



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:50 PM GMT

PDB ID : 1VFP  
Title : Crystal structure of the SR CA2+-ATPase with bound AMPPCP  
Authors : Toyoshima, C.; Mizutani, T.  
Deposited on : 2004-04-18  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

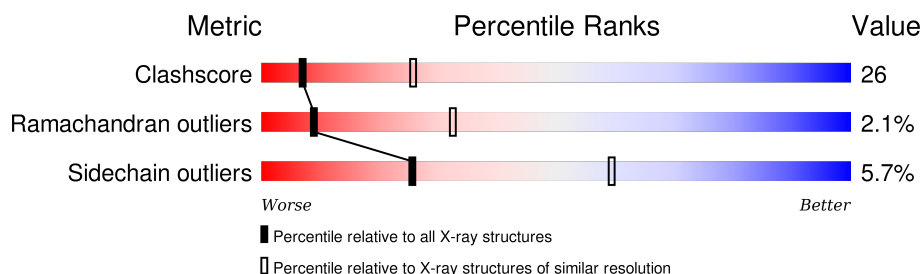
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15418 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			

There are 2 discrepancies between the modelled and reference sequences:

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

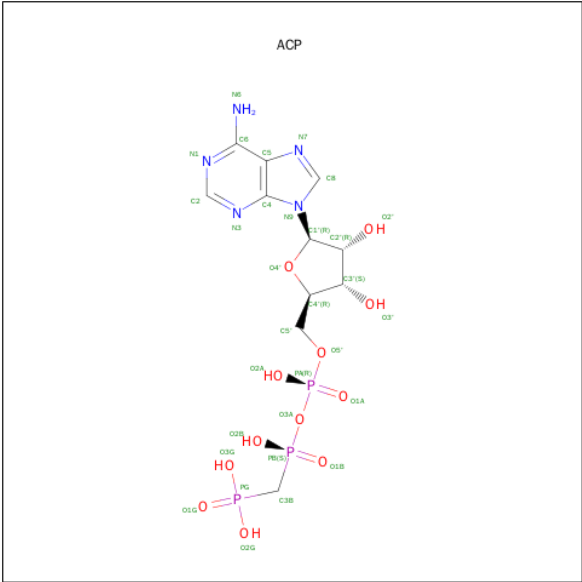
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

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

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

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is water.

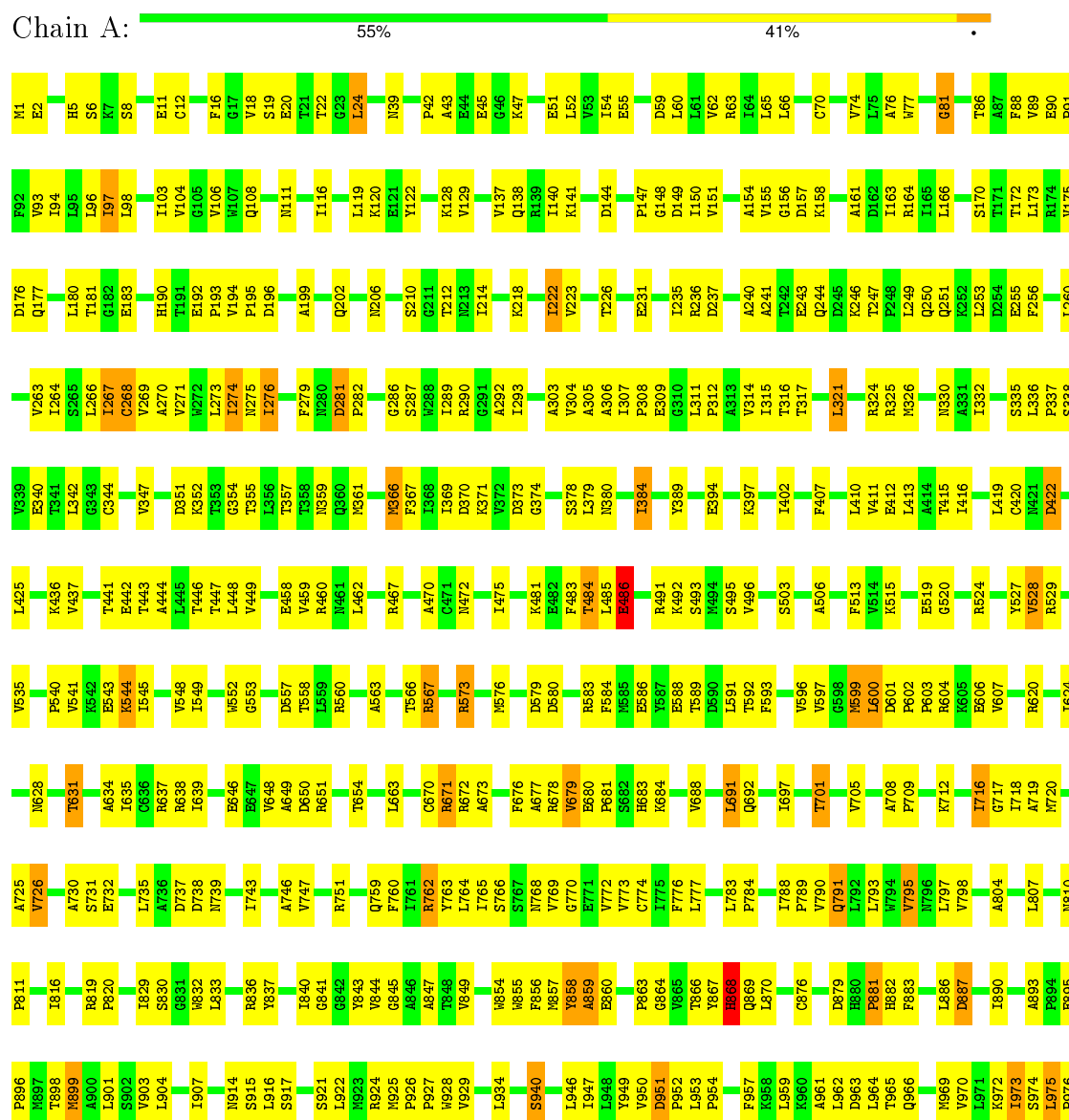
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

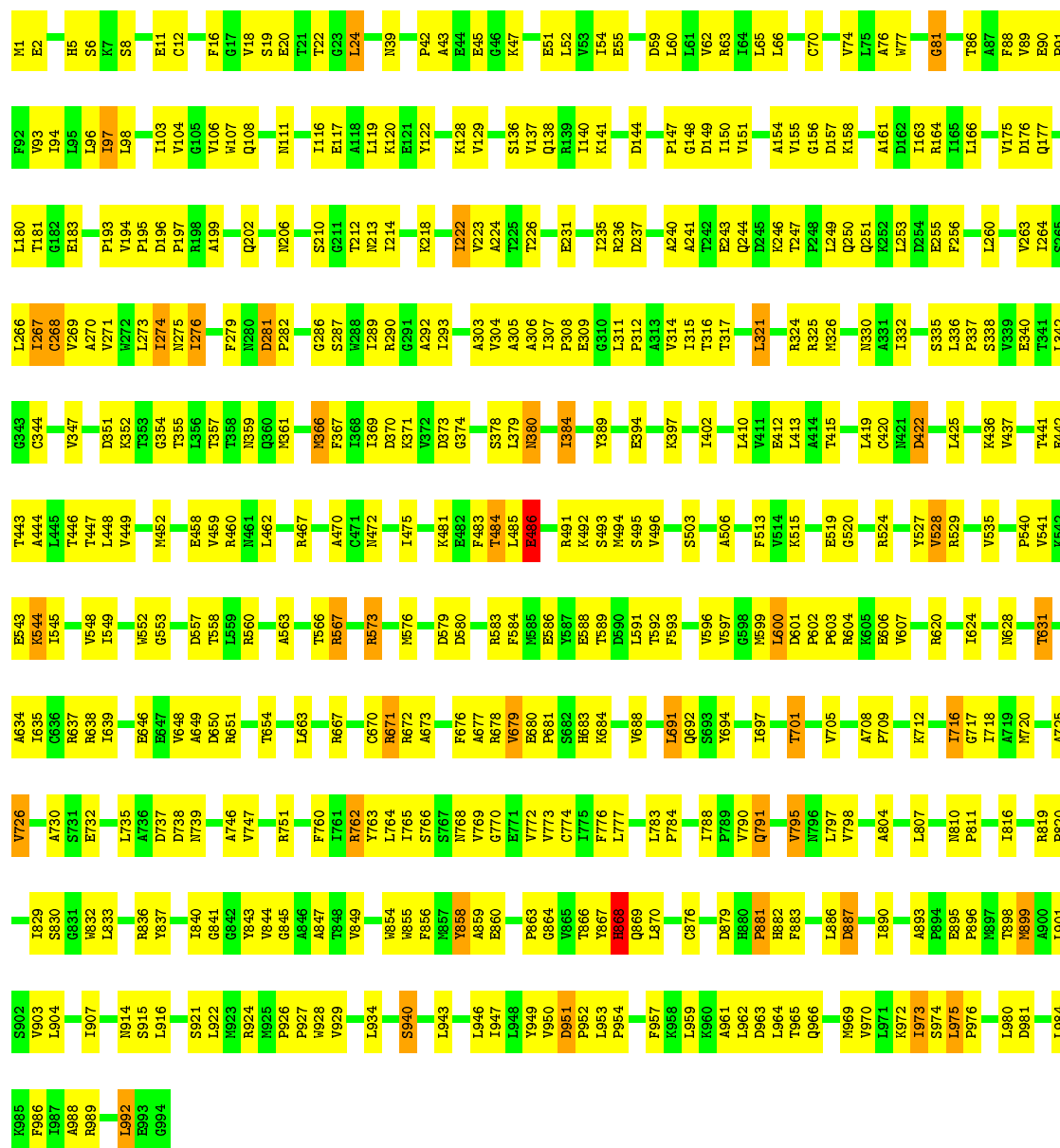
- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain B: 56% 40%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.92Å 123.62Å 151.82Å 90.00° 107.21° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.9 (15.00-2.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.247 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	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: CA, ACP, MG

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	0.43	0/7812	0.62	2/10592 (0.0%)
1	B	0.47	0/7812	0.64	2/10592 (0.0%)
All	All	0.45	0/15624	0.63	4/21184 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	LEU	CA-CB-CG	7.94	133.56	115.30
1	A	413	LEU	CA-CB-CG	7.78	133.18	115.30
1	A	81	GLY	N-CA-C	6.03	128.17	113.10
1	B	81	GLY	N-CA-C	5.98	128.04	113.10

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	7763	414	0
1	B	7671	0	7763	409	0
2	A	2	0	0	0	0
2	B	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
4	A	31	0	14	1	0
4	B	31	0	14	1	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	15418	0	15554	820	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 26.

All (820) 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:52:LEU:HB3	1:A:106:VAL:HG23	1.41	1.01
1:B:52:LEU:HB3	1:B:106:VAL:HG23	1.41	1.00
1:B:600:LEU:HD12	1:B:602:PRO:HD3	1.50	0.92
1:B:140:ILE:HD12	1:B:141:LYS:H	1.36	0.90
1:A:773:VAL:HG23	1:A:845:GLY:HA3	1.54	0.90
1:A:246:LYS:HE3	1:A:251:GLN:HG2	1.54	0.89
1:A:600:LEU:HD12	1:A:602:PRO:HD3	1.53	0.89
1:A:573:ARG:HH11	1:A:573:ARG:HG2	1.37	0.88
1:B:246:LYS:HE3	1:B:251:GLN:HG2	1.54	0.87
1:B:773:VAL:HG23	1:B:845:GLY:HA3	1.54	0.87
1:A:963:ASP:HB2	1:A:966:GLN:HG3	1.57	0.86
1:A:952:PRO:HG3	1:B:111:ASN:HD21	1.41	0.86
1:B:573:ARG:HH11	1:B:573:ARG:HG2	1.41	0.84
1:A:140:ILE:HD12	1:A:141:LYS:H	1.41	0.84
1:B:963:ASP:HB2	1:B:966:GLN:HG3	1.58	0.83
1:A:156:GLY:HA2	1:A:726:VAL:CG1	2.07	0.83
1:B:156:GLY:HA2	1:B:726:VAL:CG1	2.09	0.82
1:B:65:LEU:CD2	1:B:309:GLU:HG2	2.09	0.82
1:A:247:THR:HG22	1:A:337:PRO:HG3	1.61	0.82
1:A:65:LEU:CD2	1:A:309:GLU:HG2	2.10	0.82
1:B:770:GLY:HA3	1:B:844:VAL:HG23	1.63	0.81
1:A:947:ILE:HA	1:A:953:LEU:HD23	1.62	0.81
1:A:287:SER:HB2	1:A:289:ILE:HG22	1.62	0.81
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.63	0.81
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.63	0.81
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.63	0.81
1:B:947:ILE:HA	1:B:953:LEU:HD23	1.61	0.81
1:B:558:THR:HG22	1:B:634:ALA:HB1	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:HA	1:A:210:SER:HB2	1.64	0.80
1:B:287:SER:HB2	1:B:289:ILE:HG22	1.62	0.80
1:B:247:THR:HG22	1:B:337:PRO:HG3	1.62	0.80
1:B:679:VAL:HG22	1:B:683:HIS:CB	2.11	0.80
1:B:903:VAL:HA	1:B:970:VAL:HG13	1.64	0.80
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.63	0.79
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.64	0.79
1:B:181:THR:OG1	1:B:183:GLU:HG2	1.83	0.79
1:A:840:ILE:HD13	1:A:980:LEU:HD23	1.65	0.79
1:B:65:LEU:HD22	1:B:309:GLU:HG2	1.65	0.79
1:B:161:ALA:HA	1:B:210:SER:HB2	1.65	0.78
1:A:679:VAL:HG22	1:A:683:HIS:CB	2.14	0.78
1:B:844:VAL:HG12	1:B:907:ILE:HD13	1.66	0.78
1:B:964:LEU:HD12	1:B:964:LEU:H	1.49	0.78
1:B:541:VAL:O	1:B:545:ILE:HG12	1.85	0.77
1:A:65:LEU:HD22	1:A:309:GLU:HG2	1.66	0.77
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.67	0.77
1:A:181:THR:OG1	1:A:183:GLU:HG2	1.85	0.77
1:A:964:LEU:HD12	1:A:964:LEU:H	1.50	0.77
1:B:624:ILE:HG21	1:B:684:LYS:HG2	1.67	0.76
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.67	0.76
1:A:773:VAL:CG2	1:A:845:GLY:HA3	2.15	0.76
1:B:876:CYS:HB3	1:B:883:PHE:CE2	2.21	0.76
1:A:271:VAL:HG22	1:A:776:PHE:HE1	1.50	0.76
1:A:567:ARG:HG2	1:A:591:LEU:HD23	1.68	0.76
1:B:773:VAL:CG2	1:B:845:GLY:HA3	2.15	0.75
1:A:847:ALA:HB1	1:A:973:ILE:HD12	1.68	0.75
1:A:876:CYS:HB3	1:A:883:PHE:CE2	2.20	0.75
1:A:705:VAL:HG12	1:A:726:VAL:CG1	2.17	0.75
1:B:271:VAL:HG22	1:B:776:PHE:HE1	1.50	0.75
1:B:567:ARG:HG2	1:B:591:LEU:HD23	1.68	0.75
1:B:847:ALA:HB1	1:B:973:ILE:HD12	1.67	0.75
1:A:90:GLU:HG2	1:A:790:VAL:HG22	1.68	0.74
1:A:844:VAL:HG12	1:A:907:ILE:HD13	1.67	0.74
1:A:777:LEU:O	1:A:777:LEU:HD23	1.87	0.74
1:B:840:ILE:HD13	1:B:980:LEU:HD23	1.67	0.74
1:B:90:GLU:HG2	1:B:790:VAL:HG22	1.68	0.74
1:A:541:VAL:O	1:A:545:ILE:HG12	1.88	0.74
1:B:129:VAL:HG12	1:B:151:VAL:HG22	1.70	0.74
1:B:777:LEU:O	1:B:777:LEU:HD23	1.87	0.73
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:VAL:HG12	1:A:726:VAL:HG11	1.71	0.73
1:B:705:VAL:HG12	1:B:726:VAL:CG1	2.18	0.73
1:B:549:ILE:HD11	1:B:596:VAL:HG21	1.70	0.73
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.71	0.73
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.70	0.73
1:B:679:VAL:HG22	1:B:683:HIS:HB3	1.71	0.73
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.69	0.73
1:A:855:TRP:O	1:A:859:ALA:HB2	1.89	0.72
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.71	0.72
1:B:895:GLU:HB2	1:B:896:PRO:HD3	1.72	0.72
1:B:495:SER:HB2	1:B:588:GLU:OE1	1.89	0.72
1:A:271:VAL:HG22	1:A:776:PHE:CE1	2.25	0.72
1:A:854:TRP:HE1	1:A:858:TYR:HD2	1.38	0.72
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.72	0.72
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.71	0.72
1:B:420:CYS:O	1:B:515:LYS:HE2	1.90	0.71
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.25	0.71
1:B:855:TRP:O	1:B:859:ALA:HB2	1.90	0.71
1:B:705:VAL:HG12	1:B:726:VAL:HG11	1.73	0.71
1:B:957:PHE:O	1:B:959:LEU:HG	1.91	0.71
1:B:1:MET:HG3	1:B:2:GLU:N	2.05	0.71
1:B:855:TRP:CE3	1:B:896:PRO:HG3	2.25	0.71
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.91	0.70
1:B:271:VAL:HG22	1:B:776:PHE:CE1	2.25	0.70
1:A:957:PHE:O	1:A:959:LEU:HG	1.91	0.70
1:A:895:GLU:HB2	1:A:896:PRO:HD3	1.71	0.70
1:B:96:LEU:HD23	1:B:797:LEU:HD11	1.74	0.70
1:A:620:ARG:NH2	1:A:671:ARG:HA	2.06	0.70
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.92	0.70
1:A:308:PRO:CB	1:A:764:LEU:HD23	2.22	0.70
1:A:840:ILE:HD13	1:A:980:LEU:CD2	2.21	0.69
1:A:528:VAL:HG11	1:A:541:VAL:HG11	1.72	0.69
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.75	0.69
1:A:306:ALA:HA	1:A:768:ASN:HD22	1.57	0.69
1:B:166:LEU:HD11	1:B:222:ILE:HB	1.74	0.69
1:B:628:ASN:HB3	1:B:631:THR:HG23	1.75	0.69
1:B:854:TRP:HE1	1:B:858:TYR:HD2	1.39	0.69
1:B:308:PRO:CB	1:B:764:LEU:HD23	2.22	0.69
1:B:306:ALA:HA	1:B:768:ASN:ND2	2.08	0.69
1:A:420:CYS:O	1:A:515:LYS:HE2	1.93	0.69
1:B:528:VAL:HG11	1:B:541:VAL:HG11	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:ARG:NH2	1:B:671:ARG:HA	2.08	0.68
1:A:770:GLY:HA2	1:A:773:VAL:HG22	1.74	0.68
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.75	0.68
1:A:679:VAL:HG22	1:A:683:HIS:HB3	1.74	0.68
1:B:840:ILE:HD13	1:B:980:LEU:CD2	2.23	0.68
1:A:306:ALA:HA	1:A:768:ASN:ND2	2.08	0.68
1:A:628:ASN:HB3	1:A:631:THR:HG23	1.75	0.68
1:A:495:SER:HB2	1:A:588:GLU:OE1	1.94	0.68
1:B:306:ALA:HA	1:B:768:ASN:HD22	1.57	0.68
1:B:389:TYR:HB3	1:B:425:LEU:HD11	1.75	0.67
1:B:893:ALA:O	1:B:896:PRO:HD2	1.95	0.67
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.76	0.67
1:A:96:LEU:HD23	1:A:797:LEU:HD11	1.75	0.67
1:B:770:GLY:HA2	1:B:773:VAL:HG22	1.75	0.67
1:B:366:MET:HG2	1:B:384:ILE:HD11	1.77	0.67
1:B:804:ALA:O	1:B:807:LEU:HB2	1.93	0.67
1:B:716:ILE:HD13	1:B:717:GLY:N	2.10	0.66
1:B:86:THR:HG22	1:B:790:VAL:HG21	1.78	0.66
1:A:308:PRO:HB3	1:A:764:LEU:HD23	1.77	0.66
1:A:893:ALA:O	1:A:896:PRO:HD2	1.96	0.66
1:A:716:ILE:HD13	1:A:717:GLY:N	2.11	0.66
1:A:737:ASP:O	1:A:738:ASP:HB2	1.96	0.66
1:B:128:LYS:HD3	1:B:437:VAL:HG13	1.78	0.65
1:B:369:ILE:HD11	1:B:545:ILE:HD11	1.78	0.65
1:A:86:THR:HG22	1:A:790:VAL:HG21	1.78	0.65
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.76	0.65
1:A:65:LEU:HG	1:A:304:VAL:HG13	1.79	0.65
1:A:804:ALA:O	1:A:807:LEU:HB2	1.95	0.65
1:B:90:GLU:CG	1:B:790:VAL:HG22	2.27	0.65
1:A:128:LYS:HD3	1:A:437:VAL:HG13	1.77	0.65
1:B:65:LEU:HG	1:B:304:VAL:HG13	1.79	0.64
1:A:90:GLU:CG	1:A:790:VAL:HG22	2.27	0.64
1:B:308:PRO:HB3	1:B:764:LEU:HD23	1.78	0.64
1:B:163:ILE:CD1	1:B:223:VAL:HG22	2.27	0.64
1:A:1:MET:HG3	1:A:2:GLU:N	2.11	0.64
1:A:163:ILE:CD1	1:A:223:VAL:HG22	2.27	0.64
1:B:737:ASP:OD2	1:B:739:ASN:HB2	1.98	0.64
1:A:42:PRO:HG2	1:A:236:ARG:HH12	1.62	0.64
1:B:156:GLY:HA2	1:B:726:VAL:HG12	1.80	0.64
1:B:449:VAL:HG21	1:B:472:ASN:OD1	1.96	0.64
1:B:276:ILE:H	1:B:276:ILE:HD13	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.28	0.63
1:A:553:GLY:O	1:A:558:THR:HA	1.97	0.63
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.81	0.63
1:A:276:ILE:H	1:A:276:ILE:HD13	1.63	0.63
1:B:335:SER:OG	1:B:337:PRO:HD2	1.99	0.63
1:B:737:ASP:O	1:B:738:ASP:HB2	1.96	0.63
1:A:8:SER:OG	1:A:11:GLU:HG3	1.99	0.63
1:B:646:GLU:OE1	1:B:651:ARG:NH1	2.32	0.63
1:A:737:ASP:OD2	1:A:739:ASN:HB2	1.97	0.63
1:B:176:ASP:O	1:B:212:THR:HB	1.99	0.63
1:B:42:PRO:HG2	1:B:236:ARG:HH12	1.64	0.63
1:B:8:SER:OG	1:B:11:GLU:HG3	1.98	0.63
1:A:864:GLY:HA3	1:A:890:ILE:HD11	1.81	0.62
1:B:864:GLY:HA3	1:B:890:ILE:HD11	1.81	0.62
1:A:335:SER:OG	1:A:337:PRO:HD2	1.99	0.62
1:B:573:ARG:NH1	1:B:573:ARG:HG2	2.14	0.62
1:A:854:TRP:NE1	1:A:858:TYR:HD2	1.98	0.62
1:B:916:LEU:CD1	1:B:927:PRO:HA	2.28	0.62
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.31	0.62
1:A:156:GLY:HA2	1:A:726:VAL:HG12	1.78	0.62
1:B:881:PRO:HG2	1:B:882:HIS:H	1.64	0.62
1:A:352:LYS:HD2	1:A:635:ILE:HD12	1.82	0.62
1:A:573:ARG:NH1	1:A:573:ARG:HG2	2.11	0.62
1:B:553:GLY:O	1:B:558:THR:HA	1.98	0.62
1:B:352:LYS:HD2	1:B:635:ILE:HD12	1.81	0.62
1:A:881:PRO:HG2	1:A:882:HIS:H	1.64	0.62
1:A:51:GLU:O	1:A:54:ILE:HG22	2.01	0.61
1:B:321:LEU:HD13	1:B:325:ARG:HH22	1.65	0.61
1:A:361:MET:CE	1:A:560:ARG:HD3	2.30	0.61
1:B:361:MET:CE	1:B:560:ARG:HD3	2.30	0.61
1:A:810:ASN:ND2	1:A:916:LEU:HA	2.16	0.61
1:B:51:GLU:O	1:B:54:ILE:HG22	2.00	0.61
1:B:854:TRP:NE1	1:B:858:TYR:HD2	1.98	0.60
1:A:42:PRO:HG2	1:A:236:ARG:NH1	2.15	0.60
1:A:366:MET:CE	1:A:448:LEU:HD11	2.31	0.60
1:A:65:LEU:HD21	1:A:309:GLU:HG2	1.84	0.60
1:A:486:GLU:O	1:A:491:ARG:NH2	2.33	0.60
1:B:819:ARG:HG3	1:B:820:PRO:HD2	1.84	0.60
1:B:975:LEU:N	1:B:976:PRO:HD2	2.16	0.60
1:B:243:GLU:HG2	1:B:244:GLN:N	2.16	0.60
1:B:24:LEU:HD22	1:B:149:ASP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:LEU:N	1:A:976:PRO:HD2	2.15	0.60
1:B:273:LEU:O	1:B:276:ILE:HG23	2.02	0.60
1:B:366:MET:CE	1:B:448:LEU:HD11	2.31	0.60
1:B:810:ASN:ND2	1:B:916:LEU:HA	2.17	0.60
1:A:273:LEU:O	1:A:276:ILE:HG23	2.02	0.60
1:A:321:LEU:HD13	1:A:325:ARG:HH22	1.67	0.60
1:A:243:GLU:HG2	1:A:244:GLN:N	2.17	0.60
1:B:42:PRO:HG2	1:B:236:ARG:NH1	2.17	0.60
1:A:249:LEU:HD22	1:A:340:GLU:HG3	1.83	0.60
1:B:357:THR:HA	1:B:603:PRO:HA	1.84	0.59
1:A:156:GLY:HA2	1:A:726:VAL:HG11	1.85	0.59
1:B:604:ARG:HB2	1:B:607:VAL:HG23	1.83	0.59
1:A:176:ASP:O	1:A:212:THR:HB	2.00	0.59
1:B:486:GLU:O	1:B:491:ARG:NH2	2.35	0.59
1:A:819:ARG:HG3	1:A:820:PRO:HD2	1.83	0.59
1:B:442:GLU:HG2	1:B:515:LYS:NZ	2.18	0.59
1:B:119:LEU:HB3	1:B:332:ILE:HD11	1.83	0.59
1:B:624:ILE:CG2	1:B:684:LYS:HG2	2.32	0.59
1:A:351:ASP:O	1:A:355:THR:HB	2.01	0.59
1:B:836:ARG:HD3	1:B:984:LEU:HD13	1.85	0.59
1:A:326:MET:HE1	1:A:746:ALA:HB2	1.85	0.59
1:B:351:ASP:O	1:B:355:THR:HB	2.03	0.59
1:A:357:THR:HA	1:A:603:PRO:HA	1.85	0.59
1:B:947:ILE:HD12	1:B:953:LEU:HD23	1.85	0.59
1:B:24:LEU:HD22	1:B:149:ASP:CB	2.33	0.59
1:B:70:CYS:O	1:B:74:VAL:HG23	2.02	0.59
1:B:65:LEU:HD21	1:B:309:GLU:HG2	1.83	0.58
1:A:181:THR:HB	1:A:202:GLN:HG2	1.86	0.58
1:A:442:GLU:HG2	1:A:515:LYS:NZ	2.18	0.58
1:A:449:VAL:HG21	1:A:472:ASN:OD1	2.03	0.58
1:A:326:MET:CE	1:A:746:ALA:HB2	2.34	0.58
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.86	0.58
1:B:783:LEU:HB3	1:B:784:PRO:HD2	1.85	0.58
1:A:458:GLU:HA	1:A:460:ARG:HH12	1.69	0.58
1:B:458:GLU:HA	1:B:460:ARG:HH12	1.68	0.58
1:B:140:ILE:CD1	1:B:141:LYS:H	2.12	0.58
1:B:147:PRO:HA	1:B:223:VAL:HG12	1.86	0.58
1:B:596:VAL:HG12	1:B:597:VAL:N	2.18	0.58
1:B:249:LEU:HD22	1:B:340:GLU:HG3	1.84	0.58
1:B:51:GLU:O	1:B:55:GLU:HG3	2.04	0.58
1:A:119:LEU:HB3	1:A:332:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLU:HA	1:A:150:ILE:HG12	1.85	0.58
1:B:515:LYS:HG3	1:B:515:LYS:O	2.03	0.57
1:B:760:PHE:HA	1:B:807:LEU:HD23	1.86	0.57
1:A:70:CYS:O	1:A:74:VAL:HG23	2.04	0.57
1:A:361:MET:HE2	1:A:560:ARG:HD3	1.86	0.57
1:A:51:GLU:O	1:A:55:GLU:HG3	2.04	0.57
1:B:1:MET:HG3	1:B:2:GLU:H	1.68	0.57
1:A:76:ALA:HB1	1:A:88:PHE:CD1	2.40	0.57
1:B:326:MET:CE	1:B:746:ALA:HB2	2.33	0.57
1:B:844:VAL:HG12	1:B:907:ILE:CD1	2.33	0.57
1:A:947:ILE:HD12	1:A:953:LEU:HD23	1.87	0.57
1:A:347:VAL:HG11	1:A:691:LEU:HD21	1.87	0.57
1:B:181:THR:HB	1:B:202:GLN:HG2	1.87	0.57
1:A:788:ILE:HG12	1:A:791:GLN:HB2	1.86	0.57
1:B:156:GLY:HA2	1:B:726:VAL:HG11	1.87	0.57
1:B:24:LEU:HB2	1:B:149:ASP:HB3	1.87	0.57
1:B:788:ILE:HG12	1:B:791:GLN:HB2	1.86	0.57
1:B:86:THR:CG2	1:B:790:VAL:HG21	2.35	0.56
1:B:315:ILE:HG23	1:B:316:THR:N	2.20	0.56
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.36	0.56
1:B:354:GLY:HA2	1:B:359:ASN:HB2	1.87	0.56
1:B:701:THR:HG23	1:B:718:ILE:HB	1.88	0.56
1:A:836:ARG:HD3	1:A:984:LEU:HD13	1.86	0.56
1:A:903:VAL:HG22	1:A:970:VAL:HG13	1.87	0.56
1:A:515:LYS:O	1:A:515:LYS:HG3	2.03	0.56
1:B:119:LEU:HD23	1:B:332:ILE:HD13	1.87	0.56
1:B:903:VAL:HG22	1:B:970:VAL:HG13	1.87	0.56
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.36	0.56
1:A:628:ASN:HB3	1:A:631:THR:CG2	2.35	0.56
1:B:76:ALA:HB1	1:B:88:PHE:CD1	2.40	0.56
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.87	0.56
1:A:86:THR:CG2	1:A:790:VAL:HG21	2.36	0.56
1:B:947:ILE:HD12	1:B:953:LEU:CD2	2.36	0.56
1:A:760:PHE:HA	1:A:807:LEU:HD23	1.87	0.56
1:B:20:GLU:HA	1:B:150:ILE:HG12	1.87	0.56
1:B:247:THR:O	1:B:251:GLN:HG3	2.06	0.56
1:A:620:ARG:HH22	1:A:671:ARG:HA	1.70	0.56
1:A:330:ASN:HB2	1:A:737:ASP:HB2	1.87	0.56
1:B:330:ASN:HB2	1:B:737:ASP:HB2	1.88	0.56
1:B:361:MET:HE2	1:B:599:MET:SD	2.46	0.56
1:B:147:PRO:HA	1:B:223:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:ASN:HD22	1:B:916:LEU:HA	1.71	0.56
1:B:281:ASP:OD1	1:B:282:PRO:HD2	2.06	0.56
1:B:584:PHE:N	1:B:584:PHE:CD2	2.72	0.56
1:B:140:ILE:HD12	1:B:141:LYS:N	2.13	0.56
1:A:222:ILE:HD13	1:A:223:VAL:N	2.20	0.56
1:B:140:ILE:HD11	1:B:144:ASP:OD2	2.06	0.55
1:A:161:ALA:CA	1:A:210:SER:HB2	2.35	0.55
1:A:810:ASN:HD22	1:A:916:LEU:HA	1.70	0.55
1:B:402:ILE:HD12	1:B:402:ILE:C	2.27	0.55
1:A:952:PRO:HG3	1:B:111:ASN:ND2	2.17	0.55
1:A:24:LEU:HB2	1:A:149:ASP:HB3	1.88	0.55
1:A:140:ILE:HD12	1:A:141:LYS:N	2.17	0.55
1:A:763:TYR:HB2	1:A:915:SER:OG	2.06	0.55
1:B:161:ALA:CA	1:B:210:SER:HB2	2.37	0.55
1:B:975:LEU:O	1:B:975:LEU:HD13	2.06	0.55
1:B:436:LYS:CB	1:B:443:THR:HG21	2.36	0.55
1:B:347:VAL:HG11	1:B:691:LEU:HD21	1.89	0.55
1:B:843:TYR:OH	1:B:976:PRO:HG2	2.07	0.55
1:B:867:TYR:HD2	1:B:868:HIS:CE1	2.25	0.54
1:A:158:LYS:HE2	1:A:725:ALA:HB1	1.89	0.54
1:A:111:ASN:HB3	1:A:324:ARG:NE	2.22	0.54
1:A:119:LEU:HD23	1:A:332:ILE:HD13	1.89	0.54
1:A:315:ILE:HG23	1:A:316:THR:N	2.22	0.54
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.90	0.54
1:A:247:THR:O	1:A:251:GLN:HG3	2.07	0.54
1:B:947:ILE:HD11	1:B:957:PHE:CE1	2.43	0.54
1:A:811:PRO:HG2	1:A:929:VAL:HG12	1.90	0.54
1:A:947:ILE:HD12	1:A:953:LEU:CD2	2.37	0.54
1:B:951:ASP:HB3	1:B:952:PRO:HD3	1.89	0.54
1:B:491:ARG:NH1	1:B:588:GLU:OE1	2.40	0.54
1:A:281:ASP:OD1	1:A:282:PRO:HD2	2.07	0.54
1:B:111:ASN:HB3	1:B:324:ARG:NE	2.23	0.54
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.89	0.54
1:B:326:MET:HE2	1:B:746:ALA:HB2	1.90	0.54
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.89	0.54
1:B:237:ASP:HA	1:B:240:ALA:O	2.08	0.54
1:B:963:ASP:C	1:B:965:THR:H	2.10	0.54
1:A:705:VAL:HG12	1:A:726:VAL:HG13	1.90	0.54
1:B:628:ASN:HB3	1:B:631:THR:CG2	2.37	0.54
1:B:620:ARG:HH22	1:B:671:ARG:HA	1.73	0.54
1:B:222:ILE:HD13	1:B:223:VAL:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ILE:C	1:B:716:ILE:HD13	2.29	0.53
1:A:436:LYS:CB	1:A:443:THR:HG21	2.38	0.53
1:A:237:ASP:HA	1:A:240:ALA:O	2.07	0.53
1:A:963:ASP:C	1:A:965:THR:H	2.10	0.53
1:B:763:TYR:HB2	1:B:915:SER:OG	2.07	0.53
1:A:24:LEU:HD22	1:A:149:ASP:CB	2.38	0.53
1:A:867:TYR:HD2	1:A:868:HIS:CE1	2.26	0.53
1:B:158:LYS:HE2	1:B:725:ALA:HB1	1.90	0.53
1:A:688:VAL:O	1:A:692:GLN:HG3	2.09	0.53
1:B:688:VAL:O	1:B:692:GLN:HG3	2.08	0.53
1:A:338:SER:OG	1:A:732:GLU:HB3	2.08	0.53
1:B:491:ARG:O	1:B:492:LYS:HB2	2.09	0.53
1:B:355:THR:HG23	1:B:720:MET:HE2	1.91	0.53
1:A:584:PHE:CD2	1:A:584:PHE:N	2.72	0.53
1:B:679:VAL:HG22	1:B:683:HIS:HB2	1.89	0.53
1:A:879:ASP:OD1	1:A:881:PRO:HD3	2.09	0.53
1:A:844:VAL:HG12	1:A:907:ILE:CD1	2.35	0.53
1:A:515:LYS:O	4:A:1001:ACP:H2	2.09	0.53
1:A:273:LEU:C	1:A:275:ASN:H	2.12	0.53
1:A:947:ILE:HD11	1:A:957:PHE:CE1	2.44	0.53
1:B:545:ILE:O	1:B:549:ILE:HG12	2.09	0.53
1:A:235:ILE:O	1:A:240:ALA:HB3	2.08	0.53
1:A:975:LEU:HD13	1:A:975:LEU:O	2.09	0.53
1:A:974:SER:C	1:A:976:PRO:HD2	2.29	0.53
1:B:367:PHE:HD1	1:B:552:TRP:CH2	2.26	0.53
1:B:338:SER:OG	1:B:732:GLU:HB3	2.08	0.53
1:B:6:SER:HA	1:B:194:VAL:O	2.09	0.53
1:B:895:GLU:O	1:B:899:MET:HB2	2.09	0.52
1:B:235:ILE:O	1:B:240:ALA:HB3	2.10	0.52
1:A:716:ILE:HD13	1:A:716:ILE:C	2.28	0.52
1:A:321:LEU:O	1:A:325:ARG:HG3	2.08	0.52
1:B:879:ASP:OD1	1:B:881:PRO:HD3	2.09	0.52
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.41	0.52
1:A:807:LEU:HD21	1:A:915:SER:CB	2.39	0.52
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.39	0.52
1:B:635:ILE:O	1:B:639:ILE:HG12	2.10	0.52
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.09	0.52
1:A:76:ALA:HB1	1:A:88:PHE:CE1	2.45	0.52
1:B:119:LEU:HB3	1:B:332:ILE:CD1	2.40	0.52
1:B:974:SER:C	1:B:976:PRO:HD2	2.30	0.52
1:A:712:LYS:HG3	1:A:730:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:VAL:HG23	1:B:970:VAL:HG22	1.92	0.52
1:B:361:MET:HE2	1:B:560:ARG:HD3	1.91	0.52
1:A:6:SER:HA	1:A:194:VAL:O	2.10	0.52
1:B:712:LYS:HG3	1:B:730:ALA:HB1	1.92	0.52
1:B:705:VAL:HG12	1:B:726:VAL:HG13	1.90	0.51
1:B:515:LYS:O	4:B:2001:ACP:H2	2.10	0.51
1:A:491:ARG:O	1:A:492:LYS:HB2	2.10	0.51
1:B:389:TYR:HA	1:B:447:THR:HG21	1.92	0.51
1:B:366:MET:HE2	1:B:448:LEU:HD11	1.91	0.51
1:B:276:ILE:H	1:B:276:ILE:CD1	2.23	0.51
1:A:701:THR:HG23	1:A:718:ILE:HB	1.92	0.51
1:A:266:LEU:C	1:A:268:CYS:H	2.14	0.51
1:B:266:LEU:C	1:B:268:CYS:H	2.14	0.51
1:A:402:ILE:HD12	1:A:402:ILE:C	2.30	0.51
1:A:596:VAL:HG12	1:A:597:VAL:N	2.23	0.51
1:B:389:TYR:O	1:B:447:THR:CG2	2.59	0.51
1:B:637:ARG:HG2	1:B:637:ARG:HH11	1.76	0.51
1:B:950:VAL:O	1:B:954:PRO:HD2	2.11	0.51
1:B:273:LEU:C	1:B:275:ASN:H	2.13	0.51
1:B:76:ALA:HB1	1:B:88:PHE:CE1	2.45	0.51
1:B:485:LEU:HB2	1:B:495:SER:HB3	1.92	0.51
1:B:484:THR:HB	1:B:496:VAL:HG22	1.92	0.51
1:A:903:VAL:HG23	1:A:970:VAL:HG22	1.91	0.51
1:B:777:LEU:HD22	1:B:849:VAL:HG21	1.93	0.51
1:B:540:PRO:O	1:B:543:GLU:HB3	2.10	0.51
1:B:903:VAL:HA	1:B:970:VAL:CG1	2.39	0.51
1:B:276:ILE:HA	1:B:279:PHE:CE2	2.45	0.51
1:A:768:ASN:O	1:A:772:VAL:HG23	2.11	0.51
1:A:243:GLU:HG2	1:A:244:GLN:H	1.75	0.51
1:A:540:PRO:O	1:A:543:GLU:HB3	2.11	0.51
1:A:276:ILE:H	1:A:276:ILE:CD1	2.24	0.50
1:B:24:LEU:HD22	1:B:149:ASP:N	2.26	0.50
1:A:367:PHE:HD1	1:A:552:TRP:CH2	2.29	0.50
1:B:811:PRO:HG2	1:B:929:VAL:HG12	1.92	0.50
1:B:807:LEU:HD21	1:B:915:SER:CB	2.41	0.50
1:A:389:TYR:HA	1:A:447:THR:HG21	1.93	0.50
1:A:276:ILE:HA	1:A:279:PHE:CE2	2.46	0.50
1:B:243:GLU:HG2	1:B:244:GLN:H	1.75	0.50
1:B:342:LEU:O	1:B:747:VAL:HG22	2.11	0.50
1:A:903:VAL:HA	1:A:970:VAL:CG1	2.39	0.50
1:B:768:ASN:O	1:B:772:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:THR:HG22	1:A:962:LEU:CD1	2.42	0.50
1:A:950:VAL:HB	1:A:953:LEU:HD22	1.94	0.50
1:B:361:MET:CE	1:B:599:MET:HG3	2.41	0.50
1:A:867:TYR:O	1:A:869:GLN:N	2.45	0.50
1:B:214:ILE:N	1:B:214:ILE:HD12	2.27	0.50
1:A:140:ILE:HD11	1:A:144:ASP:OD2	2.12	0.50
1:A:679:VAL:HG22	1:A:683:HIS:HB2	1.91	0.50
1:A:260:LEU:O	1:A:264:ILE:HG12	2.12	0.50
1:B:276:ILE:HD13	1:B:276:ILE:N	2.27	0.50
1:B:762:ARG:HG2	1:B:837:TYR:HE1	1.77	0.50
1:A:19:SER:HB2	1:A:22:THR:HB	1.93	0.50
1:A:950:VAL:O	1:A:954:PRO:HD2	2.12	0.50
1:B:19:SER:HB2	1:B:22:THR:HB	1.93	0.50
1:A:60:LEU:O	1:A:63:ARG:HB2	2.12	0.50
1:B:361:MET:HE1	1:B:560:ARG:HD3	1.93	0.49
1:B:558:THR:HG22	1:B:634:ALA:CB	2.40	0.49
1:A:119:LEU:HD21	1:A:330:ASN:HA	1.94	0.49
1:A:545:ILE:O	1:A:549:ILE:HG12	2.11	0.49
1:B:670:CYS:HB3	1:B:691:LEU:HD13	1.94	0.49
1:B:60:LEU:O	1:B:63:ARG:HB2	2.12	0.49
1:A:436:LYS:HB3	1:A:443:THR:HG21	1.95	0.49
1:A:795:VAL:HG22	1:A:901:LEU:HD11	1.94	0.49
1:A:286:GLY:HA3	1:A:290:ARG:HD3	1.95	0.49
1:A:798:VAL:HG13	1:A:940:SER:OG	2.12	0.49
1:A:103:ILE:HA	1:A:106:VAL:HG12	1.94	0.49
1:A:762:ARG:HG2	1:A:837:TYR:HE1	1.77	0.49
1:B:769:VAL:HB	1:B:841:GLY:HA3	1.95	0.49
1:B:306:ALA:CA	1:B:768:ASN:HD22	2.25	0.49
1:B:89:VAL:O	1:B:93:VAL:HG23	2.12	0.49
1:B:795:VAL:HG22	1:B:901:LEU:HD11	1.93	0.49
1:B:419:LEU:HD12	1:B:513:PHE:CE2	2.48	0.49
1:B:898:THR:HG22	1:B:962:LEU:CD1	2.42	0.49
1:A:163:ILE:HD12	1:A:223:VAL:HG22	1.95	0.49
1:B:389:TYR:O	1:B:447:THR:HG22	2.12	0.49
1:A:119:LEU:HB3	1:A:332:ILE:CD1	2.42	0.49
1:B:867:TYR:O	1:B:869:GLN:N	2.45	0.49
1:A:342:LEU:O	1:A:747:VAL:HG22	2.13	0.49
1:A:270:ALA:O	1:A:274:ILE:HG12	2.13	0.48
1:A:777:LEU:HD22	1:A:849:VAL:HG21	1.95	0.48
1:B:193:PRO:HA	1:B:206:ASN:ND2	2.28	0.48
1:A:366:MET:HE2	1:A:448:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:2:GLU:H	1.74	0.48
1:A:276:ILE:N	1:A:276:ILE:HD13	2.28	0.48
1:A:459:VAL:HA	1:A:462:LEU:HD12	1.94	0.48
1:B:286:GLY:HA3	1:B:290:ARG:HD3	1.94	0.48
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.96	0.48
1:B:764:LEU:O	1:B:768:ASN:HB2	2.12	0.48
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.27	0.48
1:A:24:LEU:HD22	1:A:149:ASP:N	2.28	0.48
1:B:811:PRO:HG2	1:B:929:VAL:CG1	2.44	0.48
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.28	0.48
1:A:952:PRO:HG2	1:B:107:TRP:NE1	2.29	0.48
1:B:163:ILE:HD11	1:B:223:VAL:HG22	1.95	0.48
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.95	0.48
1:A:218:LYS:HD2	1:A:422:ASP:OD2	2.13	0.48
1:B:52:LEU:HB3	1:B:106:VAL:CG2	2.30	0.48
1:A:140:ILE:CD1	1:A:141:LYS:H	2.18	0.48
1:A:764:LEU:O	1:A:768:ASN:HB2	2.14	0.48
1:B:97:ILE:O	1:B:97:ILE:HD13	2.13	0.48
1:A:52:LEU:HB3	1:A:106:VAL:CG2	2.29	0.48
1:A:1:MET:HB2	1:A:16:PHE:CZ	2.49	0.48
1:B:231:GLU:HA	1:B:231:GLU:OE1	2.13	0.48
1:B:966:GLN:O	1:B:969:MET:HB3	2.14	0.48
1:B:119:LEU:HD21	1:B:330:ASN:HA	1.96	0.48
1:A:317:THR:O	1:A:321:LEU:HB2	2.14	0.48
1:B:765:ILE:O	1:B:769:VAL:HG23	2.13	0.48
1:B:1:MET:HB2	1:B:16:PHE:CZ	2.49	0.48
1:B:446:THR:HG23	1:B:472:ASN:ND2	2.28	0.48
1:B:436:LYS:HB3	1:B:443:THR:HG21	1.95	0.48
1:A:231:GLU:HA	1:A:231:GLU:OE1	2.13	0.48
1:A:306:ALA:CA	1:A:768:ASN:HD22	2.26	0.48
1:B:317:THR:O	1:B:321:LEU:HB2	2.13	0.48
1:B:459:VAL:HA	1:B:462:LEU:HD12	1.95	0.48
1:A:895:GLU:O	1:A:899:MET:HB2	2.13	0.47
1:B:321:LEU:O	1:B:325:ARG:HG3	2.13	0.47
1:B:218:LYS:HD2	1:B:422:ASP:OD2	2.13	0.47
1:A:370:ASP:HB3	1:A:378:SER:OG	2.14	0.47
1:A:765:ILE:O	1:A:769:VAL:HG23	2.14	0.47
1:A:769:VAL:HB	1:A:841:GLY:HA3	1.96	0.47
1:A:97:ILE:HD13	1:A:97:ILE:O	2.14	0.47
1:B:260:LEU:O	1:B:264:ILE:HG12	2.14	0.47
1:A:864:GLY:CA	1:A:890:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ILE:CD1	1:A:596:VAL:HG11	2.44	0.47
1:B:867:TYR:C	1:B:869:GLN:H	2.17	0.47
1:B:832:TRP:CE2	1:B:988:ALA:HB2	2.49	0.47
1:A:303:ALA:O	1:A:307:ILE:HG12	2.13	0.47
1:B:654:THR:HA	1:B:677:ALA:O	2.15	0.47
1:B:39:ASN:OD1	1:B:226:THR:HB	2.14	0.47
1:B:679:VAL:CG2	1:B:683:HIS:HB3	2.44	0.47
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.50	0.47
1:B:519:GLU:OE2	1:B:678:ARG:NH1	2.47	0.47
1:B:303:ALA:O	1:B:307:ILE:HG12	2.14	0.47
1:B:270:ALA:O	1:B:274:ILE:HG12	2.14	0.47
1:A:279:PHE:CE1	1:A:292:ALA:HA	2.50	0.47
1:B:321:LEU:HD22	1:B:325:ARG:CZ	2.44	0.47
1:B:361:MET:HB2	1:B:444:ALA:HB2	1.97	0.47
1:B:856:PHE:O	1:B:866:THR:HG22	2.15	0.47
1:A:870:LEU:HD12	1:A:870:LEU:N	2.30	0.47
1:A:898:THR:HG22	1:A:962:LEU:HD11	1.96	0.47
1:B:527:TYR:O	1:B:592:THR:HA	2.15	0.47
1:B:336:LEU:HB2	1:B:337:PRO:HD3	1.97	0.47
1:A:832:TRP:CE2	1:A:988:ALA:HB2	2.49	0.47
1:A:867:TYR:C	1:A:869:GLN:H	2.17	0.47
1:B:870:LEU:N	1:B:870:LEU:HD12	2.30	0.47
1:B:701:THR:HA	1:B:718:ILE:O	2.15	0.47
1:B:798:VAL:HG13	1:B:940:SER:OG	2.15	0.47
1:B:963:ASP:C	1:B:965:THR:N	2.69	0.47
1:B:158:LYS:NZ	1:B:213:ASN:OD1	2.41	0.47
1:B:483:PHE:HZ	1:B:576:MET:HE1	1.80	0.47
1:B:858:TYR:O	1:B:858:TYR:CG	2.68	0.46
1:A:485:LEU:HB2	1:A:495:SER:HB3	1.96	0.46
1:A:361:MET:HG3	1:A:441:THR:HA	1.97	0.46
1:B:155:VAL:HA	1:B:214:ILE:HG22	1.97	0.46
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.97	0.46
1:B:379:LEU:CD1	1:B:544:LYS:HD2	2.44	0.46
1:A:986:PHE:HA	1:A:989:ARG:HH21	1.81	0.46
1:A:858:TYR:CG	1:A:858:TYR:O	2.67	0.46
1:A:321:LEU:HD22	1:A:325:ARG:CZ	2.45	0.46
1:B:371:LYS:HE2	1:B:373:ASP:HB2	1.96	0.46
1:B:904:LEU:O	1:B:907:ILE:HG22	2.15	0.46
1:A:963:ASP:C	1:A:965:THR:N	2.69	0.46
1:A:389:TYR:O	1:A:447:THR:CG2	2.63	0.46
1:B:898:THR:HG22	1:B:962:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:CD1	1:A:544:LYS:HD2	2.45	0.46
1:A:371:LYS:HE2	1:A:373:ASP:HB2	1.96	0.46
1:B:103:ILE:HA	1:B:106:VAL:HG12	1.96	0.46
1:B:950:VAL:HB	1:B:953:LEU:HD22	1.96	0.46
1:A:973:ILE:HD13	1:A:973:ILE:O	2.16	0.46
1:B:103:ILE:HG23	1:B:104:VAL:N	2.31	0.46
1:B:947:ILE:HD12	1:B:953:LEU:HG	1.97	0.46
1:B:864:GLY:CA	1:B:890:ILE:HD11	2.46	0.46
1:A:214:ILE:HD12	1:A:214:ILE:N	2.30	0.46
1:A:483:PHE:HZ	1:A:576:MET:HE1	1.81	0.46
1:B:928:TRP:HA	1:B:934:LEU:HD11	1.96	0.46
1:A:264:ILE:HD12	1:A:306:ALA:HB1	1.98	0.46
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.98	0.46
1:A:484:THR:HB	1:A:496:VAL:HG22	1.98	0.46
1:A:249:LEU:O	1:A:253:LEU:HG	2.16	0.46
1:A:856:PHE:O	1:A:866:THR:HG22	2.15	0.46
1:A:924:ARG:O	1:A:926:PRO:HD3	2.16	0.46
1:A:654:THR:HA	1:A:677:ALA:O	2.14	0.46
1:B:680:GLU:HB3	1:B:681:PRO:HD2	1.98	0.46
1:B:279:PHE:CE1	1:B:292:ALA:HA	2.50	0.46
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.45	0.46
1:A:458:GLU:HG2	1:A:460:ARG:HH12	1.81	0.46
1:A:194:VAL:O	1:A:194:VAL:HG13	2.16	0.46
1:A:59:ASP:O	1:A:63:ARG:HG3	2.15	0.46
1:B:344:CYS:HB2	1:B:697:ILE:HG13	1.98	0.46
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.98	0.46
1:B:116:ILE:HG22	1:B:120:LYS:HE3	1.98	0.46
1:A:103:ILE:HG23	1:A:104:VAL:N	2.31	0.46
1:A:904:LEU:O	1:A:907:ILE:HG22	2.16	0.46
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.97	0.46
1:A:966:GLN:O	1:A:969:MET:HB3	2.15	0.46
1:B:832:TRP:NE1	1:B:988:ALA:HB2	2.30	0.46
1:B:973:ILE:HD13	1:B:973:ILE:O	2.15	0.46
1:B:59:ASP:O	1:B:63:ARG:HG3	2.16	0.46
1:A:361:MET:HE1	1:A:560:ARG:HD3	1.98	0.45
1:B:359:ASN:N	1:B:601:ASP:OD1	2.49	0.45
1:A:784:PRO:HG3	1:A:856:PHE:HE1	1.81	0.45
1:B:986:PHE:HA	1:B:989:ARG:HH21	1.80	0.45
1:B:890:ILE:HG12	1:B:890:ILE:O	2.15	0.45
1:A:175:VAL:HG12	1:A:176:ASP:N	2.31	0.45
1:B:772:VAL:C	1:B:774:CYS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MET:CE	1:A:599:MET:HG3	2.45	0.45
1:B:584:PHE:N	1:B:584:PHE:HD2	2.15	0.45
1:A:947:ILE:HD12	1:A:953:LEU:HG	1.97	0.45
1:A:890:ILE:O	1:A:890:ILE:HG12	2.17	0.45
1:A:720:MET:HE1	1:A:735:LEU:HD12	1.97	0.45
1:A:947:ILE:HD12	1:A:953:LEU:CG	2.47	0.45
1:B:596:VAL:CG1	1:B:597:VAL:N	2.79	0.45
1:A:635:ILE:O	1:A:639:ILE:HG12	2.15	0.45
1:A:103:ILE:HG23	1:A:104:VAL:H	1.82	0.45
1:A:558:THR:HG22	1:A:634:ALA:CB	2.40	0.45
1:B:515:LYS:HA	1:B:563:ALA:O	2.17	0.45
1:B:163:ILE:HD12	1:B:223:VAL:HG22	1.96	0.45
1:A:807:LEU:HD21	1:A:915:SER:HB3	1.98	0.45
1:A:914:ASN:HB3	1:A:981:ASP:OD1	2.17	0.45
1:B:947:ILE:HD12	1:B:953:LEU:CG	2.46	0.45
1:A:772:VAL:C	1:A:774:CYS:H	2.19	0.45
1:B:344:CYS:O	1:B:697:ILE:HB	2.17	0.45
1:A:116:ILE:HG22	1:A:120:LYS:HE3	1.97	0.45
1:A:832:TRP:NE1	1:A:988:ALA:HB2	2.31	0.45
1:B:797:LEU:HD23	1:B:797:LEU:C	2.37	0.45
1:B:379:LEU:HD11	1:B:544:LYS:HD2	1.98	0.45
1:A:527:TYR:O	1:A:592:THR:HA	2.17	0.45
1:A:89:VAL:O	1:A:93:VAL:HG23	2.17	0.45
1:A:528:VAL:HG12	1:A:593:PHE:HB3	1.99	0.45
1:A:491:ARG:HD2	1:A:493:SER:OG	2.17	0.45
1:A:355:THR:HG23	1:A:720:MET:HE2	1.98	0.45
1:A:311:LEU:HA	1:A:314:VAL:HG12	1.99	0.45
1:B:264:ILE:HD12	1:B:306:ALA:HB1	1.99	0.45
1:A:39:ASN:OD1	1:A:226:THR:HB	2.17	0.45
1:A:264:ILE:HD13	1:A:267:ILE:HD11	2.00	0.44
1:B:830:SER:OG	1:B:833:LEU:HD13	2.17	0.44
1:A:503:SER:HA	1:A:506:ALA:HB2	1.99	0.44
1:A:52:LEU:O	1:A:55:GLU:HB2	2.17	0.44
1:B:528:VAL:HG12	1:B:593:PHE:HB3	2.00	0.44
1:B:549:ILE:CD1	1:B:596:VAL:HG11	2.48	0.44
1:A:389:TYR:O	1:A:447:THR:HG22	2.17	0.44
1:A:163:ILE:HD11	1:A:223:VAL:HG22	1.99	0.44
1:B:249:LEU:O	1:B:253:LEU:HG	2.17	0.44
1:A:701:THR:HA	1:A:718:ILE:O	2.18	0.44
1:B:751:ARG:HB3	1:B:816:ILE:HD11	1.99	0.44
1:B:103:ILE:HG23	1:B:104:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ILE:HD12	1:A:593:PHE:CE1	2.53	0.44
1:B:412:GLU:OE2	1:B:566:THR:HG21	2.17	0.44
1:B:604:ARG:HB2	1:B:607:VAL:CG2	2.47	0.44
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.99	0.44
1:A:311:LEU:O	1:A:314:VAL:HG12	2.18	0.44
1:B:807:LEU:HD21	1:B:915:SER:HB3	1.98	0.44
1:B:361:MET:HG3	1:B:441:THR:HA	1.97	0.44
1:B:520:GLY:O	1:B:524:ARG:HG3	2.18	0.44
1:A:602:PRO:HA	1:A:603:PRO:HD2	1.91	0.44
1:B:545:ILE:HD12	1:B:593:PHE:CE1	2.52	0.44
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.17	0.44
1:A:975:LEU:N	1:A:976:PRO:CD	2.80	0.44
1:A:866:THR:OG1	1:A:867:TYR:N	2.51	0.44
1:A:795:VAL:HG22	1:A:901:LEU:CD1	2.48	0.44
1:B:380:ASN:HA	1:B:380:ASN:HD22	1.67	0.44
1:A:528:VAL:HG23	1:A:535:VAL:CG2	2.48	0.44
1:A:515:LYS:HA	1:A:563:ALA:O	2.17	0.44
1:A:361:MET:HB2	1:A:444:ALA:HB2	1.99	0.44
1:B:1:MET:CG	1:B:2:GLU:N	2.79	0.44
1:B:914:ASN:HB3	1:B:981:ASP:OD1	2.18	0.44
1:A:624:ILE:CG2	1:A:679:VAL:HG11	2.48	0.44
1:A:352:LYS:HD2	1:A:635:ILE:CD1	2.48	0.44
1:B:975:LEU:N	1:B:976:PRO:CD	2.81	0.44
1:B:784:PRO:HG3	1:B:856:PHE:HE1	1.82	0.44
1:A:263:VAL:O	1:A:267:ILE:HG12	2.17	0.44
1:B:273:LEU:O	1:B:276:ILE:HD12	2.18	0.44
1:B:458:GLU:HG2	1:B:460:ARG:HH12	1.82	0.44
1:B:5:HIS:CD2	1:B:194:VAL:HG13	2.53	0.44
1:A:503:SER:HA	1:A:506:ALA:CB	2.48	0.44
1:A:90:GLU:N	1:A:91:PRO:HD2	2.33	0.43
1:A:916:LEU:HD11	1:A:927:PRO:HA	2.00	0.43
1:B:175:VAL:HG12	1:B:176:ASP:N	2.33	0.43
1:A:379:LEU:HD11	1:A:544:LYS:HD2	2.00	0.43
1:B:370:ASP:HB3	1:B:378:SER:OG	2.18	0.43
1:B:148:GLY:HA2	1:B:222:ILE:HD11	2.00	0.43
1:B:263:VAL:O	1:B:267:ILE:HG12	2.18	0.43
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.18	0.43
1:A:1:MET:HE1	1:A:12:CYS:HA	1.99	0.43
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.73	0.43
1:B:45:GLU:O	1:B:47:LYS:HG3	2.18	0.43
1:A:637:ARG:HH11	1:A:637:ARG:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:SER:HB2	1:B:840:ILE:HB	2.00	0.43
1:A:361:MET:HE2	1:A:599:MET:SD	2.57	0.43
1:A:719:ALA:HB2	1:A:731:SER:OG	2.19	0.43
1:A:45:GLU:O	1:A:47:LYS:HG3	2.18	0.43
1:B:720:MET:HE1	1:B:735:LEU:HD12	2.01	0.43
1:B:866:THR:OG1	1:B:867:TYR:N	2.51	0.43
1:B:795:VAL:HG22	1:B:901:LEU:CD1	2.47	0.43
1:B:503:SER:HA	1:B:506:ALA:HB2	1.99	0.43
1:B:52:LEU:O	1:B:55:GLU:HB2	2.19	0.43
1:A:797:LEU:C	1:A:797:LEU:HD23	2.39	0.43
1:B:366:MET:HE1	1:B:452:MET:SD	2.58	0.43
1:B:924:ARG:O	1:B:926:PRO:HD3	2.18	0.43
1:A:586:GLU:O	1:A:589:THR:HG22	2.18	0.43
1:B:311:LEU:HA	1:B:314:VAL:HG12	2.00	0.43
1:A:170:SER:HB2	1:A:486:GLU:HG2	2.00	0.43
1:A:330:ASN:CB	1:A:737:ASP:HB2	2.48	0.43
1:B:624:ILE:CG2	1:B:679:VAL:HG11	2.49	0.43
1:B:1:MET:HE1	1:B:12:CYS:HA	1.99	0.43
1:B:264:ILE:HD13	1:B:267:ILE:HD11	1.99	0.43
1:A:177:GLN:HB3	1:A:212:THR:HG21	2.01	0.43
1:B:315:ILE:CG2	1:B:316:THR:N	2.82	0.43
1:A:986:PHE:CA	1:A:989:ARG:HH21	2.32	0.43
1:A:62:VAL:O	1:A:66:LEU:HB2	2.18	0.43
1:A:557:ASP:O	1:A:558:THR:C	2.56	0.43
1:B:557:ASP:O	1:B:558:THR:C	2.57	0.43
1:B:412:GLU:CD	1:B:529:ARG:HH11	2.22	0.43
1:A:5:HIS:CD2	1:A:194:VAL:HG13	2.53	0.43
1:B:503:SER:HA	1:B:506:ALA:CB	2.49	0.43
1:B:90:GLU:N	1:B:91:PRO:HD2	2.34	0.43
1:B:491:ARG:HD2	1:B:493:SER:OG	2.18	0.43
1:B:389:TYR:CA	1:B:447:THR:HG21	2.48	0.43
1:A:788:ILE:HG12	1:A:791:GLN:CD	2.39	0.43
1:A:519:GLU:OE2	1:A:678:ARG:NH1	2.52	0.43
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.86	0.43
1:A:766:SER:HB2	1:A:840:ILE:HB	2.00	0.43
1:B:855:TRP:CZ3	1:B:896:PRO:HG3	2.54	0.43
1:A:273:LEU:O	1:A:276:ILE:HD12	2.18	0.43
1:A:830:SER:OG	1:A:833:LEU:HD13	2.18	0.43
1:B:62:VAL:O	1:B:66:LEU:HB2	2.19	0.43
1:A:336:LEU:N	1:A:337:PRO:CD	2.82	0.42
1:A:705:VAL:CG1	1:A:726:VAL:HG11	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:PHE:CA	1:B:989:ARG:HH21	2.32	0.42
1:A:344:CYS:O	1:A:697:ILE:HB	2.19	0.42
1:B:988:ALA:CA	1:B:992:LEU:HD12	2.42	0.42
1:A:442:GLU:HG2	1:A:515:LYS:HZ1	1.84	0.42
1:B:870:LEU:H	1:B:870:LEU:HD12	1.84	0.42
1:B:886:LEU:O	1:B:887:ASP:C	2.57	0.42
1:B:586:GLU:O	1:B:589:THR:HG22	2.18	0.42
1:B:269:VAL:O	1:B:273:LEU:HG	2.19	0.42
1:A:269:VAL:O	1:A:273:LEU:HG	2.19	0.42
1:B:788:ILE:HG12	1:B:791:GLN:CD	2.40	0.42
1:A:520:GLY:O	1:A:524:ARG:HG3	2.19	0.42
1:A:650:ASP:OD2	1:A:672:ARG:HD2	2.19	0.42
1:B:943:LEU:HD12	1:B:943:LEU:HA	1.85	0.42
1:B:606:GLU:HG3	1:B:739:ASN:OD1	2.20	0.42
1:A:359:ASN:N	1:A:601:ASP:OD1	2.50	0.42
1:A:256:PHE:CE1	1:A:829:ILE:HD11	2.54	0.42
1:B:673:ALA:HB3	1:B:676:PHE:CZ	2.54	0.42
1:A:904:LEU:HD12	1:A:904:LEU:HA	1.89	0.42
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.50	0.42
1:B:326:MET:HE1	1:B:746:ALA:HB2	1.99	0.42
1:A:701:THR:HG21	1:A:743:ILE:HD11	2.02	0.42
1:A:266:LEU:C	1:A:268:CYS:N	2.72	0.42
1:B:650:ASP:OD2	1:B:672:ARG:HD2	2.19	0.42
1:A:886:LEU:O	1:A:887:ASP:C	2.57	0.42
1:B:289:ILE:O	1:B:293:ILE:HG13	2.19	0.42
1:A:870:LEU:HD12	1:A:870:LEU:H	1.84	0.42
1:B:691:LEU:HA	1:B:691:LEU:HD12	1.72	0.42
1:B:970:VAL:C	1:B:972:LYS:H	2.23	0.42
1:B:271:VAL:HA	1:B:274:ILE:HG12	2.01	0.42
1:A:810:ASN:HA	1:A:811:PRO:HD3	1.89	0.42
1:B:330:ASN:CB	1:B:737:ASP:HB2	2.49	0.42
1:B:154:ALA:O	1:B:155:VAL:C	2.58	0.42
1:A:949:TYR:N	1:A:949:TYR:CD1	2.88	0.42
1:B:140:ILE:CG1	1:B:141:LYS:N	2.82	0.42
1:B:1:MET:HB3	1:B:224:ALA:O	2.20	0.42
1:B:18:VAL:HG21	1:B:24:LEU:CD1	2.49	0.42
1:A:18:VAL:HG21	1:A:24:LEU:CD1	2.50	0.42
1:A:397:LYS:HB3	1:A:402:ILE:HG21	2.01	0.42
1:B:986:PHE:HA	1:B:989:ARG:HE	1.85	0.42
1:A:247:THR:OG1	1:A:250:GLN:HB2	2.20	0.42
1:A:158:LYS:HB2	1:A:158:LYS:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:C	1:B:268:CYS:N	2.73	0.42
1:B:410:LEU:HD23	1:B:410:LEU:HA	1.89	0.42
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.54	0.42
1:A:412:GLU:CD	1:A:529:ARG:HH11	2.24	0.42
1:B:379:LEU:CD1	1:B:548:VAL:HG21	2.50	0.42
1:A:481:LYS:HG3	1:A:496:VAL:HG13	2.01	0.42
1:A:344:CYS:HB2	1:A:697:ILE:HG13	2.00	0.42
1:A:289:ILE:O	1:A:293:ILE:HG13	2.20	0.41
1:B:311:LEU:O	1:B:314:VAL:HG12	2.19	0.41
1:B:177:GLN:HB3	1:B:212:THR:HG21	2.01	0.41
1:B:361:MET:SD	1:B:601:ASP:HB2	2.59	0.41
1:A:458:GLU:HA	1:A:460:ARG:NH1	2.33	0.41
1:B:94:ILE:O	1:B:97:ILE:HG22	2.19	0.41
1:B:579:ASP:CG	1:B:580:ASP:N	2.74	0.41
1:B:305:ALA:O	1:B:768:ASN:ND2	2.53	0.41
1:A:347:VAL:HG11	1:A:691:LEU:CD2	2.49	0.41
1:A:194:VAL:HA	1:A:195:PRO:HD2	1.79	0.41
1:A:266:LEU:O	1:A:268:CYS:N	2.53	0.41
1:A:94:ILE:O	1:A:97:ILE:HG22	2.20	0.41
1:B:949:TYR:CD1	1:B:949:TYR:N	2.87	0.41
1:B:336:LEU:N	1:B:337:PRO:CD	2.83	0.41
1:A:783:LEU:HD22	1:A:870:LEU:HB3	2.02	0.41
1:B:458:GLU:HA	1:B:460:ARG:NH1	2.33	0.41
1:B:194:VAL:HG13	1:B:194:VAL:O	2.19	0.41
1:A:986:PHE:HA	1:A:989:ARG:HE	1.84	0.41
1:B:66:LEU:HD13	1:B:98:LEU:HD23	2.02	0.41
1:A:624:ILE:HG22	1:A:679:VAL:HG11	2.02	0.41
1:A:412:GLU:OE2	1:A:529:ARG:NH1	2.53	0.41
1:A:315:ILE:CG2	1:A:316:THR:N	2.83	0.41
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.90	0.41
1:A:579:ASP:CG	1:A:580:ASP:N	2.74	0.41
1:A:573:ARG:NH1	1:A:573:ARG:CG	2.78	0.41
1:B:247:THR:OG1	1:B:250:GLN:HB2	2.20	0.41
1:B:624:ILE:HG22	1:B:679:VAL:HG11	2.02	0.41
1:A:970:VAL:C	1:A:972:LYS:H	2.23	0.41
1:A:148:GLY:HA2	1:A:222:ILE:HD11	2.02	0.41
1:A:762:ARG:NH2	1:A:836:ARG:NH1	2.69	0.41
1:B:347:VAL:HG11	1:B:691:LEU:CD2	2.50	0.41
1:B:481:LYS:HG3	1:B:496:VAL:HG13	2.02	0.41
1:A:648:VAL:O	1:A:650:ASP:N	2.53	0.41
1:B:964:LEU:CD1	1:B:964:LEU:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HA	1:A:274:ILE:HG12	2.01	0.41
1:A:857:MET:HB2	1:A:858:TYR:H	1.66	0.41
1:A:94:ILE:HG12	1:A:793:LEU:HD22	2.03	0.41
1:B:528:VAL:HG23	1:B:535:VAL:CG2	2.51	0.41
1:B:783:LEU:HD22	1:B:870:LEU:HB3	2.03	0.41
1:A:154:ALA:N	1:A:157:ASP:OD2	2.44	0.41
1:B:903:VAL:CG2	1:B:970:VAL:HG13	2.51	0.41
1:A:305:ALA:O	1:A:768:ASN:ND2	2.54	0.41
1:A:389:TYR:CA	1:A:447:THR:HG21	2.50	0.41
1:A:361:MET:SD	1:A:601:ASP:HB2	2.59	0.41
1:A:483:PHE:HZ	1:A:576:MET:CE	2.33	0.41
1:A:903:VAL:CG2	1:A:970:VAL:HG13	2.50	0.41
1:A:596:VAL:CG1	1:A:597:VAL:N	2.83	0.41
1:B:916:LEU:HD11	1:B:927:PRO:HA	2.01	0.41
1:A:584:PHE:N	1:A:584:PHE:HD2	2.15	0.41
1:B:266:LEU:O	1:B:268:CYS:N	2.54	0.41
1:A:379:LEU:HD12	1:A:548:VAL:HG21	2.03	0.41
1:A:66:LEU:HD13	1:A:98:LEU:HD23	2.03	0.41
1:B:667:ARG:HG2	1:B:694:TYR:CE2	2.56	0.41
1:A:415:THR:HA	1:A:475:ILE:HG21	2.02	0.41
1:B:195:PRO:O	1:B:197:PRO:HD3	2.20	0.41
1:B:196:ASP:HB3	1:B:199:ALA:HB2	2.03	0.41
1:A:407:PHE:O	1:A:411:VAL:HG23	2.21	0.41
1:B:602:PRO:HA	1:B:603:PRO:HD2	1.92	0.41
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.86	0.41
1:B:836:ARG:HD3	1:B:984:LEU:CD1	2.50	0.41
1:A:921:SER:HB2	1:A:989:ARG:HH12	1.85	0.41
1:A:172:THR:HG22	1:A:173:LEU:N	2.36	0.41
1:B:256:PHE:CE1	1:B:829:ILE:HD11	2.55	0.41
1:A:192:GLU:HG3	1:A:192:GLU:H	1.69	0.41
1:B:369:ILE:HD11	1:B:545:ILE:CD1	2.50	0.40
1:A:807:LEU:HA	1:A:810:ASN:OD1	2.21	0.40
1:A:964:LEU:H	1:A:964:LEU:CD1	2.27	0.40
1:B:442:GLU:HG2	1:B:515:LYS:HZ1	1.84	0.40
1:B:154:ALA:N	1:B:157:ASP:OD2	2.45	0.40
1:B:921:SER:HB2	1:B:989:ARG:HH12	1.86	0.40
1:B:648:VAL:O	1:B:650:ASP:N	2.53	0.40
1:B:415:THR:HA	1:B:475:ILE:HG21	2.03	0.40
1:B:287:SER:HB2	1:B:289:ILE:CG2	2.42	0.40
1:B:494:MET:HG2	1:B:495:SER:N	2.36	0.40
1:B:397:LYS:HB3	1:B:402:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:CD1	1:A:548:VAL:HG21	2.51	0.40
1:A:917:SER:HB2	1:A:925:MET:HE2	2.04	0.40
1:B:86:THR:O	1:B:86:THR:HG22	2.22	0.40
1:B:807:LEU:HA	1:B:810:ASN:OD1	2.21	0.40
1:A:190:HIS:O	1:A:206:ASN:HA	2.20	0.40
1:A:751:ARG:C	1:A:816:ILE:HD11	2.42	0.40
1:A:988:ALA:O	1:A:993:GLU:HG2	2.21	0.40
1:B:412:GLU:OE2	1:B:529:ARG:NH1	2.54	0.40
1:B:513:PHE:HD1	1:B:566:THR:HG22	1.87	0.40
1:A:366:MET:HE1	1:A:448:LEU:HD11	2.03	0.40
1:A:1:MET:CG	1:A:2:GLU:N	2.83	0.40
1:B:762:ARG:NH2	1:B:836:ARG:NH1	2.69	0.40
1:A:673:ALA:HB3	1:A:676:PHE:CZ	2.55	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%)	875 (88%)	95 (10%)	22 (2%)	8	31
1	B	992/994 (100%)	878 (88%)	94 (10%)	20 (2%)	9	33
All	All	1984/1988 (100%)	1753 (88%)	189 (10%)	42 (2%)	9	32

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	TYR
1	A	486	GLU
1	A	860	GLU
1	A	881	PRO
1	A	951	ASP

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Mol	Chain	Res	Type
1	A	992	LEU
1	B	122	TYR
1	B	486	GLU
1	B	860	GLU
1	B	881	PRO
1	B	951	ASP
1	B	992	LEU
1	A	274	ILE
1	A	858	TYR
1	A	868	HIS
1	B	274	ILE
1	B	858	TYR
1	B	868	HIS
1	A	470	ALA
1	A	649	ALA
1	A	887	ASP
1	A	961	ALA
1	B	470	ALA
1	B	649	ALA
1	B	887	ASP
1	B	961	ALA
1	A	241	ALA
1	A	859	ALA
1	B	241	ALA
1	A	43	ALA
1	A	267	ILE
1	A	573	ARG
1	B	43	ALA
1	B	267	ILE
1	B	573	ARG
1	A	81	GLY
1	B	81	GLY
1	A	374	GLY
1	B	374	GLY
1	B	863	PRO
1	A	789	PRO
1	A	863	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	792 (94%)	48 (6%)	25	59
1	B	840/840 (100%)	792 (94%)	48 (6%)	25	59
All	All	1680/1680 (100%)	1584 (94%)	96 (6%)	25	59

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	77	TRP
1	A	97	ILE
1	A	108	GLN
1	A	137	VAL
1	A	138	GLN
1	A	164	ARG
1	A	180	LEU
1	A	222	ILE
1	A	255	GLU
1	A	268	CYS
1	A	276	ILE
1	A	281	ASP
1	A	321	LEU
1	A	366	MET
1	A	380	ASN
1	A	384	ILE
1	A	394	GLU
1	A	422	ASP
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	528	VAL
1	A	544	LYS
1	A	567	ARG
1	A	583	ARG
1	A	599	MET
1	A	600	LEU
1	A	631	THR
1	A	638	ARG
1	A	663	LEU

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Mol	Chain	Res	Type
1	A	671	ARG
1	A	679	VAL
1	A	691	LEU
1	A	701	THR
1	A	716	ILE
1	A	726	VAL
1	A	759	GLN
1	A	762	ARG
1	A	791	GLN
1	A	795	VAL
1	A	868	HIS
1	A	899	MET
1	A	922	LEU
1	A	940	SER
1	A	946	LEU
1	A	973	ILE
1	A	975	LEU
1	B	24	LEU
1	B	77	TRP
1	B	97	ILE
1	B	108	GLN
1	B	117	GLU
1	B	136	SER
1	B	137	VAL
1	B	138	GLN
1	B	164	ARG
1	B	180	LEU
1	B	222	ILE
1	B	255	GLU
1	B	268	CYS
1	B	276	ILE
1	B	281	ASP
1	B	321	LEU
1	B	366	MET
1	B	380	ASN
1	B	384	ILE
1	B	394	GLU
1	B	422	ASP
1	B	467	ARG
1	B	484	THR
1	B	486	GLU
1	B	528	VAL

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Mol	Chain	Res	Type
1	B	544	LYS
1	B	567	ARG
1	B	583	ARG
1	B	600	LEU
1	B	631	THR
1	B	638	ARG
1	B	663	LEU
1	B	671	ARG
1	B	679	VAL
1	B	691	LEU
1	B	701	THR
1	B	716	ILE
1	B	726	VAL
1	B	762	ARG
1	B	791	GLN
1	B	795	VAL
1	B	868	HIS
1	B	899	MET
1	B	922	LEU
1	B	940	SER
1	B	946	LEU
1	B	973	ILE
1	B	975	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	ASN
1	A	114	ASN
1	A	138	GLN
1	A	244	GLN
1	A	359	ASN
1	A	380	ASN
1	A	706	ASN
1	A	755	ASN
1	A	869	GLN
1	A	875	GLN
1	A	919	ASN
1	A	920	GLN
1	B	108	GLN
1	B	111	ASN

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Mol	Chain	Res	Type
1	B	114	ASN
1	B	138	GLN
1	B	244	GLN
1	B	359	ASN
1	B	380	ASN
1	B	706	ASN
1	B	755	ASN
1	B	869	GLN
1	B	875	GLN
1	B	919	ASN
1	B	920	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z  > 2$
4	ACP	A	1001	3	25,33,33	1.87	4 (16%)	31,52,52	2.24	7 (22%)
4	ACP	B	2001	3	25,33,33	1.95	5 (20%)	31,52,52	2.28	7 (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
4	ACP	A	1001	3	-	0/15/38/38	0/3/3/3
4	ACP	B	2001	3	-	0/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	ACP	PB-O2B	-4.11	1.46	1.56
4	A	1001	ACP	PB-O2B	-3.67	1.47	1.56
4	A	1001	ACP	PG-O2G	-2.19	1.49	1.54
4	B	2001	ACP	C5-N7	-2.14	1.32	1.39
4	B	2001	ACP	C2-N3	2.21	1.36	1.32
4	B	2001	ACP	O4'-C1'	2.39	1.44	1.41
4	A	1001	ACP	C2-N3	3.18	1.37	1.32
4	A	1001	ACP	PB-O3A	6.08	1.65	1.58
4	B	2001	ACP	PB-O3A	7.01	1.66	1.58

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	ACP	N3-C2-N1	-7.40	123.23	128.89
4	A	1001	ACP	N3-C2-N1	-7.07	123.48	128.89
4	A	1001	ACP	C5'-C4'-C3'	-4.70	96.57	115.21
4	B	2001	ACP	C5'-C4'-C3'	-4.63	96.82	115.21
4	A	1001	ACP	O1B-PB-C3B	-4.06	98.80	109.02
4	B	2001	ACP	O1B-PB-C3B	-3.58	100.02	109.02
4	A	1001	ACP	C1'-N9-C4	-2.25	123.55	126.94
4	B	2001	ACP	O3G-PG-O2G	2.06	114.17	108.13
4	A	1001	ACP	O2B-PB-C3B	2.94	119.69	106.88
4	B	2001	ACP	C4-C5-N7	3.03	112.26	109.48
4	A	1001	ACP	C4-C5-N7	3.07	112.31	109.48
4	B	2001	ACP	O2B-PB-C3B	3.30	121.25	106.88
4	B	2001	ACP	O5'-C5'-C4'	4.36	125.21	109.12
4	A	1001	ACP	O5'-C5'-C4'	4.42	125.41	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	ACP	1	0
4	B	2001	ACP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.