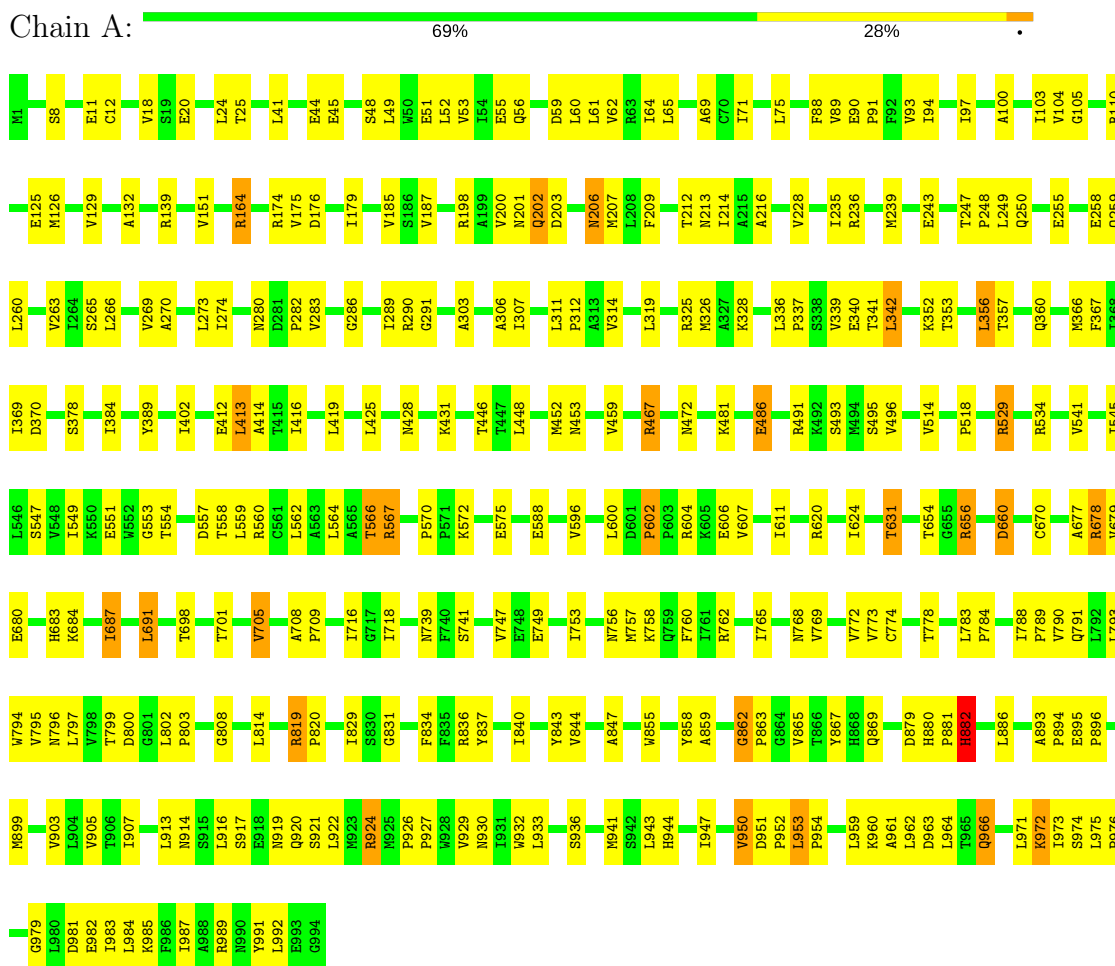
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	165	Total	O	0	0
			165	165		
7	B	180	Total	O	0	0
			180	180		
7	C	180	Total	O	0	0
			180	180		
7	D	165	Total	O	0	0
			165	165		

3 Residue-property plots

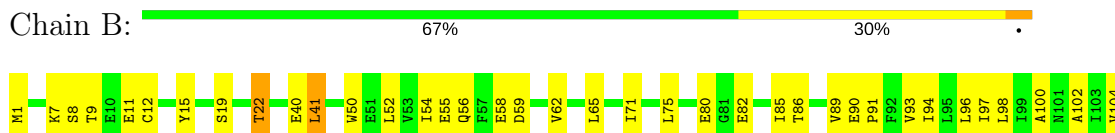
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

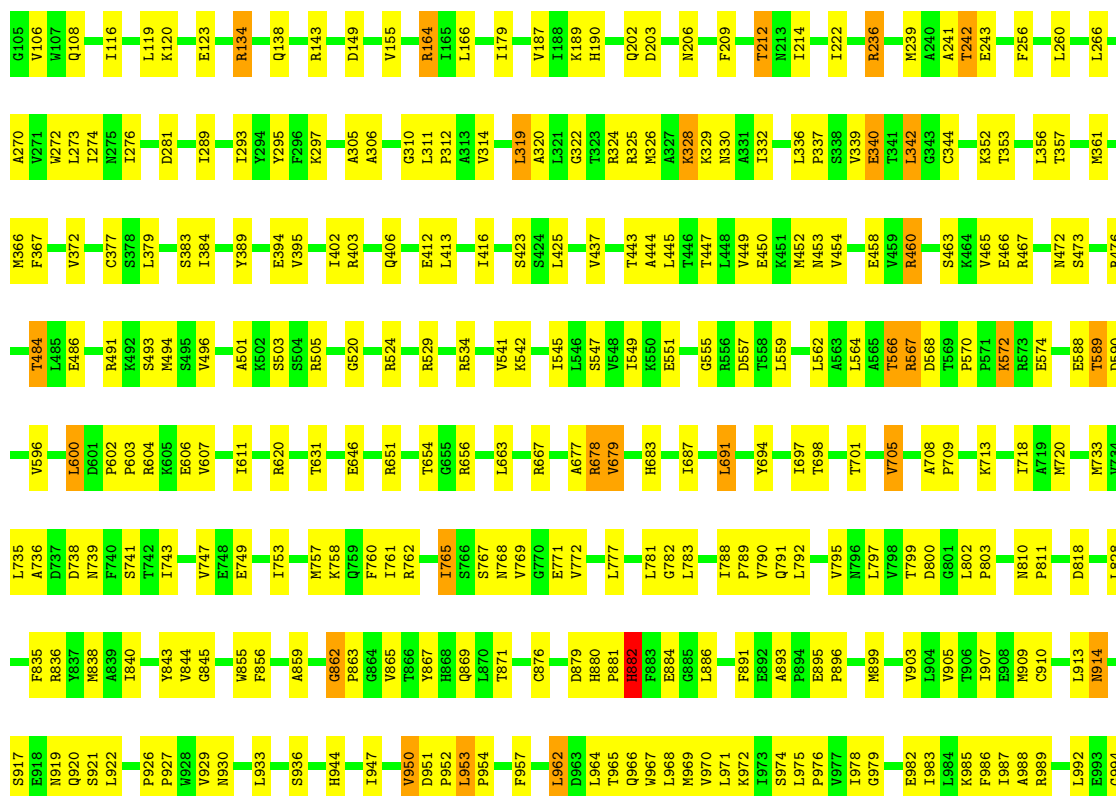
Note EDS was not executed.

• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



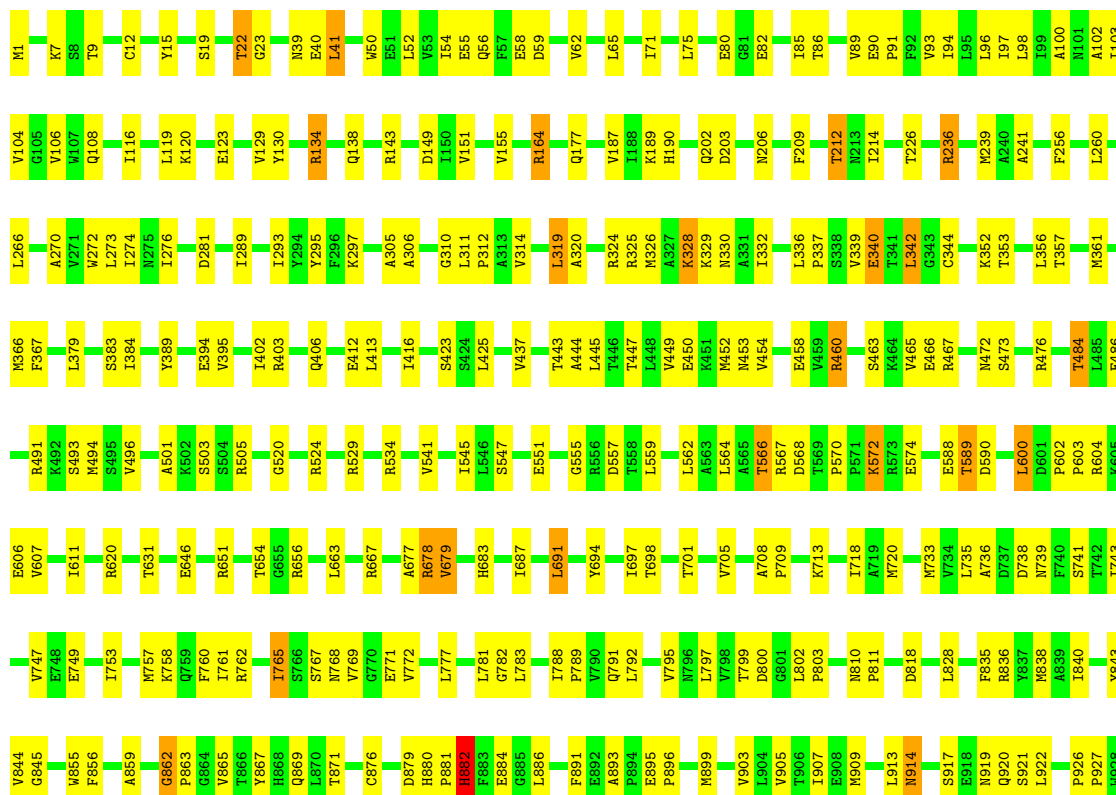
• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

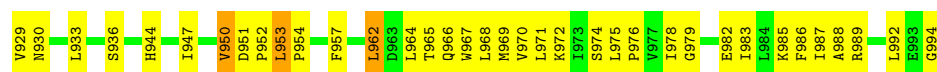




• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

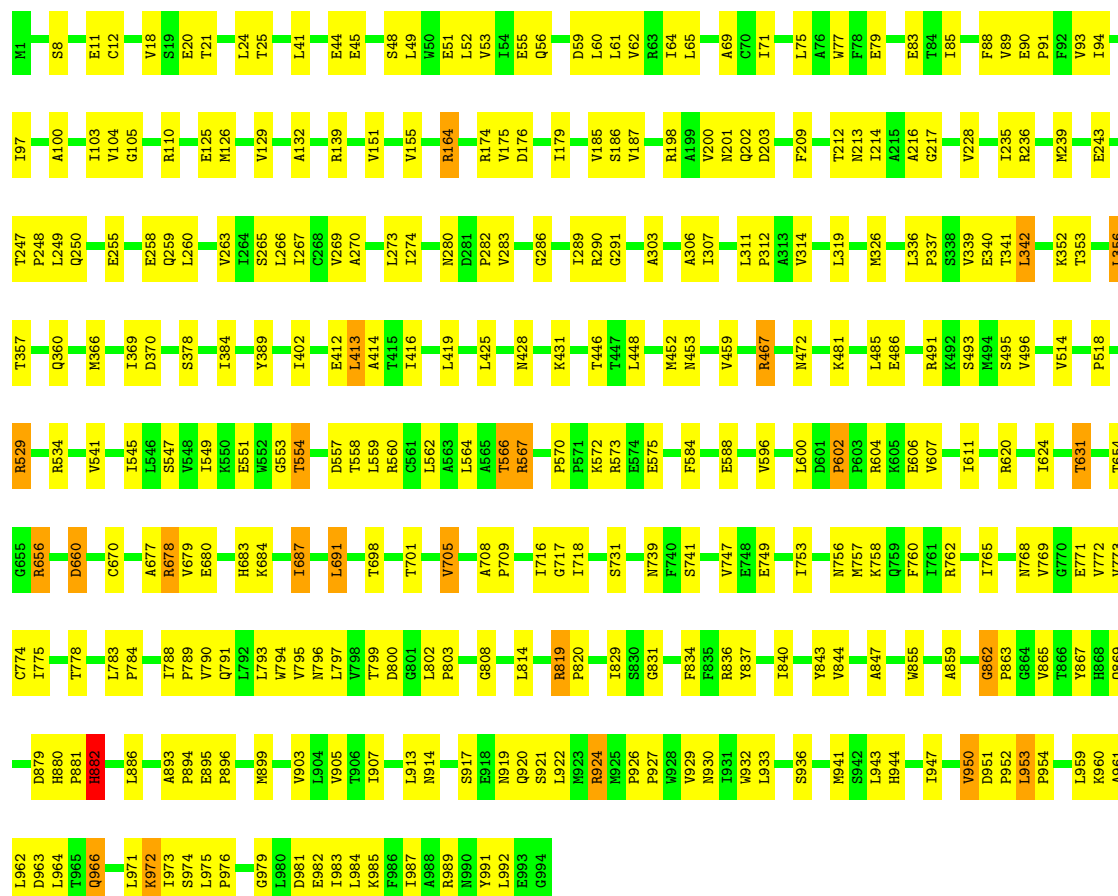
Chain C: 68% 29% •





● Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain D: 68% 29% .



4 Data and refinement statistics

Xtriage (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, α , β , γ	102.21Å 275.39Å 109.94Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	93.4 (15.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31698	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: NA, MG, TG1, MF4, ADP

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	0.38	0/7812	0.58	0/10592
1	B	0.41	0/7812	0.59	0/10592
1	C	0.41	0/7812	0.59	0/10592
1	D	0.38	0/7812	0.58	0/10592
All	All	0.40	0/31248	0.58	0/42368

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	7671	0	7764	240	0
1	B	7671	0	7764	267	0
1	C	7671	0	7764	258	0
1	D	7671	0	7764	238	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	2	0
5	C	27	0	12	2	0
5	D	27	0	12	0	0
6	A	46	0	50	0	0
6	B	46	0	50	2	0
6	C	46	0	50	2	0
6	D	46	0	50	0	0
7	A	165	0	0	5	0
7	B	180	0	0	9	0
7	C	180	0	0	7	0
7	D	165	0	0	6	0
All	All	31698	0	31304	999	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 16.

All (999) 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:C:460:ARG:H	1:C:460:ARG:HD3	1.09	1.15
1:B:460:ARG:HD3	1:B:460:ARG:H	1.10	1.13
1:D:679:VAL:HG13	1:D:683:HIS:HB2	1.47	0.96
1:C:921:SER:HB2	1:C:989:ARG:HH22	1.30	0.95
1:B:921:SER:HB2	1:B:989:ARG:HH22	1.31	0.94
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.49	0.93
1:A:202:GLN:H	1:A:202:GLN:HE21	1.13	0.92
1:B:494:MET:HE3	5:B:1102:ADP:HN62	1.36	0.90
1:C:484:THR:HB	1:C:496:VAL:HG12	1.56	0.88
1:B:484:THR:HB	1:B:496:VAL:HG12	1.57	0.87
1:B:319:LEU:HB3	1:B:336:LEU:HD12	1.58	0.85
1:C:319:LEU:HB3	1:C:336:LEU:HD12	1.59	0.84
1:C:494:MET:HE2	7:C:4036:HOH:O	1.78	0.84
1:C:1:MET:HE1	1:C:7:LYS:HD2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ARG:HD3	1:C:460:ARG:N	1.93	0.81
1:A:289:ILE:HG22	1:A:290:ARG:HH11	1.46	0.80
1:D:289:ILE:HG22	1:D:290:ARG:HH11	1.46	0.80
1:B:460:ARG:HD3	1:B:460:ARG:N	1.94	0.80
1:D:174:ARG:HG3	1:D:216:ALA:HB3	1.63	0.79
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.65	0.79
1:A:174:ARG:HG3	1:A:216:ALA:HB3	1.65	0.78
1:A:125:GLU:HG3	1:A:126:MET:HG2	1.65	0.77
1:D:125:GLU:HG3	1:D:126:MET:HG2	1.65	0.77
1:D:260:LEU:HD11	1:D:306:ALA:HB1	1.67	0.77
1:B:1:MET:HE1	1:B:7:LYS:HD2	1.67	0.77
1:B:865:VAL:HG11	1:B:869:GLN:HB2	1.67	0.76
1:B:921:SER:H	1:B:989:ARG:HH12	1.29	0.76
1:D:413:LEU:HD22	1:D:564:LEU:HD12	1.66	0.76
1:A:247:THR:HB	1:A:248:PRO:HD2	1.68	0.76
1:C:865:VAL:HG11	1:C:869:GLN:HB2	1.68	0.76
1:C:921:SER:H	1:C:989:ARG:HH12	1.29	0.75
1:D:247:THR:HB	1:D:248:PRO:HD2	1.69	0.75
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.88	0.74
1:B:972:LYS:HA	1:B:972:LYS:HE2	1.69	0.74
1:C:972:LYS:HE2	1:C:972:LYS:HA	1.70	0.74
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.68	0.74
1:B:209:PHE:O	1:B:212:THR:HB	1.87	0.74
1:A:553:GLY:O	1:A:554:THR:CG2	2.37	0.73
1:D:412:GLU:OE1	1:D:529:ARG:HD2	1.88	0.73
1:B:80:GLU:HG3	1:B:82:GLU:HG2	1.70	0.73
1:C:80:GLU:HG3	1:C:82:GLU:HG2	1.70	0.73
1:C:458:GLU:HB2	1:C:460:ARG:HE	1.54	0.73
1:B:458:GLU:HB2	1:B:460:ARG:HE	1.54	0.72
1:C:212:THR:HG21	7:C:4082:HOH:O	1.87	0.72
1:B:844:VAL:HG22	1:B:907:ILE:HG21	1.71	0.72
1:C:844:VAL:HG22	1:C:907:ILE:HG21	1.71	0.72
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.72	0.71
1:B:212:THR:HG21	7:B:3082:HOH:O	1.88	0.71
1:B:922:LEU:HD23	1:B:927:PRO:HG3	1.72	0.71
1:C:567:ARG:HD3	1:C:570:PRO:HA	1.72	0.71
1:B:260:LEU:HD11	1:B:306:ALA:HB1	1.72	0.71
1:C:260:LEU:HD11	1:C:306:ALA:HB1	1.73	0.71
1:D:319:LEU:HB3	1:D:336:LEU:HD12	1.71	0.71
1:C:922:LEU:HD23	1:C:927:PRO:HG3	1.73	0.70
1:C:735:LEU:HD11	1:C:743:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HA	1:A:987:ILE:HD12	1.73	0.70
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.72	0.70
1:C:735:LEU:HD21	1:C:743:ILE:HD13	1.74	0.69
1:D:90:GLU:HB3	1:D:91:PRO:HD3	1.72	0.69
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.72	0.69
1:B:735:LEU:HD21	1:B:743:ILE:HD13	1.74	0.69
1:C:1:MET:HE3	1:C:12:CYS:HA	1.74	0.69
1:C:913:LEU:HD22	1:C:927:PRO:HB3	1.73	0.69
1:A:202:GLN:H	1:A:202:GLN:NE2	1.90	0.69
1:B:913:LEU:HD22	1:B:927:PRO:HB3	1.73	0.69
1:D:984:LEU:HA	1:D:987:ILE:HD12	1.75	0.69
1:B:735:LEU:HD11	1:B:743:ILE:HD11	1.74	0.68
1:D:176:ASP:O	1:D:212:THR:HG23	1.92	0.68
1:A:553:GLY:O	1:A:554:THR:HG23	1.93	0.68
1:C:209:PHE:O	1:C:212:THR:HB	1.94	0.68
1:C:90:GLU:HB3	1:C:91:PRO:HD3	1.76	0.68
1:D:369:ILE:HD11	1:D:545:ILE:HD11	1.75	0.67
1:D:749:GLU:O	1:D:753:ILE:HG12	1.94	0.67
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.75	0.67
1:A:749:GLU:O	1:A:753:ILE:HG12	1.94	0.67
1:B:782:GLY:HA3	1:B:871:THR:HG23	1.77	0.67
1:A:202:GLN:HE21	1:A:202:GLN:N	1.90	0.67
1:D:413:LEU:CD2	1:D:564:LEU:HD12	2.25	0.67
1:D:61:LEU:HD22	1:D:307:ILE:HD12	1.76	0.67
1:A:176:ASP:O	1:A:212:THR:HG23	1.94	0.67
1:B:90:GLU:HB3	1:B:91:PRO:HD3	1.76	0.67
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.76	0.67
1:D:412:GLU:OE2	1:D:566:THR:HG21	1.95	0.67
1:C:782:GLY:HA3	1:C:871:THR:HG23	1.77	0.67
1:D:756:ASN:HB3	1:D:808:GLY:HA2	1.75	0.66
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.77	0.66
1:B:416:ILE:HD11	1:B:566:THR:HG22	1.77	0.66
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.94	0.66
1:D:567:ARG:HD2	1:D:570:PRO:HA	1.77	0.66
1:C:412:GLU:OE1	1:C:529:ARG:HD2	1.95	0.66
1:A:65:LEU:HD11	1:A:307:ILE:HG13	1.77	0.66
1:A:235:ILE:O	1:A:239:MET:HG2	1.96	0.65
1:A:49:LEU:HD12	1:A:52:LEU:HD11	1.77	0.65
1:C:979:GLY:O	1:C:983:ILE:HG12	1.96	0.65
1:D:708:ALA:HB3	1:D:709:PRO:HD3	1.78	0.65
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ARG:HG2	1:A:820:PRO:HD2	1.76	0.65
1:C:412:GLU:OE2	1:C:566:THR:HG21	1.96	0.65
1:D:65:LEU:HD11	1:D:307:ILE:HG13	1.78	0.65
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.77	0.65
1:D:126:MET:HG3	1:D:139:ARG:NH1	2.12	0.65
1:D:49:LEU:HD12	1:D:52:LEU:HD11	1.77	0.65
1:D:235:ILE:O	1:D:239:MET:HG2	1.97	0.65
1:D:8:SER:OG	1:D:11:GLU:HG3	1.97	0.65
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.78	0.65
1:D:788:ILE:HG12	1:D:791:GLN:NE2	2.12	0.65
1:A:788:ILE:HG12	1:A:791:GLN:NE2	2.12	0.64
1:C:950:VAL:HG12	1:C:952:PRO:HD2	1.79	0.64
1:C:416:ILE:HD11	1:C:566:THR:HG22	1.79	0.64
1:C:65:LEU:HD23	1:C:98:LEU:HD11	1.79	0.64
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.97	0.64
1:A:126:MET:HG3	1:A:139:ARG:NH1	2.13	0.64
1:B:41:LEU:HB2	1:B:123:GLU:OE1	1.98	0.64
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.79	0.64
1:B:384:ILE:HD12	1:B:395:VAL:HG22	1.80	0.64
1:B:718:ILE:HD13	1:B:743:ILE:HD12	1.80	0.64
1:B:979:GLY:O	1:B:983:ILE:HG12	1.98	0.63
1:C:384:ILE:HD12	1:C:395:VAL:HG22	1.80	0.63
1:D:174:ARG:CG	1:D:216:ALA:HB3	2.29	0.63
1:D:819:ARG:HG2	1:D:820:PRO:HD2	1.78	0.63
1:B:19:SER:HB3	1:B:22:THR:HG23	1.80	0.63
1:B:65:LEU:HD23	1:B:98:LEU:HD11	1.81	0.63
1:B:412:GLU:OE2	1:B:566:THR:HG21	1.98	0.63
1:B:342:LEU:HD12	1:B:733:MET:CE	2.28	0.62
1:D:963:ASP:H	1:D:966:GLN:HG3	1.63	0.62
1:C:342:LEU:HD22	1:C:747:VAL:HG22	1.82	0.62
1:C:988:ALA:HA	1:C:992:LEU:HD12	1.80	0.62
1:A:894:PRO:HB2	1:A:960:LYS:HB2	1.81	0.62
1:B:119:LEU:HD22	1:B:239:MET:CE	2.29	0.62
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.80	0.62
1:D:342:LEU:HD22	1:D:747:VAL:HG22	1.80	0.62
1:D:894:PRO:HB2	1:D:960:LYS:HB2	1.82	0.62
1:A:963:ASP:H	1:A:966:GLN:HG3	1.63	0.62
1:B:1:MET:HE3	1:B:12:CYS:HA	1.82	0.62
1:C:367:PHE:CE2	1:C:379:LEU:HD13	2.35	0.62
1:B:326:MET:HG2	1:B:749:GLU:HG2	1.81	0.62
1:B:367:PHE:CE2	1:B:379:LEU:HD13	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:SER:HB3	1:C:22:THR:HG23	1.81	0.62
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.81	0.61
1:C:933:LEU:O	1:C:936:SER:HB3	2.00	0.61
1:A:174:ARG:CG	1:A:216:ALA:HB3	2.30	0.61
1:B:326:MET:HE1	1:B:339:VAL:HG22	1.82	0.61
1:C:119:LEU:HD22	1:C:239:MET:CE	2.29	0.61
1:C:326:MET:HG2	1:C:749:GLU:HG2	1.81	0.61
1:B:933:LEU:O	1:B:936:SER:HB3	2.00	0.61
1:B:986:PHE:HA	1:B:989:ARG:HE	1.65	0.61
1:A:8:SER:OG	1:A:11:GLU:HG3	2.01	0.61
1:D:802:LEU:HB2	1:D:803:PRO:HD3	1.82	0.61
1:B:679:VAL:HG13	1:B:683:HIS:HB2	1.83	0.61
1:C:41:LEU:HB2	1:C:123:GLU:OE1	2.01	0.61
1:C:326:MET:HE1	1:C:339:VAL:HG22	1.83	0.61
1:B:449:VAL:CG2	1:B:472:ASN:ND2	2.64	0.61
1:C:810:ASN:HA	1:C:930:ASN:HD22	1.66	0.60
1:C:986:PHE:HA	1:C:989:ARG:HE	1.65	0.60
1:A:983:ILE:O	1:A:987:ILE:HG13	2.01	0.60
1:D:198:ARG:HH22	1:D:660:ASP:HA	1.64	0.60
1:D:983:ILE:O	1:D:987:ILE:HG13	2.01	0.60
1:C:272:TRP:HA	1:C:295:TYR:HE2	1.67	0.60
1:B:155:VAL:HA	1:B:214:ILE:HG22	1.83	0.60
1:B:691:LEU:HB3	1:B:698:THR:HG21	1.83	0.60
1:A:270:ALA:O	1:A:274:ILE:HG13	2.02	0.60
1:B:332:ILE:N	1:B:332:ILE:HD12	2.17	0.60
1:B:810:ASN:HA	1:B:930:ASN:HD22	1.66	0.60
1:C:975:LEU:N	1:C:976:PRO:HD2	2.15	0.60
1:A:198:ARG:HH22	1:A:660:ASP:HA	1.65	0.60
1:B:272:TRP:HA	1:B:295:TYR:HE2	1.67	0.60
1:C:449:VAL:CG2	1:C:472:ASN:ND2	2.65	0.60
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.83	0.60
1:B:951:ASP:HB3	1:B:952:PRO:HD3	1.84	0.60
1:B:975:LEU:N	1:B:976:PRO:HD2	2.15	0.60
1:C:951:ASP:HB3	1:C:952:PRO:HD3	1.84	0.59
1:C:342:LEU:HD12	1:C:733:MET:CE	2.31	0.59
1:C:802:LEU:HB2	1:C:803:PRO:HD3	1.83	0.59
1:D:270:ALA:O	1:D:274:ILE:HG13	2.02	0.59
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.83	0.59
1:B:342:LEU:HD22	1:B:747:VAL:HG22	1.85	0.59
1:B:55:GLU:HA	1:B:58:GLU:HG3	1.84	0.59
1:C:332:ILE:N	1:C:332:ILE:HD12	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:953:LEU:HB2	1:D:954:PRO:HD3	1.85	0.59
1:D:963:ASP:H	1:D:966:GLN:CG	2.16	0.59
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.83	0.59
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.85	0.59
1:C:55:GLU:HA	1:C:58:GLU:HG3	1.85	0.59
1:D:865:VAL:HG11	1:D:869:GLN:HB2	1.83	0.59
1:A:448:LEU:HG	1:A:452:MET:HE2	1.83	0.59
1:A:342:LEU:HD22	1:A:747:VAL:HG22	1.83	0.59
1:B:879:ASP:O	1:B:882:HIS:HB2	2.02	0.59
1:D:691:LEU:HB3	1:D:698:THR:HG21	1.83	0.59
1:C:718:ILE:HD13	1:C:743:ILE:HD12	1.85	0.58
1:A:963:ASP:H	1:A:966:GLN:CG	2.17	0.58
1:A:829:ILE:HD12	1:A:837:TYR:HD1	1.68	0.58
1:C:879:ASP:O	1:C:882:HIS:HB2	2.03	0.58
1:D:979:GLY:O	1:D:983:ILE:HG12	2.04	0.58
1:B:203:ASP:OD1	1:B:678:ARG:NH1	2.36	0.58
1:C:491:ARG:HD2	1:C:588:GLU:OE2	2.02	0.58
1:D:416:ILE:HD11	1:D:566:THR:HG22	1.85	0.58
1:B:855:TRP:HA	1:B:859:ALA:HB2	1.86	0.58
1:B:494:MET:HE3	5:B:1102:ADP:N6	2.13	0.58
1:C:679:VAL:HG13	1:C:683:HIS:HB2	1.86	0.58
1:C:855:TRP:HA	1:C:859:ALA:HB2	1.86	0.58
1:D:829:ILE:HD12	1:D:837:TYR:HD1	1.69	0.58
1:C:691:LEU:HB3	1:C:698:THR:HG21	1.85	0.57
1:A:979:GLY:O	1:A:983:ILE:HG12	2.05	0.57
1:B:491:ARG:HD2	1:B:588:GLU:OE2	2.03	0.57
1:C:964:LEU:O	1:C:968:LEU:HG	2.04	0.57
1:A:553:GLY:C	1:A:554:THR:HG23	2.25	0.57
1:C:155:VAL:HA	1:C:214:ILE:HG22	1.85	0.57
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.85	0.57
1:B:326:MET:HE1	1:B:339:VAL:CG2	2.34	0.57
1:D:340:GLU:HG3	1:D:341:THR:N	2.20	0.57
1:B:921:SER:H	1:B:989:ARG:NH1	2.02	0.57
1:B:836:ARG:HH22	1:B:985:LYS:HE2	1.70	0.57
1:C:1:MET:CE	1:C:12:CYS:HA	2.33	0.57
1:C:256:PHE:CZ	1:C:765:ILE:HD11	2.40	0.57
1:C:491:ARG:HG2	1:C:493:SER:OG	2.04	0.57
1:C:708:ALA:HB3	1:C:709:PRO:HD3	1.86	0.57
1:D:844:VAL:HG22	1:D:907:ILE:HG21	1.86	0.57
1:C:656:ARG:HG3	7:C:4516:HOH:O	2.05	0.57
1:A:340:GLU:HG3	1:A:341:THR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.86	0.56
1:B:718:ILE:HG21	1:B:743:ILE:CD1	2.35	0.56
1:B:953:LEU:H	1:B:954:PRO:HD2	1.69	0.56
1:B:964:LEU:O	1:B:968:LEU:HG	2.05	0.56
1:C:921:SER:H	1:C:989:ARG:NH1	2.02	0.56
1:C:953:LEU:H	1:C:954:PRO:HD2	1.69	0.56
1:A:879:ASP:O	1:A:882:HIS:HB2	2.04	0.56
1:B:1:MET:CE	1:B:12:CYS:HA	2.34	0.56
1:B:491:ARG:HG2	1:B:493:SER:OG	2.04	0.56
1:B:256:PHE:CZ	1:B:765:ILE:HD11	2.40	0.56
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.86	0.56
1:B:572:LYS:H	1:B:572:LYS:HD2	1.71	0.56
1:B:944:HIS:O	1:B:947:ILE:HG22	2.04	0.56
1:A:491:ARG:HD2	1:A:588:GLU:OE2	2.05	0.56
1:C:944:HIS:O	1:C:947:ILE:HG22	2.04	0.56
1:D:879:ASP:O	1:D:882:HIS:HB2	2.04	0.56
1:B:1:MET:HE3	1:B:15:TYR:HB3	1.87	0.56
1:B:656:ARG:HG3	7:B:3516:HOH:O	2.06	0.56
1:C:791:GLN:O	1:C:795:VAL:HG23	2.05	0.56
1:A:311:LEU:N	1:A:312:PRO:HD2	2.20	0.56
1:B:293:ILE:O	1:B:297:LYS:HB2	2.06	0.56
1:B:458:GLU:CB	1:B:460:ARG:HE	2.18	0.56
1:C:460:ARG:CD	1:C:460:ARG:H	1.96	0.56
1:C:572:LYS:H	1:C:572:LYS:HD2	1.71	0.56
1:D:975:LEU:N	1:D:976:PRO:HD2	2.21	0.56
1:C:458:GLU:CB	1:C:460:ARG:HE	2.18	0.56
1:D:90:GLU:HB2	1:D:790:VAL:HG22	1.87	0.56
1:B:357:THR:HA	1:B:603:PRO:HA	1.86	0.56
1:C:836:ARG:HH22	1:C:985:LYS:HE2	1.71	0.56
1:A:52:LEU:HD12	1:A:53:VAL:HG23	1.88	0.56
1:A:975:LEU:N	1:A:976:PRO:HD2	2.21	0.56
1:C:293:ILE:O	1:C:297:LYS:HB2	2.06	0.56
1:C:357:THR:HA	1:C:603:PRO:HA	1.87	0.56
1:C:607:VAL:O	1:C:611:ILE:HG12	2.06	0.56
1:D:865:VAL:HG12	1:D:867:TYR:H	1.70	0.56
1:A:247:THR:OG1	1:A:250:GLN:HG3	2.05	0.55
1:A:865:VAL:HG12	1:A:867:TYR:H	1.69	0.55
1:C:270:ALA:O	1:C:274:ILE:HG12	2.06	0.55
1:C:326:MET:HE1	1:C:339:VAL:CG2	2.36	0.55
1:C:718:ILE:HG21	1:C:743:ILE:CD1	2.36	0.55
1:B:460:ARG:CD	1:B:460:ARG:H	1.97	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:972:LYS:HA	1:D:972:LYS:NZ	2.22	0.55
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.89	0.55
1:D:52:LEU:HD12	1:D:53:VAL:HG23	1.88	0.55
1:A:60:LEU:O	1:A:64:ILE:HG12	2.06	0.55
1:B:895:GLU:N	1:B:896:PRO:HD2	2.22	0.55
1:B:962:LEU:HD23	1:B:962:LEU:N	2.22	0.55
1:D:247:THR:OG1	1:D:250:GLN:HG3	2.05	0.55
1:D:341:THR:HG22	1:D:716:ILE:HD11	1.87	0.55
1:A:972:LYS:NZ	1:A:972:LYS:HA	2.22	0.55
1:D:311:LEU:N	1:D:312:PRO:HD2	2.21	0.55
1:A:794:TRP:NE1	1:A:947:ILE:HD11	2.22	0.55
1:D:788:ILE:HB	1:D:789:PRO:HD2	1.89	0.55
1:C:895:GLU:N	1:C:896:PRO:HD2	2.22	0.55
1:C:962:LEU:N	1:C:962:LEU:HD23	2.22	0.55
1:D:60:LEU:O	1:D:64:ILE:HG12	2.07	0.55
1:A:206:ASN:ND2	1:A:207:MET:HG2	2.22	0.54
1:B:270:ALA:O	1:B:274:ILE:HG12	2.07	0.54
1:B:791:GLN:O	1:B:795:VAL:HG23	2.06	0.54
1:D:793:LEU:O	1:D:797:LEU:HB2	2.07	0.54
1:B:607:VAL:O	1:B:611:ILE:HG12	2.07	0.54
1:C:336:LEU:HB2	1:C:337:PRO:HD3	1.89	0.54
1:A:419:LEU:O	1:A:481:LYS:HE2	2.07	0.54
1:A:774:CYS:O	1:A:778:THR:HG22	2.06	0.54
1:A:793:LEU:O	1:A:797:LEU:HB2	2.08	0.54
1:A:966:GLN:HA	1:A:966:GLN:HE21	1.73	0.54
1:B:104:VAL:HG12	1:B:108:GLN:HE21	1.72	0.54
1:B:567:ARG:CD	1:B:570:PRO:HA	2.37	0.54
1:C:757:MET:HA	1:C:760:PHE:CE2	2.42	0.54
1:B:336:LEU:HB2	1:B:337:PRO:HD3	1.89	0.54
1:D:794:TRP:NE1	1:D:947:ILE:HD11	2.23	0.54
1:B:757:MET:HA	1:B:760:PHE:CE2	2.42	0.54
1:C:104:VAL:HG12	1:C:108:GLN:HE21	1.72	0.54
1:A:93:VAL:O	1:A:97:ILE:HG12	2.07	0.54
1:C:914:ASN:HD22	1:C:922:LEU:HD11	1.72	0.54
1:D:966:GLN:HE21	1:D:966:GLN:HA	1.73	0.54
1:D:987:ILE:O	1:D:991:TYR:HB2	2.08	0.54
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.90	0.54
1:C:494:MET:HE1	5:C:1202:ADP:HN62	1.73	0.54
1:C:458:GLU:HB3	1:C:460:ARG:HH21	1.73	0.54
1:D:353:THR:HA	1:D:357:THR:OG1	2.07	0.54
1:D:491:ARG:HD2	1:D:588:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:VAL:O	1:D:97:ILE:HG12	2.07	0.54
1:B:795:VAL:HG12	1:B:800:ASP:OD2	2.08	0.54
1:B:914:ASN:HD22	1:B:922:LEU:HD11	1.73	0.54
1:A:265:SER:O	1:A:269:VAL:HG23	2.08	0.53
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.90	0.53
1:A:572:LYS:HB2	1:A:575:GLU:HG3	1.89	0.53
1:A:670:CYS:SG	1:A:687:ILE:HG22	2.48	0.53
1:A:987:ILE:O	1:A:991:TYR:HB2	2.09	0.53
1:B:917:SER:OG	1:B:920:GLN:HB2	2.07	0.53
1:C:567:ARG:CD	1:C:570:PRO:HA	2.38	0.53
1:C:325:ARG:HH12	1:C:753:ILE:HD11	1.71	0.53
1:D:265:SER:O	1:D:269:VAL:HG23	2.08	0.53
1:B:988:ALA:O	1:B:992:LEU:HB2	2.07	0.53
1:C:203:ASP:OD1	1:C:678:ARG:NH1	2.41	0.53
1:C:879:ASP:HB3	1:C:882:HIS:ND1	2.23	0.53
1:D:419:LEU:O	1:D:481:LYS:HE2	2.08	0.53
1:D:557:ASP:HB3	1:D:559:LEU:HG	1.90	0.53
1:C:795:VAL:HG12	1:C:800:ASP:OD2	2.09	0.53
1:D:549:ILE:HD11	1:D:596:VAL:HG21	1.90	0.53
1:B:962:LEU:HB2	1:B:966:GLN:CB	2.38	0.53
1:C:413:LEU:HG	1:C:564:LEU:HD12	1.91	0.53
1:C:988:ALA:O	1:C:992:LEU:HB2	2.08	0.53
1:B:449:VAL:HG22	1:B:472:ASN:HD21	1.74	0.53
1:C:962:LEU:HB2	1:C:966:GLN:CB	2.38	0.53
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.38	0.53
1:C:735:LEU:HD21	1:C:743:ILE:CD1	2.38	0.53
1:A:71:ILE:O	1:A:75:LEU:HD13	2.09	0.53
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.90	0.53
1:B:458:GLU:HB3	1:B:460:ARG:HH21	1.74	0.53
1:B:879:ASP:HB3	1:B:882:HIS:ND1	2.24	0.53
1:C:328:LYS:NZ	1:C:328:LYS:HB3	2.24	0.53
1:A:547:SER:O	1:A:551:GLU:HG3	2.09	0.53
1:B:735:LEU:HD21	1:B:743:ILE:CD1	2.38	0.53
1:B:94:ILE:O	1:B:98:LEU:HD13	2.09	0.53
1:D:774:CYS:O	1:D:778:THR:HG22	2.07	0.53
1:B:325:ARG:HH12	1:B:753:ILE:HD11	1.72	0.52
1:C:917:SER:OG	1:C:920:GLN:HB2	2.09	0.52
1:C:94:ILE:O	1:C:98:LEU:HD13	2.09	0.52
1:D:572:LYS:HB2	1:D:575:GLU:HG3	1.90	0.52
1:A:794:TRP:CE2	1:A:947:ILE:HD11	2.44	0.52
1:C:843:TYR:OH	1:C:976:PRO:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:794:TRP:CE2	1:D:947:ILE:HD11	2.44	0.52
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.91	0.52
1:A:341:THR:HG22	1:A:716:ILE:HD11	1.90	0.52
1:D:175:VAL:CG1	1:D:212:THR:HG21	2.40	0.52
1:D:847:ALA:HA	1:D:973:ILE:HD11	1.90	0.52
1:A:353:THR:HA	1:A:357:THR:OG1	2.08	0.52
1:D:739:ASN:OD1	1:D:741:SER:HB2	2.10	0.52
1:D:962:LEU:HB3	1:D:966:GLN:HB2	1.91	0.52
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.39	0.52
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.92	0.52
1:B:749:GLU:O	1:B:753:ILE:HG12	2.09	0.52
1:C:366:MET:CE	1:C:384:ILE:HD11	2.40	0.52
1:C:449:VAL:HG22	1:C:472:ASN:HD21	1.75	0.52
1:D:670:CYS:SG	1:D:687:ILE:HG22	2.50	0.52
1:A:89:VAL:O	1:A:93:VAL:HG23	2.09	0.52
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.91	0.52
1:B:843:TYR:OH	1:B:976:PRO:HG2	2.09	0.52
1:A:326:MET:HG3	1:A:749:GLU:HG2	1.91	0.52
1:D:212:THR:HG22	1:D:213:ASN:N	2.23	0.52
1:D:71:ILE:O	1:D:75:LEU:HD13	2.09	0.52
1:D:547:SER:O	1:D:551:GLU:HG3	2.10	0.52
1:A:739:ASN:OD1	1:A:741:SER:HB2	2.10	0.52
1:B:328:LYS:NZ	1:B:328:LYS:HB3	2.26	0.52
1:D:326:MET:HG3	1:D:749:GLU:HG2	1.92	0.52
1:C:749:GLU:O	1:C:753:ILE:HG12	2.10	0.51
1:C:926:PRO:O	1:C:929:VAL:HG23	2.08	0.51
1:A:541:VAL:O	1:A:545:ILE:HG12	2.10	0.51
1:B:718:ILE:HG21	1:B:743:ILE:HD11	1.90	0.51
1:A:921:SER:H	1:A:989:ARG:HH12	1.58	0.51
1:B:926:PRO:O	1:B:929:VAL:HG23	2.09	0.51
1:B:962:LEU:HD23	1:B:962:LEU:H	1.75	0.51
1:C:85:ILE:HD13	1:D:110:ARG:CZ	2.40	0.51
1:D:366:MET:CE	1:D:384:ILE:HD11	2.40	0.51
1:B:572:LYS:N	1:B:572:LYS:HD2	2.26	0.51
1:B:739:ASN:OD1	1:B:741:SER:HB2	2.10	0.51
1:C:12:CYS:SG	1:C:164:ARG:HG3	2.51	0.51
1:C:273:LEU:O	1:C:276:ILE:HG13	2.09	0.51
1:D:369:ILE:CD1	1:D:545:ILE:HD11	2.40	0.51
1:D:921:SER:H	1:D:989:ARG:HH12	1.58	0.51
1:A:369:ILE:CD1	1:A:545:ILE:HD11	2.41	0.51
1:A:921:SER:H	1:A:989:ARG:NH1	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:VAL:HA	1:A:799:THR:HB	1.93	0.51
1:B:769:VAL:HG21	6:B:1103:TG1:H332	1.93	0.51
1:D:129:VAL:HG12	1:D:151:VAL:HG12	1.93	0.51
1:D:89:VAL:O	1:D:93:VAL:HG23	2.10	0.51
1:B:893:ALA:O	1:B:896:PRO:HD2	2.11	0.51
1:D:921:SER:H	1:D:989:ARG:NH1	2.08	0.51
1:A:947:ILE:O	1:A:954:PRO:HG3	2.10	0.51
1:B:12:CYS:SG	1:B:164:ARG:HG3	2.51	0.51
1:B:604:ARG:HB2	1:B:607:VAL:HG23	1.92	0.51
1:D:795:VAL:HA	1:D:799:THR:HB	1.93	0.51
1:C:572:LYS:N	1:C:572:LYS:HD2	2.26	0.51
1:C:589:THR:HG23	7:C:4006:HOH:O	2.11	0.51
1:A:48:SER:O	1:A:52:LEU:HG	2.11	0.51
1:B:950:VAL:O	1:B:954:PRO:HD2	2.10	0.51
1:C:589:THR:CG2	1:C:590:ASP:N	2.74	0.51
1:C:893:ALA:O	1:C:896:PRO:HD2	2.11	0.51
1:D:340:GLU:HG3	1:D:341:THR:H	1.76	0.51
1:D:947:ILE:O	1:D:954:PRO:HG3	2.10	0.51
1:B:520:GLY:O	1:B:524:ARG:HG3	2.11	0.50
1:B:332:ILE:HD13	1:B:736:ALA:HB2	1.93	0.50
1:C:962:LEU:H	1:C:962:LEU:HD23	1.76	0.50
1:A:339:VAL:HG23	1:A:340:GLU:N	2.26	0.50
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.93	0.50
1:D:757:MET:HA	1:D:760:PHE:CE2	2.47	0.50
1:A:631:THR:HG21	7:A:2517:HOH:O	2.10	0.50
1:B:557:ASP:HB3	1:B:559:LEU:HG	1.93	0.50
1:C:769:VAL:HG21	6:C:1203:TG1:H332	1.94	0.50
1:C:950:VAL:O	1:C:954:PRO:HD2	2.11	0.50
1:D:352:LYS:HE2	7:D:5068:HOH:O	2.11	0.50
1:A:249:LEU:HB3	1:A:340:GLU:OE2	2.12	0.50
1:A:880:HIS:N	1:A:881:PRO:HD2	2.26	0.50
1:B:273:LEU:O	1:B:276:ILE:HG13	2.10	0.50
1:A:25:THR:HA	1:A:132:ALA:HB3	1.93	0.50
1:A:340:GLU:HG3	1:A:341:THR:H	1.77	0.50
1:D:100:ALA:O	1:D:103:ILE:HG22	2.11	0.50
1:D:125:GLU:HG3	1:D:126:MET:N	2.27	0.50
1:D:541:VAL:O	1:D:545:ILE:HG12	2.12	0.50
1:A:212:THR:HG22	1:A:213:ASN:N	2.25	0.50
1:A:757:MET:HA	1:A:760:PHE:CE2	2.47	0.50
1:A:903:VAL:O	1:A:907:ILE:HG13	2.10	0.50
1:A:895:GLU:OE2	1:A:960:LYS:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:MET:CG	1:B:749:GLU:HG2	2.42	0.50
1:B:761:ILE:HG21	1:B:828:LEU:HD13	1.93	0.50
1:D:48:SER:O	1:D:52:LEU:HG	2.12	0.50
1:A:366:MET:CE	1:A:384:ILE:HD11	2.42	0.50
1:B:366:MET:CE	1:B:384:ILE:HD11	2.42	0.50
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.93	0.50
1:D:339:VAL:HG23	1:D:340:GLU:N	2.26	0.50
1:C:326:MET:CG	1:C:749:GLU:HG2	2.42	0.50
1:D:880:HIS:N	1:D:881:PRO:HD2	2.26	0.50
1:B:85:ILE:HG23	1:B:86:THR:HG23	1.94	0.50
1:C:795:VAL:HA	1:C:799:THR:HB	1.93	0.50
1:D:249:LEU:HB3	1:D:340:GLU:OE2	2.12	0.50
1:D:428:ASN:OD1	1:D:431:LYS:HG3	2.12	0.50
1:D:758:LYS:HE3	1:D:762:ARG:NH2	2.27	0.50
1:A:125:GLU:HG3	1:A:126:MET:N	2.27	0.49
1:A:428:ASN:OD1	1:A:431:LYS:HG3	2.12	0.49
1:B:93:VAL:O	1:B:97:ILE:HG13	2.11	0.49
1:C:311:LEU:N	1:C:312:PRO:HD2	2.26	0.49
1:C:332:ILE:HD13	1:C:736:ALA:HB2	1.94	0.49
1:C:520:GLY:O	1:C:524:ARG:HG3	2.12	0.49
1:C:989:ARG:HA	1:C:994:GLY:HA2	1.93	0.49
1:B:289:ILE:O	1:B:293:ILE:HG13	2.13	0.49
1:B:989:ARG:HA	1:B:994:GLY:HA2	1.93	0.49
1:C:557:ASP:HB3	1:C:559:LEU:HG	1.93	0.49
1:D:25:THR:HA	1:D:132:ALA:HB3	1.94	0.49
1:C:739:ASN:OD1	1:C:741:SER:HB2	2.12	0.49
1:D:311:LEU:O	1:D:314:VAL:HG12	2.13	0.49
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.12	0.49
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.94	0.49
1:A:110:ARG:CZ	1:B:85:ILE:HD13	2.42	0.49
1:C:463:SER:OG	1:C:465:VAL:HG22	2.12	0.49
1:D:895:GLU:OE2	1:D:960:LYS:HD3	2.12	0.49
1:A:895:GLU:N	1:A:896:PRO:HD2	2.27	0.49
1:B:836:ARG:O	1:B:840:ILE:HG12	2.12	0.49
1:C:353:THR:HA	1:C:357:THR:OG1	2.13	0.49
1:C:93:VAL:O	1:C:97:ILE:HG13	2.12	0.49
1:B:880:HIS:N	1:B:881:PRO:HD2	2.27	0.49
1:C:880:HIS:N	1:C:881:PRO:HD2	2.27	0.49
1:D:389:TYR:HB3	1:D:425:LEU:HD11	1.95	0.49
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.95	0.49
1:C:604:ARG:HB2	1:C:607:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:LYS:HE3	1:A:762:ARG:NH2	2.28	0.49
1:B:403:ARG:HH11	1:B:403:ARG:HG3	1.77	0.49
1:B:795:VAL:HA	1:B:799:THR:HB	1.94	0.49
1:C:769:VAL:HA	6:C:1203:TG1:H231	1.95	0.49
1:C:85:ILE:HG23	1:C:86:THR:HG23	1.95	0.49
1:D:260:LEU:HD21	1:D:307:ILE:HD13	1.95	0.49
1:A:100:ALA:O	1:A:103:ILE:HG22	2.13	0.49
1:B:534:ARG:HH21	1:B:568:ASP:HB2	1.77	0.49
1:B:865:VAL:HG11	1:B:869:GLN:CB	2.41	0.49
1:C:781:LEU:HD23	1:C:783:LEU:CD1	2.43	0.49
1:D:903:VAL:O	1:D:907:ILE:HG13	2.11	0.49
1:B:134:ARG:HG2	1:B:138:GLN:NE2	2.27	0.49
1:C:85:ILE:HD13	1:D:110:ARG:NH1	2.28	0.49
1:A:311:LEU:O	1:A:314:VAL:HG12	2.13	0.48
1:A:65:LEU:CD1	1:A:307:ILE:HG13	2.41	0.48
1:B:383:SER:O	1:B:384:ILE:HD13	2.12	0.48
1:B:769:VAL:HA	6:B:1103:TG1:H231	1.95	0.48
1:C:761:ILE:HG21	1:C:828:LEU:HD13	1.94	0.48
1:D:560:ARG:HG2	1:D:560:ARG:HH11	1.76	0.48
1:D:56:GLN:OE1	1:D:105:GLY:HA3	2.12	0.48
1:B:311:LEU:N	1:B:312:PRO:HD2	2.27	0.48
1:C:134:ARG:HG2	1:C:138:GLN:NE2	2.27	0.48
1:C:361:MET:HB3	1:C:444:ALA:HB2	1.94	0.48
1:C:800:ASP:C	1:C:803:PRO:HD2	2.33	0.48
1:D:203:ASP:OD1	1:D:678:ARG:NH1	2.46	0.48
1:D:553:GLY:O	1:D:554:THR:HG23	2.12	0.48
1:D:895:GLU:N	1:D:896:PRO:HD2	2.27	0.48
1:A:486:GLU:O	1:A:491:ARG:NH2	2.40	0.48
1:B:463:SER:OG	1:B:465:VAL:HG22	2.13	0.48
1:B:50:TRP:CD1	1:B:54:ILE:HD11	2.48	0.48
1:B:777:LEU:O	1:B:781:LEU:HB2	2.12	0.48
1:C:289:ILE:O	1:C:293:ILE:HG13	2.14	0.48
1:B:402:ILE:HD12	1:B:402:ILE:C	2.33	0.48
1:C:777:LEU:O	1:C:781:LEU:HB2	2.12	0.48
1:C:865:VAL:HG11	1:C:869:GLN:CB	2.41	0.48
1:B:606:GLU:HG3	1:B:739:ASN:OD1	2.14	0.48
1:C:1:MET:HE3	1:C:15:TYR:HB3	1.94	0.48
1:C:383:SER:O	1:C:384:ILE:HD13	2.13	0.48
1:C:718:ILE:HG21	1:C:743:ILE:HD11	1.94	0.48
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.13	0.48
1:B:1:MET:HE3	1:B:15:TYR:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:GLU:CB	1:C:460:ARG:HH21	2.26	0.48
1:C:899:MET:O	1:C:903:VAL:HG23	2.13	0.48
1:D:65:LEU:CD1	1:D:307:ILE:HG13	2.41	0.48
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.77	0.48
1:B:449:VAL:HG22	1:B:472:ASN:ND2	2.29	0.48
1:C:836:ARG:O	1:C:840:ILE:HG12	2.14	0.48
1:D:126:MET:HG3	1:D:139:ARG:HH12	1.77	0.48
1:A:769:VAL:O	1:A:773:VAL:HG23	2.14	0.48
1:A:917:SER:OG	1:A:920:GLN:HB2	2.14	0.48
1:B:600:LEU:O	1:B:602:PRO:HD3	2.14	0.48
1:C:486:GLU:O	1:C:491:ARG:NH2	2.41	0.48
1:C:50:TRP:CD1	1:C:54:ILE:HD11	2.49	0.48
1:A:51:GLU:O	1:A:55:GLU:HG3	2.13	0.48
1:A:203:ASP:OD1	1:A:678:ARG:NH1	2.46	0.48
1:C:403:ARG:HG3	1:C:403:ARG:HH11	1.78	0.48
1:B:589:THR:CG2	1:B:590:ASP:N	2.77	0.48
1:A:886:LEU:HD23	1:A:886:LEU:N	2.29	0.47
1:D:917:SER:OG	1:D:920:GLN:HB2	2.14	0.47
1:A:52:LEU:HD12	1:A:53:VAL:N	2.29	0.47
1:B:190:HIS:O	1:B:206:ASN:HA	2.14	0.47
1:B:353:THR:HA	1:B:357:THR:OG1	2.15	0.47
1:B:758:LYS:HG3	1:B:828:LEU:HD22	1.95	0.47
1:C:914:ASN:ND2	1:C:922:LEU:HD11	2.30	0.47
1:D:52:LEU:HD12	1:D:53:VAL:N	2.29	0.47
1:D:893:ALA:HB1	1:D:895:GLU:OE1	2.13	0.47
1:A:239:MET:CE	1:A:708:ALA:HB1	2.44	0.47
1:A:259:GLN:O	1:A:263:VAL:HG23	2.14	0.47
1:A:59:ASP:O	1:A:62:VAL:HG22	2.14	0.47
1:B:800:ASP:C	1:B:803:PRO:HD2	2.34	0.47
1:B:899:MET:O	1:B:903:VAL:HG23	2.14	0.47
1:B:914:ASN:ND2	1:B:922:LEU:HD11	2.30	0.47
1:D:624:ILE:CG2	1:D:684:LYS:HG2	2.44	0.47
1:A:678:ARG:HB3	7:A:2069:HOH:O	2.13	0.47
1:B:366:MET:HE2	1:B:384:ILE:HD11	1.95	0.47
1:B:486:GLU:O	1:B:491:ARG:NH2	2.41	0.47
1:B:547:SER:O	1:B:551:GLU:HG3	2.15	0.47
1:D:800:ASP:C	1:D:803:PRO:HD2	2.34	0.47
1:B:458:GLU:CB	1:B:460:ARG:HH21	2.27	0.47
1:B:781:LEU:HD23	1:B:783:LEU:CD1	2.44	0.47
1:C:449:VAL:HG22	1:C:472:ASN:ND2	2.29	0.47
1:D:51:GLU:O	1:D:55:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:VAL:O	1:D:611:ILE:HG12	2.15	0.47
1:D:836:ARG:NH2	1:D:985:LYS:HE2	2.29	0.47
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.96	0.47
1:A:926:PRO:O	1:A:929:VAL:HG23	2.15	0.47
1:B:242:THR:HB	1:B:243:GLU:H	1.54	0.47
1:B:361:MET:HB3	1:B:444:ALA:HB2	1.95	0.47
1:B:494:MET:HE1	7:B:3036:HOH:O	2.13	0.47
1:C:97:ILE:HD13	1:C:797:LEU:HD11	1.97	0.47
1:D:259:GLN:O	1:D:263:VAL:HG23	2.15	0.47
1:D:769:VAL:O	1:D:773:VAL:HG23	2.15	0.47
1:A:100:ALA:O	1:A:104:VAL:HG23	2.14	0.47
1:A:607:VAL:O	1:A:611:ILE:HG12	2.15	0.47
1:B:97:ILE:HD13	1:B:797:LEU:HD11	1.97	0.47
1:C:310:GLY:O	1:C:314:VAL:HG23	2.15	0.47
1:D:687:ILE:O	1:D:691:LEU:HD22	2.14	0.47
1:D:933:LEU:O	1:D:936:SER:HB3	2.15	0.47
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.44	0.47
1:B:50:TRP:O	1:B:54:ILE:HG13	2.15	0.47
1:B:811:PRO:HG3	1:B:929:VAL:CG1	2.45	0.47
1:C:366:MET:HE2	1:C:384:ILE:HD11	1.95	0.47
1:C:758:LYS:HG3	1:C:828:LEU:HD22	1.96	0.47
1:D:100:ALA:O	1:D:104:VAL:HG23	2.15	0.47
1:D:679:VAL:HG13	1:D:683:HIS:CB	2.33	0.47
1:B:589:THR:HG23	7:B:3006:HOH:O	2.15	0.47
1:B:836:ARG:NH2	1:B:985:LYS:HE2	2.28	0.47
1:D:486:GLU:O	1:D:491:ARG:NH2	2.41	0.47
1:D:631:THR:HG21	7:D:5517:HOH:O	2.13	0.47
1:D:962:LEU:HB3	1:D:966:GLN:CB	2.44	0.47
1:B:667:ARG:HG2	1:B:694:TYR:CE1	2.49	0.47
1:C:534:ARG:HH21	1:C:568:ASP:HB2	1.79	0.47
1:C:781:LEU:HD23	1:C:783:LEU:HD11	1.96	0.47
1:D:624:ILE:HG21	1:D:684:LYS:HG2	1.97	0.47
1:D:799:THR:HG21	1:D:905:VAL:HG22	1.97	0.47
1:A:553:GLY:O	1:A:554:THR:HG22	2.14	0.46
1:A:836:ARG:NH2	1:A:985:LYS:HE2	2.29	0.46
1:B:865:VAL:HG12	1:B:867:TYR:H	1.81	0.46
1:D:59:ASP:O	1:D:62:VAL:HG22	2.15	0.46
1:D:239:MET:CE	1:D:708:ALA:HB1	2.45	0.46
1:A:933:LEU:O	1:A:936:SER:HB3	2.16	0.46
1:B:305:ALA:HB2	1:B:792:LEU:HD13	1.97	0.46
1:B:966:GLN:O	1:B:969:MET:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:VAL:O	1:C:545:ILE:HG12	2.16	0.46
1:C:683:HIS:O	1:C:687:ILE:HG13	2.15	0.46
1:C:811:PRO:HG3	1:C:929:VAL:CG1	2.46	0.46
1:C:865:VAL:HG12	1:C:867:TYR:H	1.81	0.46
1:C:947:ILE:HD11	1:C:957:PHE:CD2	2.50	0.46
1:A:126:MET:HG3	1:A:139:ARG:HH12	1.79	0.46
1:A:370:ASP:HB3	1:A:378:SER:OG	2.15	0.46
1:D:836:ARG:O	1:D:840:ILE:HG12	2.15	0.46
1:A:200:VAL:CG1	1:A:201:ASN:N	2.78	0.46
1:B:865:VAL:CG1	1:B:869:GLN:HB2	2.41	0.46
1:B:96:LEU:HD23	1:B:96:LEU:O	2.15	0.46
1:C:606:GLU:HG3	1:C:739:ASN:OD1	2.16	0.46
1:C:926:PRO:HA	1:C:927:PRO:HD3	1.86	0.46
1:A:701:THR:HA	1:A:718:ILE:O	2.15	0.46
1:A:800:ASP:C	1:A:803:PRO:HD2	2.35	0.46
1:A:829:ILE:HD12	1:A:837:TYR:CD1	2.50	0.46
1:A:836:ARG:O	1:A:840:ILE:HG12	2.15	0.46
1:B:344:CYS:SG	1:B:697:ILE:HG13	2.55	0.46
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.86	0.46
1:C:667:ARG:HG2	1:C:694:TYR:CE1	2.50	0.46
1:C:966:GLN:O	1:C:969:MET:HB3	2.15	0.46
1:D:886:LEU:N	1:D:886:LEU:HD23	2.31	0.46
1:A:352:LYS:HE2	7:A:2068:HOH:O	2.16	0.46
1:B:52:LEU:O	1:B:56:GLN:HG2	2.16	0.46
1:B:71:ILE:O	1:B:75:LEU:HD13	2.16	0.46
1:B:947:ILE:HD11	1:B:957:PHE:CD2	2.51	0.46
1:C:965:THR:HA	1:C:968:LEU:HD12	1.97	0.46
1:A:110:ARG:NH1	1:B:85:ILE:HD13	2.31	0.46
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.97	0.46
1:B:337:PRO:O	1:B:340:GLU:HG3	2.16	0.46
1:B:450:GLU:OE1	1:B:467:ARG:NH2	2.47	0.46
1:C:494:MET:CE	5:C:1202:ADP:HN62	2.27	0.46
1:C:52:LEU:O	1:C:56:GLN:HG2	2.16	0.46
1:C:547:SER:O	1:C:551:GLU:HG3	2.16	0.46
1:C:71:ILE:O	1:C:75:LEU:HD13	2.16	0.46
1:D:974:SER:C	1:D:976:PRO:HD2	2.36	0.46
1:A:974:SER:C	1:A:976:PRO:HD2	2.36	0.46
1:B:310:GLY:O	1:B:314:VAL:HG23	2.16	0.46
1:B:893:ALA:HB1	1:B:895:GLU:OE1	2.16	0.46
1:B:810:ASN:HA	1:B:930:ASN:ND2	2.29	0.46
1:C:810:ASN:HA	1:C:930:ASN:ND2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:O	1:A:290:ARG:HD2	2.16	0.46
1:C:332:ILE:CD1	1:C:736:ALA:HB2	2.45	0.46
1:C:865:VAL:CG1	1:C:869:GLN:HB2	2.42	0.46
1:D:448:LEU:HG	1:D:452:MET:HE2	1.97	0.46
1:C:337:PRO:O	1:C:340:GLU:HG3	2.16	0.46
1:D:950:VAL:HB	1:D:953:LEU:HD12	1.97	0.46
1:D:971:LEU:O	1:D:975:LEU:HB2	2.17	0.46
1:B:541:VAL:O	1:B:545:ILE:HG12	2.16	0.45
1:C:50:TRP:O	1:C:54:ILE:HG13	2.17	0.45
1:C:600:LEU:O	1:C:602:PRO:HD3	2.16	0.45
1:C:757:MET:O	1:C:761:ILE:HG13	2.16	0.45
1:C:967:TRP:O	1:C:971:LEU:HG	2.17	0.45
1:D:289:ILE:O	1:D:290:ARG:HD2	2.16	0.45
1:D:518:PRO:HB3	1:D:549:ILE:HD13	1.98	0.45
1:D:862:GLY:N	1:D:863:PRO:HD3	2.30	0.45
1:D:919:ASN:O	1:D:989:ARG:HD3	2.16	0.45
1:A:200:VAL:HG13	1:A:680:GLU:CG	2.45	0.45
1:A:919:ASN:O	1:A:989:ARG:HD3	2.15	0.45
1:B:965:THR:HA	1:B:968:LEU:HD12	1.97	0.45
1:C:443:THR:O	1:C:447:THR:HG23	2.16	0.45
1:D:495:SER:HB3	1:D:514:VAL:HG22	1.97	0.45
1:A:200:VAL:HG12	1:A:202:GLN:HE21	1.81	0.45
1:A:971:LEU:O	1:A:975:LEU:HB2	2.17	0.45
1:C:97:ILE:CD1	1:C:797:LEU:HD11	2.46	0.45
1:D:59:ASP:HB3	1:D:62:VAL:HG22	1.98	0.45
1:D:913:LEU:HD22	1:D:927:PRO:HB3	1.97	0.45
1:A:352:LYS:HA	1:A:356:LEU:HB2	1.98	0.45
1:B:768:ASN:O	1:B:772:VAL:HG23	2.16	0.45
1:C:116:ILE:HD12	1:C:236:ARG:HG2	1.99	0.45
1:C:836:ARG:NH2	1:C:985:LYS:HE2	2.30	0.45
1:C:96:LEU:HD23	1:C:96:LEU:O	2.16	0.45
1:D:926:PRO:O	1:D:929:VAL:HG23	2.17	0.45
1:A:796:ASN:HA	7:A:2131:HOH:O	2.15	0.45
1:A:899:MET:O	1:A:903:VAL:HG23	2.16	0.45
1:B:449:VAL:HG21	1:B:472:ASN:CG	2.36	0.45
1:B:683:HIS:O	1:B:687:ILE:HG13	2.16	0.45
1:B:886:LEU:HD23	1:B:886:LEU:N	2.31	0.45
1:C:320:ALA:O	1:C:324:ARG:HG3	2.15	0.45
1:C:811:PRO:HG3	1:C:929:VAL:HG12	1.99	0.45
1:D:701:THR:HA	1:D:718:ILE:O	2.15	0.45
1:D:893:ALA:O	1:D:896:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:O	1:A:273:LEU:HG	2.17	0.45
1:A:862:GLY:N	1:A:863:PRO:HD3	2.31	0.45
1:B:116:ILE:HD12	1:B:236:ARG:HG2	1.99	0.45
1:B:781:LEU:HD23	1:B:783:LEU:HD11	1.97	0.45
1:B:811:PRO:HG3	1:B:929:VAL:HG12	1.99	0.45
1:B:967:TRP:O	1:B:971:LEU:HG	2.17	0.45
1:C:893:ALA:HB1	1:C:895:GLU:OE1	2.17	0.45
1:D:829:ILE:HD12	1:D:837:TYR:CD1	2.51	0.45
1:A:88:PHE:C	1:A:91:PRO:HD2	2.37	0.45
1:B:329:LYS:O	1:B:330:ASN:HB2	2.16	0.45
1:B:494:MET:CE	7:B:3036:HOH:O	2.64	0.45
1:B:555:GLY:C	1:B:557:ASP:H	2.20	0.45
1:C:305:ALA:HB2	1:C:792:LEU:HD13	1.98	0.45
1:C:971:LEU:HA	1:C:975:LEU:HD23	1.99	0.45
1:D:914:ASN:HB3	1:D:981:ASP:OD2	2.17	0.45
1:C:423:SER:HB3	1:C:437:VAL:O	2.17	0.45
1:D:228:VAL:O	1:D:228:VAL:HG12	2.16	0.45
1:D:768:ASN:O	1:D:772:VAL:HG23	2.16	0.45
1:D:950:VAL:HG12	1:D:952:PRO:HG2	1.99	0.45
1:A:360:GLN:HG2	1:A:389:TYR:CE2	2.52	0.45
1:A:414:ALA:HB2	1:A:452:MET:HE3	1.99	0.45
1:A:893:ALA:O	1:A:896:PRO:HD2	2.17	0.45
1:A:950:VAL:HG12	1:A:952:PRO:HG2	1.99	0.45
1:B:971:LEU:HA	1:B:975:LEU:HD23	1.99	0.45
1:C:190:HIS:O	1:C:206:ASN:HA	2.17	0.45
1:C:768:ASN:O	1:C:772:VAL:HG23	2.16	0.45
1:D:155:VAL:HG22	1:D:217:GLY:H	1.81	0.45
1:D:402:ILE:C	1:D:402:ILE:HD12	2.36	0.45
1:D:899:MET:O	1:D:903:VAL:HG23	2.17	0.45
1:D:943:LEU:O	1:D:947:ILE:HG13	2.16	0.45
1:D:954:PRO:HB3	1:D:959:LEU:O	2.17	0.45
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.99	0.45
1:A:950:VAL:HB	1:A:953:LEU:HD12	1.98	0.45
1:B:256:PHE:CE1	1:B:765:ILE:HD11	2.52	0.45
1:B:767:SER:O	1:B:771:GLU:HG3	2.16	0.45
1:C:352:LYS:HE2	7:C:4068:HOH:O	2.16	0.45
1:C:402:ILE:C	1:C:402:ILE:HD12	2.36	0.45
1:C:59:ASP:OD2	1:C:62:VAL:HG23	2.16	0.45
1:C:835:PHE:O	1:C:838:MET:HB3	2.17	0.45
1:D:65:LEU:HD11	1:D:307:ILE:HG21	1.99	0.45
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.98	0.44
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.17	0.44
1:B:97:ILE:CD1	1:B:797:LEU:HD11	2.47	0.44
1:C:177:GLN:NE2	1:C:189:LYS:NZ	2.65	0.44
1:C:701:THR:HA	1:C:718:ILE:O	2.17	0.44
1:D:814:LEU:N	1:D:814:LEU:HD12	2.32	0.44
1:A:303:ALA:O	1:A:307:ILE:HG12	2.17	0.44
1:D:186:SER:HB3	7:D:5524:HOH:O	2.17	0.44
1:A:954:PRO:HB3	1:A:959:LEU:O	2.17	0.44
1:C:555:GLY:C	1:C:557:ASP:H	2.21	0.44
1:C:947:ILE:HD11	1:C:957:PHE:CG	2.52	0.44
1:D:88:PHE:C	1:D:91:PRO:HD2	2.37	0.44
1:A:402:ILE:HD12	1:A:402:ILE:C	2.37	0.44
1:A:481:LYS:HG3	1:A:496:VAL:HB	1.99	0.44
1:B:116:ILE:O	1:B:120:LYS:HG3	2.18	0.44
1:B:701:THR:HA	1:B:718:ILE:O	2.17	0.44
1:C:329:LYS:O	1:C:330:ASN:HB2	2.17	0.44
1:C:886:LEU:HD23	1:C:886:LEU:N	2.33	0.44
1:D:360:GLN:HG2	1:D:389:TYR:CE2	2.52	0.44
1:A:228:VAL:HG12	1:A:228:VAL:O	2.17	0.44
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.35	0.44
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.99	0.44
1:B:332:ILE:CD1	1:B:736:ALA:HB2	2.47	0.44
1:B:947:ILE:HD11	1:B:957:PHE:CG	2.53	0.44
1:C:116:ILE:O	1:C:120:LYS:HG3	2.18	0.44
1:C:187:VAL:CG2	1:C:189:LYS:HE2	2.47	0.44
1:C:788:ILE:HG12	1:C:791:GLN:OE1	2.17	0.44
1:C:856:PHE:CZ	1:C:891:PHE:HA	2.53	0.44
1:C:914:ASN:HD22	1:C:914:ASN:HA	1.56	0.44
1:D:366:MET:HE2	1:D:384:ILE:HD11	1.98	0.44
1:D:783:LEU:HB3	1:D:784:PRO:HD2	1.98	0.44
1:D:984:LEU:HD23	1:D:987:ILE:HD12	1.99	0.44
1:A:12:CYS:SG	1:A:164:ARG:HG3	2.57	0.44
1:A:65:LEU:HD11	1:A:307:ILE:HG21	1.99	0.44
1:A:336:LEU:N	1:A:337:PRO:HD2	2.33	0.44
1:A:69:ALA:HB2	1:A:94:ILE:HG21	2.00	0.44
1:B:59:ASP:OD2	1:B:62:VAL:HG23	2.17	0.44
1:B:856:PHE:CZ	1:B:891:PHE:HA	2.53	0.44
1:C:89:VAL:O	1:C:93:VAL:HG23	2.18	0.44
1:D:269:VAL:O	1:D:273:LEU:HG	2.18	0.44
1:D:855:TRP:HA	1:D:859:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:LEU:O	1:A:947:ILE:HG13	2.17	0.44
1:B:119:LEU:HD22	1:B:239:MET:HE3	1.98	0.44
1:B:835:PHE:O	1:B:838:MET:HB3	2.18	0.44
1:B:974:SER:C	1:B:976:PRO:HD2	2.37	0.44
1:C:344:CYS:SG	1:C:697:ILE:HG13	2.58	0.44
1:C:450:GLU:OE1	1:C:467:ARG:NH2	2.49	0.44
1:C:646:GLU:OE2	1:C:651:ARG:NH1	2.51	0.44
1:A:984:LEU:HD23	1:A:987:ILE:HD12	1.99	0.44
1:B:896:PRO:O	1:B:899:MET:HB2	2.18	0.44
1:C:758:LYS:NZ	1:C:828:LEU:HD23	2.33	0.44
1:C:767:SER:O	1:C:771:GLU:HG3	2.17	0.44
1:C:921:SER:HB2	1:C:989:ARG:NH2	2.14	0.44
1:D:370:ASP:HB3	1:D:378:SER:OG	2.18	0.44
1:D:573:ARG:HG3	1:D:573:ARG:HH21	1.83	0.44
1:D:678:ARG:HB3	7:D:5069:HOH:O	2.17	0.44
1:A:814:LEU:N	1:A:814:LEU:HD12	2.33	0.44
1:A:922:LEU:N	1:A:922:LEU:HD12	2.33	0.44
1:C:978:ILE:O	1:C:982:GLU:HB2	2.18	0.44
1:D:69:ALA:HB2	1:D:94:ILE:HG21	2.00	0.44
1:A:491:ARG:HG2	1:A:493:SER:OG	2.17	0.43
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.83	0.43
1:B:320:ALA:O	1:B:324:ARG:HG3	2.17	0.43
1:D:796:ASN:HA	7:D:5131:HOH:O	2.16	0.43
1:A:768:ASN:O	1:A:772:VAL:HG23	2.18	0.43
1:B:454:VAL:HG22	7:B:3034:HOH:O	2.17	0.43
1:D:214:ILE:HD12	1:D:214:ILE:N	2.33	0.43
1:D:200:VAL:HG13	1:D:680:GLU:CG	2.48	0.43
1:A:687:ILE:O	1:A:691:LEU:HD22	2.18	0.43
1:A:855:TRP:HA	1:A:859:ALA:HB2	2.00	0.43
1:B:149:ASP:HB2	7:B:3093:HOH:O	2.19	0.43
1:B:389:TYR:HB3	1:B:425:LEU:HD11	2.00	0.43
1:B:452:MET:O	1:B:453:ASN:C	2.57	0.43
1:D:303:ALA:O	1:D:307:ILE:HG12	2.18	0.43
1:D:862:GLY:H	1:D:863:PRO:HD3	1.83	0.43
1:A:553:GLY:C	1:A:554:THR:CG2	2.85	0.43
1:A:862:GLY:H	1:A:863:PRO:HD3	1.83	0.43
1:B:443:THR:O	1:B:447:THR:HG23	2.18	0.43
1:B:80:GLU:CG	1:B:82:GLU:HG2	2.45	0.43
1:B:921:SER:HB2	1:B:989:ARG:NH2	2.14	0.43
1:C:129:VAL:HG12	1:C:151:VAL:HG22	1.98	0.43
1:C:256:PHE:CE1	1:C:765:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:953:LEU:N	1:C:954:PRO:HD2	2.33	0.43
1:C:974:SER:C	1:C:976:PRO:HD2	2.38	0.43
1:D:336:LEU:N	1:D:337:PRO:HD2	2.34	0.43
1:B:423:SER:HB3	1:B:437:VAL:O	2.19	0.43
1:B:465:VAL:HG23	1:B:466:GLU:N	2.33	0.43
1:C:80:GLU:CG	1:C:82:GLU:HG2	2.45	0.43
1:B:549:ILE:HD11	1:B:596:VAL:HG21	2.00	0.43
1:B:914:ASN:HD22	1:B:914:ASN:HA	1.57	0.43
1:B:919:ASN:HD22	1:B:988:ALA:HB3	1.83	0.43
1:C:454:VAL:HG22	7:C:4034:HOH:O	2.18	0.43
1:D:481:LYS:HG3	1:D:496:VAL:HB	2.01	0.43
1:A:20:GLU:HB3	7:A:2516:HOH:O	2.18	0.43
1:A:930:ASN:OD1	1:A:932:TRP:HB2	2.19	0.43
1:B:352:LYS:HE2	7:B:3068:HOH:O	2.17	0.43
1:C:149:ASP:HB2	7:C:4093:HOH:O	2.19	0.43
1:D:760:PHE:C	1:D:760:PHE:CD1	2.92	0.43
1:A:283:VAL:HG22	1:A:286:GLY:H	1.84	0.43
1:B:903:VAL:HG22	1:B:970:VAL:HG13	2.01	0.43
1:D:12:CYS:SG	1:D:164:ARG:HG3	2.58	0.43
1:D:926:PRO:HA	1:D:927:PRO:HD3	1.83	0.43
1:A:280:ASN:N	1:A:280:ASN:HD22	2.16	0.43
1:A:459:VAL:HB	1:A:467:ARG:HD3	2.00	0.43
1:A:831:GLY:O	1:A:834:PHE:HB3	2.19	0.43
1:B:953:LEU:N	1:B:954:PRO:HD2	2.33	0.43
1:D:200:VAL:CG1	1:D:201:ASN:N	2.82	0.43
1:D:352:LYS:HA	1:D:356:LEU:HB2	2.00	0.43
1:D:606:GLU:H	1:D:606:GLU:CD	2.22	0.43
1:D:930:ASN:OD1	1:D:932:TRP:HB2	2.19	0.43
1:A:600:LEU:O	1:A:602:PRO:HD3	2.19	0.43
1:B:332:ILE:N	1:B:332:ILE:CD1	2.82	0.43
1:B:978:ILE:O	1:B:982:GLU:HB2	2.19	0.43
1:C:788:ILE:HB	1:C:789:PRO:HD2	2.01	0.43
1:C:919:ASN:HD22	1:C:988:ALA:HB3	1.83	0.43
1:D:21:THR:HG22	1:D:21:THR:O	2.17	0.43
1:D:831:GLY:O	1:D:834:PHE:HB3	2.19	0.43
1:B:104:VAL:O	1:B:108:GLN:HG3	2.19	0.42
1:B:449:VAL:HG21	1:B:472:ASN:OD1	2.19	0.42
1:B:788:ILE:HB	1:B:789:PRO:HD2	2.01	0.42
1:B:788:ILE:HG12	1:B:791:GLN:OE1	2.19	0.42
1:C:389:TYR:HB3	1:C:425:LEU:HD11	2.00	0.42
1:C:758:LYS:HE3	1:C:762:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:THR:HA	1:D:677:ALA:O	2.18	0.42
1:A:336:LEU:O	1:A:339:VAL:HG22	2.19	0.42
1:A:452:MET:O	1:A:453:ASN:C	2.58	0.42
1:A:459:VAL:HB	1:A:467:ARG:CD	2.49	0.42
1:A:558:THR:O	1:A:558:THR:HG22	2.18	0.42
1:C:896:PRO:O	1:C:899:MET:HB2	2.19	0.42
1:C:903:VAL:HG22	1:C:970:VAL:HG13	2.01	0.42
1:D:922:LEU:HD12	1:D:922:LEU:N	2.34	0.42
1:A:18:VAL:HG12	1:A:24:LEU:HD23	2.02	0.42
1:B:473:SER:HA	1:B:476:ARG:NH1	2.34	0.42
1:B:757:MET:O	1:B:761:ILE:HG13	2.19	0.42
1:B:89:VAL:O	1:B:93:VAL:HG23	2.19	0.42
1:C:104:VAL:O	1:C:108:GLN:HG3	2.19	0.42
1:C:765:ILE:O	1:C:769:VAL:HG23	2.19	0.42
1:D:280:ASN:HD22	1:D:280:ASN:N	2.16	0.42
1:D:558:THR:O	1:D:558:THR:HG22	2.18	0.42
1:A:179:ILE:O	1:A:705:VAL:HG22	2.18	0.42
1:A:840:ILE:O	1:A:844:VAL:HG23	2.19	0.42
1:B:266:LEU:HD13	1:B:266:LEU:O	2.20	0.42
1:B:372:VAL:HG22	1:B:377:CYS:HB2	2.01	0.42
1:B:765:ILE:O	1:B:769:VAL:HG23	2.19	0.42
1:C:119:LEU:HD22	1:C:239:MET:HE3	2.00	0.42
1:D:209:PHE:O	1:D:212:THR:HB	2.20	0.42
1:D:414:ALA:HB2	1:D:452:MET:HE3	2.00	0.42
1:A:185:VAL:O	1:A:185:VAL:HG13	2.19	0.42
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.86	0.42
1:A:951:ASP:O	1:A:954:PRO:HD2	2.18	0.42
1:B:646:GLU:OE2	1:B:651:ARG:NH1	2.52	0.42
1:D:283:VAL:HG22	1:D:286:GLY:H	1.85	0.42
1:D:717:GLY:O	1:D:731:SER:HB3	2.19	0.42
1:B:542:LYS:HD2	7:B:3003:HOH:O	2.19	0.42
1:C:449:VAL:HG21	1:C:472:ASN:CG	2.40	0.42
1:D:459:VAL:HB	1:D:467:ARG:CD	2.49	0.42
1:B:862:GLY:N	1:B:863:PRO:HD3	2.35	0.42
1:C:325:ARG:NH1	1:C:753:ILE:HD11	2.35	0.42
1:D:336:LEU:O	1:D:339:VAL:HG22	2.20	0.42
1:D:765:ILE:O	1:D:769:VAL:HG23	2.20	0.42
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.34	0.42
1:A:604:ARG:HB2	1:A:607:VAL:HG23	2.02	0.42
1:A:606:GLU:H	1:A:606:GLU:CD	2.23	0.42
1:B:40:GLU:CD	1:B:143:ARG:HE	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:CG2	1:B:189:LYS:HE2	2.50	0.42
1:B:501:ALA:C	1:B:503:SER:H	2.23	0.42
1:D:448:LEU:HG	1:D:452:MET:CE	2.50	0.42
1:D:452:MET:O	1:D:453:ASN:C	2.58	0.42
1:A:760:PHE:C	1:A:760:PHE:CD1	2.93	0.42
1:B:758:LYS:NZ	1:B:828:LEU:HD23	2.35	0.42
1:C:654:THR:HA	1:C:677:ALA:O	2.20	0.42
1:C:862:GLY:N	1:C:863:PRO:HD3	2.35	0.42
1:D:459:VAL:HB	1:D:467:ARG:HD3	2.01	0.42
1:A:200:VAL:HG12	1:A:202:GLN:NE2	2.34	0.42
1:A:209:PHE:O	1:A:212:THR:HB	2.20	0.42
1:A:214:ILE:HD12	1:A:214:ILE:N	2.35	0.42
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.20	0.42
1:A:765:ILE:O	1:A:769:VAL:HG23	2.20	0.42
1:C:473:SER:HA	1:C:476:ARG:HH11	1.85	0.42
1:C:876:CYS:SG	1:C:884:GLU:OE1	2.78	0.42
1:D:239:MET:SD	1:D:708:ALA:HB1	2.60	0.42
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.97	0.41
1:B:473:SER:HA	1:B:476:ARG:HH11	1.85	0.41
1:C:452:MET:O	1:C:453:ASN:C	2.58	0.41
1:C:465:VAL:HG23	1:C:466:GLU:N	2.35	0.41
1:C:75:LEU:HD23	1:C:297:LYS:HD2	2.01	0.41
1:D:18:VAL:HG12	1:D:24:LEU:HD23	2.02	0.41
1:D:179:ILE:O	1:D:705:VAL:HG22	2.19	0.41
1:B:325:ARG:NH1	1:B:753:ILE:HD11	2.36	0.41
1:C:720:MET:HE1	1:C:738:ASP:O	2.20	0.41
1:C:905:VAL:O	1:C:909:MET:HG2	2.19	0.41
1:D:185:VAL:HG13	1:D:185:VAL:O	2.20	0.41
1:D:212:THR:CG2	1:D:213:ASN:N	2.82	0.41
1:D:428:ASN:CG	1:D:431:LYS:HG3	2.41	0.41
1:D:491:ARG:HG2	1:D:493:SER:OG	2.19	0.41
1:D:865:VAL:C	1:D:867:TYR:H	2.24	0.41
1:A:206:ASN:HD22	1:A:206:ASN:H	1.68	0.41
1:A:428:ASN:CG	1:A:431:LYS:HG3	2.41	0.41
1:A:239:MET:SD	1:A:708:ALA:HB1	2.60	0.41
1:C:574:GLU:H	1:C:574:GLU:CD	2.24	0.41
1:D:412:GLU:OE2	1:D:566:THR:CG2	2.66	0.41
1:D:604:ARG:HB2	1:D:607:VAL:HG23	2.03	0.41
1:D:893:ALA:HA	1:D:894:PRO:HD3	1.86	0.41
1:A:624:ILE:HD13	1:A:687:ILE:CD1	2.51	0.41
1:B:574:GLU:CD	1:B:574:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LYS:HE3	1:B:762:ARG:NH2	2.35	0.41
1:C:501:ALA:C	1:C:503:SER:H	2.23	0.41
1:C:983:ILE:O	1:C:987:ILE:HG13	2.19	0.41
1:C:100:ALA:O	1:C:104:VAL:HG23	2.20	0.41
1:C:473:SER:HA	1:C:476:ARG:NH1	2.35	0.41
1:D:840:ILE:O	1:D:844:VAL:HG23	2.20	0.41
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.48	0.41
1:A:865:VAL:C	1:A:867:TYR:H	2.24	0.41
1:A:924:ARG:HE	1:A:924:ARG:HA	1.86	0.41
1:C:40:GLU:CD	1:C:143:ARG:HE	2.22	0.41
1:C:975:LEU:N	1:C:976:PRO:CD	2.82	0.41
1:D:795:VAL:HA	1:D:799:THR:CB	2.49	0.41
1:D:843:TYR:OH	1:D:976:PRO:HG2	2.20	0.41
1:A:941:MET:O	1:A:944:HIS:HB3	2.20	0.41
1:B:65:LEU:HG	1:B:94:ILE:HD11	2.03	0.41
1:B:922:LEU:HD12	1:B:922:LEU:N	2.36	0.41
1:B:90:GLU:O	1:B:94:ILE:HG22	2.21	0.41
1:C:23:GLY:HA3	1:C:130:TYR:O	2.20	0.41
1:C:656:ARG:HA	1:C:656:ARG:HD3	1.92	0.41
1:D:198:ARG:HE	1:D:656:ARG:HH22	1.69	0.41
1:B:491:ARG:NH1	1:B:588:GLU:OE1	2.54	0.41
1:B:975:LEU:N	1:B:976:PRO:CD	2.82	0.41
1:D:198:ARG:HE	1:D:656:ARG:NH2	2.18	0.41
1:D:255:GLU:O	1:D:258:GLU:HB2	2.20	0.41
1:D:366:MET:HA	1:D:596:VAL:O	2.21	0.41
1:B:102:ALA:O	1:B:106:VAL:HG23	2.21	0.41
1:B:166:LEU:HD11	1:B:222:ILE:HB	2.02	0.41
1:B:876:CYS:SG	1:B:884:GLU:OE1	2.79	0.41
1:B:983:ILE:O	1:B:987:ILE:HG13	2.20	0.41
1:D:567:ARG:HD2	1:D:570:PRO:CA	2.48	0.41
1:D:491:ARG:NH1	1:D:588:GLU:OE1	2.54	0.41
1:D:941:MET:O	1:D:944:HIS:HB3	2.20	0.41
1:D:951:ASP:O	1:D:954:PRO:HD2	2.20	0.41
1:B:322:GLY:O	1:B:326:MET:HG3	2.20	0.41
1:B:656:ARG:HA	1:B:656:ARG:HD3	1.92	0.41
1:B:654:THR:HA	1:B:677:ALA:O	2.21	0.41
1:C:491:ARG:NH1	1:C:588:GLU:OE1	2.54	0.41
1:D:446:THR:HG23	1:D:472:ASN:ND2	2.35	0.41
1:D:924:ARG:HE	1:D:924:ARG:HA	1.86	0.41
1:A:198:ARG:HE	1:A:656:ARG:NH2	2.19	0.41
1:A:325:ARG:O	1:A:328:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:VAL:HA	1:A:799:THR:CB	2.50	0.41
1:B:90:GLU:HB2	1:B:790:VAL:HG22	2.03	0.41
1:C:962:LEU:HB2	1:C:966:GLN:HB2	2.02	0.41
1:A:654:THR:HA	1:A:677:ALA:O	2.21	0.40
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.20	0.40
1:C:922:LEU:HD12	1:C:922:LEU:N	2.36	0.40
1:A:255:GLU:O	1:A:258:GLU:HB2	2.21	0.40
1:A:366:MET:HA	1:A:596:VAL:O	2.21	0.40
1:B:8:SER:OG	1:B:11:GLU:HG3	2.22	0.40
1:B:179:ILE:O	1:B:705:VAL:HG22	2.21	0.40
1:B:905:VAL:O	1:B:909:MET:HG2	2.20	0.40
1:B:910:CYS:HB3	1:B:978:ILE:CG1	2.51	0.40
1:B:962:LEU:HB2	1:B:966:GLN:HB2	2.02	0.40
1:C:102:ALA:O	1:C:106:VAL:HG23	2.22	0.40
1:C:100:ALA:O	1:C:103:ILE:HG22	2.21	0.40
1:C:266:LEU:HD13	1:C:266:LEU:O	2.21	0.40
1:C:777:LEU:HD12	1:C:845:GLY:O	2.21	0.40
1:C:962:LEU:HG	1:C:967:TRP:NE1	2.36	0.40
1:D:77:TRP:C	1:D:79:GLU:H	2.25	0.40
1:A:448:LEU:HG	1:A:452:MET:CE	2.50	0.40
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.52	0.40
1:B:100:ALA:O	1:B:104:VAL:HG23	2.21	0.40
1:B:449:VAL:CG2	1:B:472:ASN:CG	2.89	0.40
1:B:777:LEU:HD12	1:B:845:GLY:O	2.21	0.40
1:B:962:LEU:HG	1:B:967:TRP:NE1	2.36	0.40
1:C:389:TYR:HA	1:C:447:THR:HG21	2.03	0.40
1:C:90:GLU:O	1:C:94:ILE:HG22	2.22	0.40
1:D:20:GLU:HB3	7:D:5516:HOH:O	2.20	0.40
1:D:485:LEU:HD22	1:D:584:PHE:CE2	2.56	0.40
1:D:600:LEU:O	1:D:602:PRO:HD3	2.22	0.40
1:D:83:GLU:C	1:D:85:ILE:H	2.24	0.40
1:D:971:LEU:HA	1:D:975:LEU:HD23	2.02	0.40
1:A:367:PHE:C	1:A:367:PHE:CD2	2.95	0.40
1:A:858:TYR:N	1:A:858:TYR:CD1	2.89	0.40
1:A:971:LEU:HA	1:A:975:LEU:HD23	2.02	0.40
1:B:720:MET:HE1	1:B:738:ASP:O	2.21	0.40
1:C:39:ASN:OD1	1:C:226:THR:HB	2.21	0.40
1:D:263:VAL:O	1:D:267:ILE:HG13	2.21	0.40
1:D:771:GLU:O	1:D:775:ILE:HG12	2.22	0.40
1:A:950:VAL:C	1:A:952:PRO:HD2	2.41	0.40
1:D:670:CYS:HB3	1:D:691:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:950:VAL:C	1:D:952:PRO:HD2	2.41	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	992/994 (100%)	932 (94%)	51 (5%)	9 (1%)	19	22
1	B	992/994 (100%)	934 (94%)	52 (5%)	6 (1%)	27	33
1	C	992/994 (100%)	933 (94%)	53 (5%)	6 (1%)	27	33
1	D	992/994 (100%)	931 (94%)	52 (5%)	9 (1%)	19	22
All	All	3968/3976 (100%)	3730 (94%)	208 (5%)	30 (1%)	21	25

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	HIS
1	B	882	HIS
1	C	882	HIS
1	D	882	HIS
1	A	961	ALA
1	D	961	ALA
1	A	992	LEU
1	B	663	LEU
1	C	663	LEU
1	D	992	LEU
1	A	243	GLU
1	A	282	PRO
1	B	241	ALA
1	D	243	GLU

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Mol	Chain	Res	Type
1	D	282	PRO
1	A	862	GLY
1	A	953	LEU
1	C	241	ALA
1	C	950	VAL
1	D	862	GLY
1	B	950	VAL
1	B	953	LEU
1	C	953	LEU
1	D	953	LEU
1	A	291	GLY
1	A	950	VAL
1	D	291	GLY
1	B	862	GLY
1	C	862	GLY
1	D	950	VAL

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%)	805 (96%)	35 (4%)	32	45
1	B	840/840 (100%)	801 (95%)	39 (5%)	29	41
1	C	840/840 (100%)	803 (96%)	37 (4%)	31	43
1	D	840/840 (100%)	806 (96%)	34 (4%)	34	48
All	All	3360/3360 (100%)	3215 (96%)	145 (4%)	32	43

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	44	GLU
1	A	45	GLU
1	A	164	ARG
1	A	187	VAL

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Mol	Chain	Res	Type
1	A	202	GLN
1	A	206	ASN
1	A	236	ARG
1	A	266	LEU
1	A	342	LEU
1	A	356	LEU
1	A	413	LEU
1	A	467	ARG
1	A	486	GLU
1	A	529	ARG
1	A	534	ARG
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	602	PRO
1	A	620	ARG
1	A	631	THR
1	A	656	ARG
1	A	660	ASP
1	A	678	ARG
1	A	687	ILE
1	A	691	LEU
1	A	705	VAL
1	A	819	ARG
1	A	882	HIS
1	A	924	ARG
1	A	964	LEU
1	A	966	GLN
1	A	972	LYS
1	A	982	GLU
1	B	9	THR
1	B	22	THR
1	B	41	LEU
1	B	134	ARG
1	B	164	ARG
1	B	202	GLN
1	B	212	THR
1	B	236	ARG
1	B	242	THR
1	B	281	ASP
1	B	319	LEU
1	B	328	LYS

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Mol	Chain	Res	Type
1	B	340	GLU
1	B	342	LEU
1	B	356	LEU
1	B	394	GLU
1	B	406	GLN
1	B	445	LEU
1	B	460	ARG
1	B	484	THR
1	B	505	ARG
1	B	562	LEU
1	B	566	THR
1	B	567	ARG
1	B	572	LYS
1	B	589	THR
1	B	600	LEU
1	B	620	ARG
1	B	631	THR
1	B	678	ARG
1	B	679	VAL
1	B	691	LEU
1	B	705	VAL
1	B	713	LYS
1	B	765	ILE
1	B	818	ASP
1	B	882	HIS
1	B	914	ASN
1	B	962	LEU
1	C	9	THR
1	C	22	THR
1	C	41	LEU
1	C	134	ARG
1	C	164	ARG
1	C	202	GLN
1	C	212	THR
1	C	236	ARG
1	C	281	ASP
1	C	319	LEU
1	C	328	LYS
1	C	340	GLU
1	C	342	LEU
1	C	356	LEU
1	C	394	GLU

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Mol	Chain	Res	Type
1	C	406	GLN
1	C	445	LEU
1	C	460	ARG
1	C	484	THR
1	C	505	ARG
1	C	562	LEU
1	C	566	THR
1	C	572	LYS
1	C	589	THR
1	C	600	LEU
1	C	620	ARG
1	C	631	THR
1	C	678	ARG
1	C	679	VAL
1	C	691	LEU
1	C	705	VAL
1	C	713	LYS
1	C	765	ILE
1	C	818	ASP
1	C	882	HIS
1	C	914	ASN
1	C	962	LEU
1	D	41	LEU
1	D	44	GLU
1	D	45	GLU
1	D	164	ARG
1	D	187	VAL
1	D	202	GLN
1	D	236	ARG
1	D	266	LEU
1	D	342	LEU
1	D	356	LEU
1	D	413	LEU
1	D	467	ARG
1	D	529	ARG
1	D	534	ARG
1	D	554	THR
1	D	562	LEU
1	D	566	THR
1	D	567	ARG
1	D	602	PRO
1	D	620	ARG

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Mol	Chain	Res	Type
1	D	631	THR
1	D	656	ARG
1	D	660	ASP
1	D	678	ARG
1	D	687	ILE
1	D	691	LEU
1	D	705	VAL
1	D	819	ARG
1	D	882	HIS
1	D	924	ARG
1	D	964	LEU
1	D	966	GLN
1	D	972	LYS
1	D	982	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	206	ASN
1	A	280	ASN
1	A	359	ASN
1	A	872	HIS
1	A	914	ASN
1	A	966	GLN
1	A	990	ASN
1	B	108	GLN
1	B	138	GLN
1	B	278	HIS
1	B	359	ASN
1	B	406	GLN
1	B	768	ASN
1	B	796	ASN
1	B	914	ASN
1	B	919	ASN
1	C	108	GLN
1	C	138	GLN
1	C	177	GLN
1	C	278	HIS
1	C	359	ASN
1	C	406	GLN
1	C	768	ASN

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Mol	Chain	Res	Type
1	C	796	ASN
1	C	914	ASN
1	C	919	ASN
1	D	280	ASN
1	D	914	ASN
1	D	966	GLN
1	D	990	ASN

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 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	ADP	A	1002	2	25,29,29	1.34	4 (16%)	25,45,45	2.83	5 (20%)
6	TG1	A	1003	-	44,48,48	2.00	12 (27%)	48,72,72	1.64	9 (18%)
4	MF4	A	998	1,2	0,4,4	0.00	-	0,6,6	0.00	-
4	MF4	B	1098	1,2	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	B	1102	2	25,29,29	1.41	6 (24%)	25,45,45	2.81	5 (20%)
6	TG1	B	1103	-	44,48,48	2.04	11 (25%)	48,72,72	1.71	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MF4	C	1198	1,2	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	1202	2	25,29,29	1.38	5 (20%)	25,45,45	2.79	5 (20%)
6	TG1	C	1203	-	44,48,48	2.05	10 (22%)	48,72,72	1.71	10 (20%)
4	MF4	D	1298	1,2	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	D	1302	2	25,29,29	1.31	3 (12%)	25,45,45	2.84	5 (20%)
6	TG1	D	1303	-	44,48,48	1.99	10 (22%)	48,72,72	1.65	11 (22%)

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	ADP	A	1002	2	-	0/12/32/32	0/3/3/3
6	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
4	MF4	A	998	1,2	-	0/0/0/0	0/0/0/0
4	MF4	B	1098	1,2	-	0/0/0/0	0/0/0/0
5	ADP	B	1102	2	-	0/12/32/32	0/3/3/3
6	TG1	B	1103	-	-	0/33/99/99	0/3/3/3
4	MF4	C	1198	1,2	-	0/0/0/0	0/0/0/0
5	ADP	C	1202	2	-	0/12/32/32	0/3/3/3
6	TG1	C	1203	-	-	0/33/99/99	0/3/3/3
4	MF4	D	1298	1,2	-	0/0/0/0	0/0/0/0
5	ADP	D	1302	2	-	0/12/32/32	0/3/3/3
6	TG1	D	1303	-	-	0/33/99/99	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1202	ADP	PB-O3A	-2.27	1.56	1.60
5	B	1102	ADP	PB-O3A	-2.21	1.56	1.60
5	B	1102	ADP	C5-N7	-2.06	1.32	1.39
6	B	1103	TG1	O1-C13	2.01	1.40	1.34
5	A	1002	ADP	C2-N1	2.01	1.37	1.33
5	C	1202	ADP	C2-N1	2.01	1.37	1.33
6	A	1003	TG1	C9-C8	2.02	1.55	1.52
6	B	1103	TG1	C1-C5	2.07	1.54	1.51
6	D	1303	TG1	O7-C27	2.08	1.40	1.34
6	A	1003	TG1	O7-C27	2.10	1.40	1.34
6	D	1303	TG1	C1-C5	2.15	1.54	1.51
6	A	1003	TG1	C1-C5	2.15	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1202	ADP	PB-O2B	2.16	1.63	1.54
5	B	1102	ADP	C2-N1	2.16	1.38	1.33
5	B	1102	ADP	PB-O2B	2.16	1.63	1.54
6	B	1103	TG1	C1-C2	2.21	1.58	1.54
6	C	1203	TG1	C1-C5	2.22	1.55	1.51
5	A	1002	ADP	PB-O2B	2.25	1.63	1.54
5	D	1302	ADP	PB-O2B	2.25	1.63	1.54
6	C	1203	TG1	C1-C2	2.25	1.58	1.54
6	A	1003	TG1	O3-C3	2.29	1.49	1.44
6	A	1003	TG1	C11-C7	2.35	1.58	1.55
5	D	1302	ADP	C4-N3	2.38	1.39	1.35
6	C	1203	TG1	C9-C8	2.40	1.55	1.52
6	B	1103	TG1	C9-C8	2.41	1.55	1.52
6	C	1203	TG1	C34-C11	2.48	1.56	1.53
5	C	1202	ADP	C4-N3	2.48	1.39	1.35
5	B	1102	ADP	C4-N3	2.53	1.39	1.35
6	D	1303	TG1	C11-C7	2.58	1.58	1.55
5	A	1002	ADP	C4-N3	2.59	1.39	1.35
6	B	1103	TG1	C34-C11	2.61	1.57	1.53
6	A	1003	TG1	C34-C11	2.61	1.57	1.53
6	B	1103	TG1	C11-C7	2.61	1.58	1.55
5	D	1302	ADP	C2-N3	2.66	1.36	1.32
6	D	1303	TG1	C9-C10	2.67	1.59	1.54
5	A	1002	ADP	C2-N3	2.69	1.36	1.32
6	A	1003	TG1	C9-C10	2.70	1.59	1.54
6	C	1203	TG1	C11-C7	2.74	1.59	1.55
6	D	1303	TG1	C34-C11	2.76	1.57	1.53
6	A	1003	TG1	C1-C2	2.77	1.59	1.54
6	D	1303	TG1	C1-C2	2.87	1.59	1.54
6	A	1003	TG1	O6-C7	3.02	1.48	1.43
6	C	1203	TG1	C9-C10	3.06	1.59	1.54
6	D	1303	TG1	O6-C7	3.06	1.48	1.43
6	B	1103	TG1	C9-C10	3.08	1.59	1.54
6	C	1203	TG1	O6-C7	3.10	1.48	1.43
5	C	1202	ADP	C2-N3	3.23	1.37	1.32
6	B	1103	TG1	O6-C7	3.26	1.48	1.43
5	B	1102	ADP	C2-N3	3.37	1.37	1.32
6	C	1203	TG1	C10-C1	4.53	1.66	1.54
6	B	1103	TG1	C10-C1	4.57	1.66	1.54
6	D	1303	TG1	C10-C1	4.82	1.67	1.54
6	A	1003	TG1	C10-C1	4.97	1.67	1.54
6	D	1303	TG1	O4-C21	5.34	1.32	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	TG1	O4-C21	5.47	1.33	1.21
6	B	1103	TG1	O4-C21	5.75	1.33	1.21
6	C	1203	TG1	O4-C21	5.88	1.33	1.21
6	A	1003	TG1	C7-C8	6.10	1.61	1.53
6	D	1303	TG1	C7-C8	6.20	1.61	1.53
6	B	1103	TG1	C7-C8	7.12	1.62	1.53
6	C	1203	TG1	C7-C8	7.23	1.62	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1302	ADP	N3-C2-N1	-12.73	117.97	128.86
5	B	1102	ADP	N3-C2-N1	-12.68	118.01	128.86
5	A	1002	ADP	N3-C2-N1	-12.66	118.02	128.86
5	C	1202	ADP	N3-C2-N1	-12.62	118.06	128.86
6	D	1303	TG1	O12-C12-C11	-4.31	124.22	128.26
6	A	1003	TG1	O12-C12-C11	-4.25	124.27	128.26
6	C	1203	TG1	O12-C12-C11	-4.10	124.42	128.26
6	B	1103	TG1	O12-C12-C11	-4.09	124.42	128.26
6	D	1303	TG1	O9-C10-C31	-3.44	94.11	107.88
6	A	1003	TG1	O9-C10-C31	-3.41	94.22	107.88
6	C	1203	TG1	O9-C10-C31	-3.24	94.89	107.88
6	B	1103	TG1	O9-C10-C31	-3.20	95.05	107.88
5	A	1002	ADP	C4-C5-N7	-3.11	106.41	109.41
5	D	1302	ADP	C4-C5-N7	-3.04	106.47	109.41
5	B	1102	ADP	C4'-O4'-C1'	-2.99	106.71	109.83
5	C	1202	ADP	C4'-O4'-C1'	-2.92	106.78	109.83
5	B	1102	ADP	C4-C5-N7	-2.89	106.62	109.41
5	D	1302	ADP	C4'-O4'-C1'	-2.73	106.99	109.83
5	A	1002	ADP	C4'-O4'-C1'	-2.72	106.99	109.83
5	C	1202	ADP	C4-C5-N7	-2.61	106.89	109.41
6	A	1003	TG1	C11-C7-C6	-2.50	98.22	103.03
6	D	1303	TG1	C11-C7-C6	-2.47	98.27	103.03
6	C	1203	TG1	C11-C7-C6	-2.44	98.32	103.03
6	B	1103	TG1	C11-C7-C6	-2.43	98.34	103.03
6	B	1103	TG1	C23-C22-C21	-2.30	110.07	116.04
6	C	1203	TG1	C23-C22-C21	-2.29	110.10	116.04
6	A	1003	TG1	O4-C21-C22	-2.22	117.91	125.20
6	D	1303	TG1	O4-C21-C22	-2.21	117.95	125.20
6	D	1303	TG1	C23-C22-C21	-2.01	110.84	116.04
5	B	1102	ADP	C2-N1-C6	2.00	122.16	118.75
6	D	1303	TG1	C2-O1-C13	2.01	121.00	117.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1102	ADP	C2'-C3'-C4'	2.06	106.57	102.62
5	C	1202	ADP	C2'-C3'-C4'	2.10	106.66	102.62
5	C	1202	ADP	C2-N1-C6	2.11	122.34	118.75
5	A	1002	ADP	C2-N1-C6	2.15	122.40	118.75
5	D	1302	ADP	C2-N1-C6	2.26	122.59	118.75
6	C	1203	TG1	O5-C12-O12	2.31	124.76	121.63
5	A	1002	ADP	C2'-C3'-C4'	2.34	107.11	102.62
5	D	1302	ADP	C2'-C3'-C4'	2.37	107.17	102.62
6	B	1103	TG1	O5-C12-O12	2.38	124.86	121.63
6	D	1303	TG1	C24-C22-C21	2.39	130.76	120.80
6	A	1003	TG1	C24-C22-C21	2.40	130.79	120.80
6	C	1203	TG1	C24-C22-C21	2.43	130.93	120.80
6	B	1103	TG1	C24-C22-C21	2.44	130.99	120.80
6	A	1003	TG1	O5-C12-O12	2.51	125.04	121.63
6	D	1303	TG1	O5-C12-O12	2.56	125.10	121.63
6	A	1003	TG1	O3-C21-O4	2.66	128.59	123.33
6	D	1303	TG1	O3-C21-O4	2.66	128.60	123.33
6	A	1003	TG1	C7-C6-C5	2.99	123.18	115.13
6	D	1303	TG1	C7-C6-C5	3.00	123.19	115.13
6	C	1203	TG1	C7-C6-C5	3.08	123.41	115.13
6	B	1103	TG1	C7-C6-C5	3.09	123.44	115.13
6	C	1203	TG1	O3-C21-O4	3.18	129.63	123.33
6	B	1103	TG1	O3-C21-O4	3.18	129.64	123.33
6	C	1203	TG1	C2-O1-C13	3.91	124.19	117.61
6	B	1103	TG1	C2-O1-C13	3.99	124.33	117.61
6	C	1203	TG1	C10-O9-C32	5.34	134.42	121.73
6	B	1103	TG1	C10-O9-C32	5.40	134.56	121.73
6	A	1003	TG1	C10-O9-C32	5.41	134.58	121.73
6	D	1303	TG1	C10-O9-C32	5.42	134.59	121.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	ADP	2	0
6	B	1103	TG1	2	0
5	C	1202	ADP	2	0
6	C	1203	TG1	2	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

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.