



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 05:37 PM EDT

PDB ID : 3B9R  
Title : SERCA Ca<sup>2+</sup>-ATPase E2 aluminium fluoride complex without thapsigargin  
Authors : Olesen, C.; Picard, M.; Winther, A.M.L.; Morth, J.P.; Moller, J.V.; Nissen, P.  
Deposited on : 2007-11-06  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

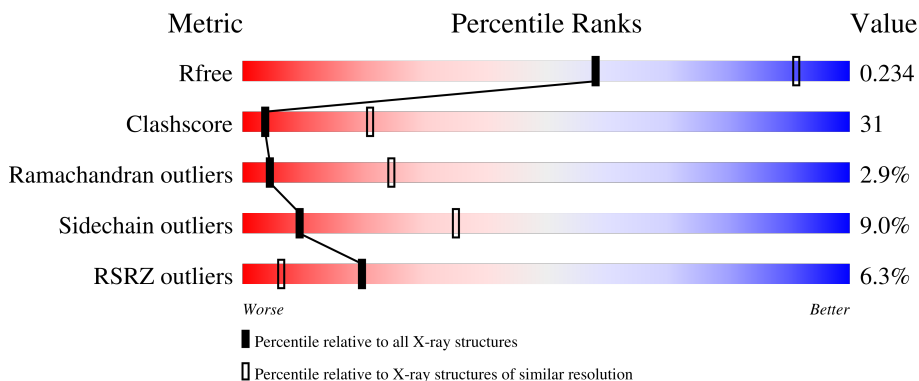
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	994	5% (Poor fit)   50% (0 outliers)   43% (1 outlier)   7% (2 outliers)
1	B	994	8% (Poor fit)   50% (0 outliers)   44% (1 outlier)   6% (2 outliers)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ALF	B	995	-	-	X	-

## 2 Entry composition [i](#)

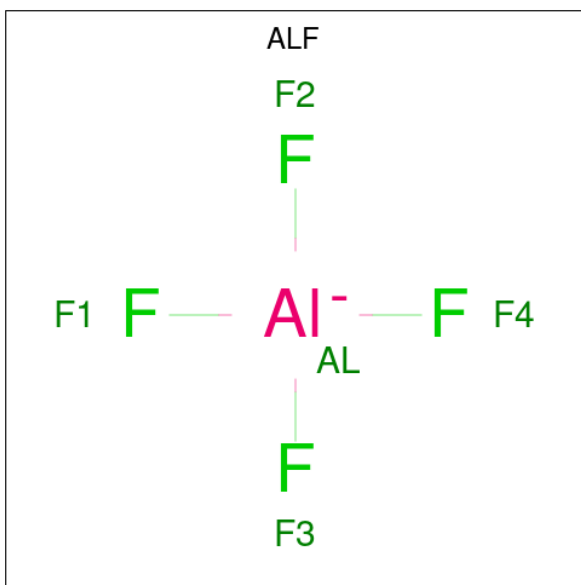
There are 6 unique types of molecules in this entry. The entry contains 15426 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0
1	B	994	7671	4876	1287	1451	57	0	0	0

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).



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

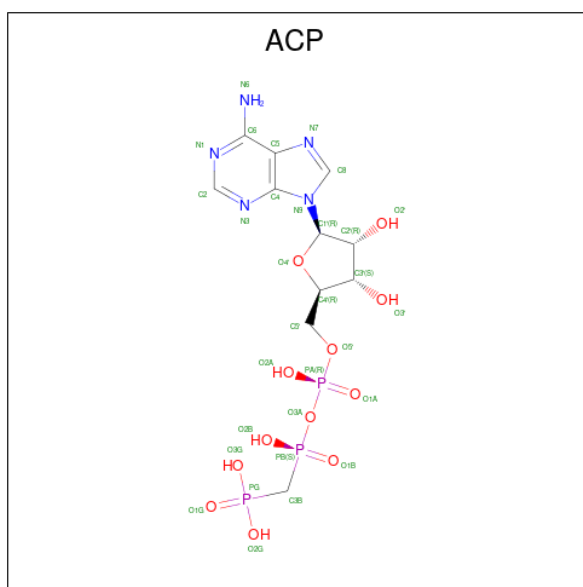
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0

- Molecule 5 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
5	A	1	Total C N O P 31 11 5 12 3	0	0
5	B	1	Total C N O P 31 11 5 12 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0

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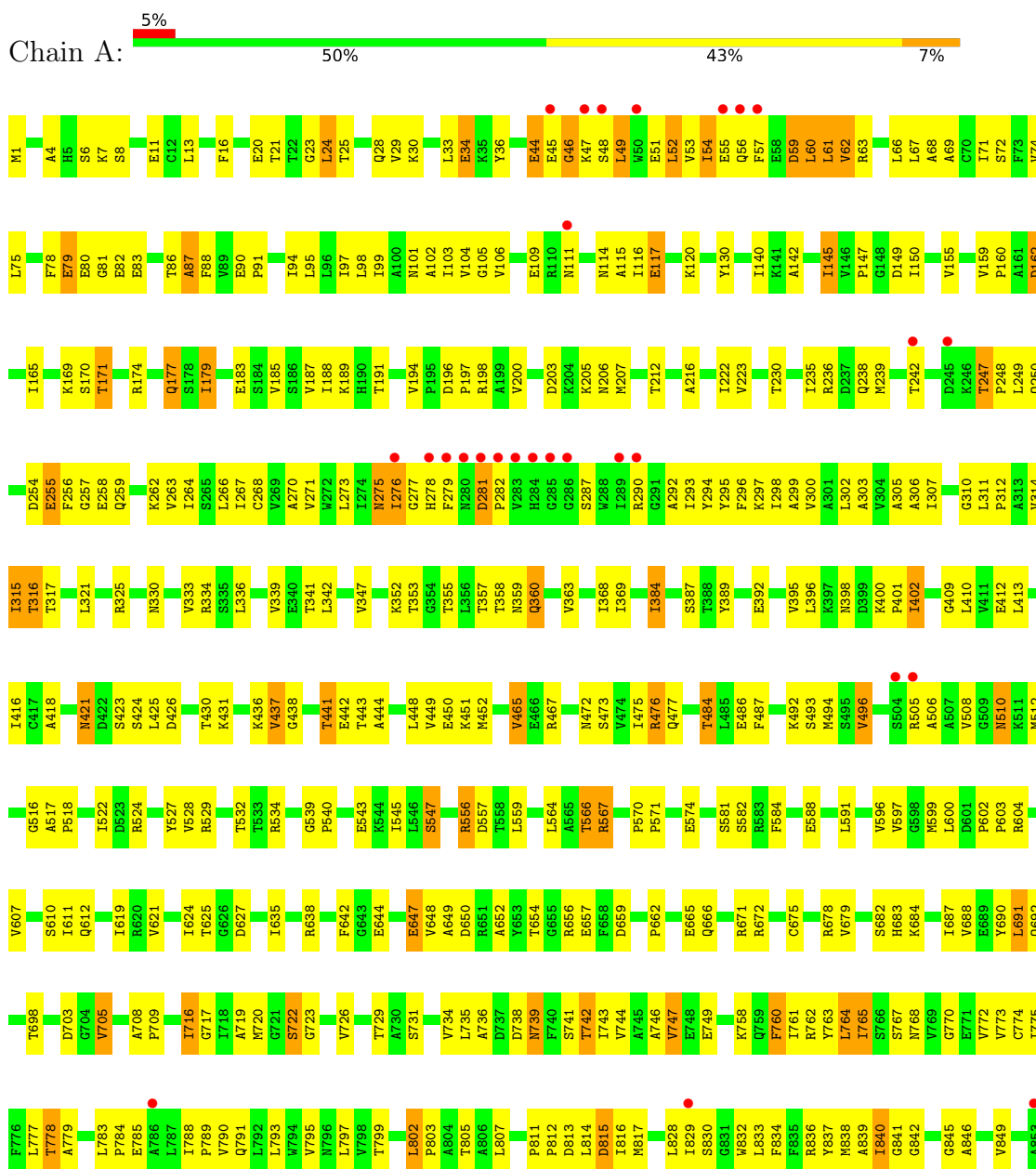
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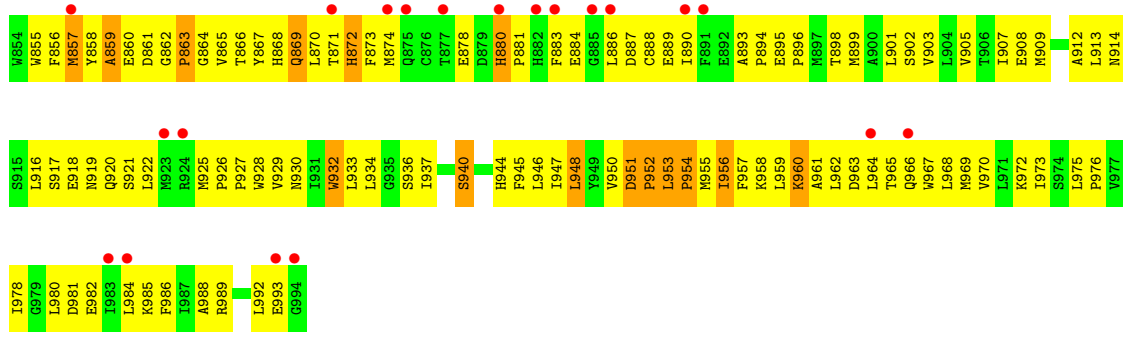
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	B	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

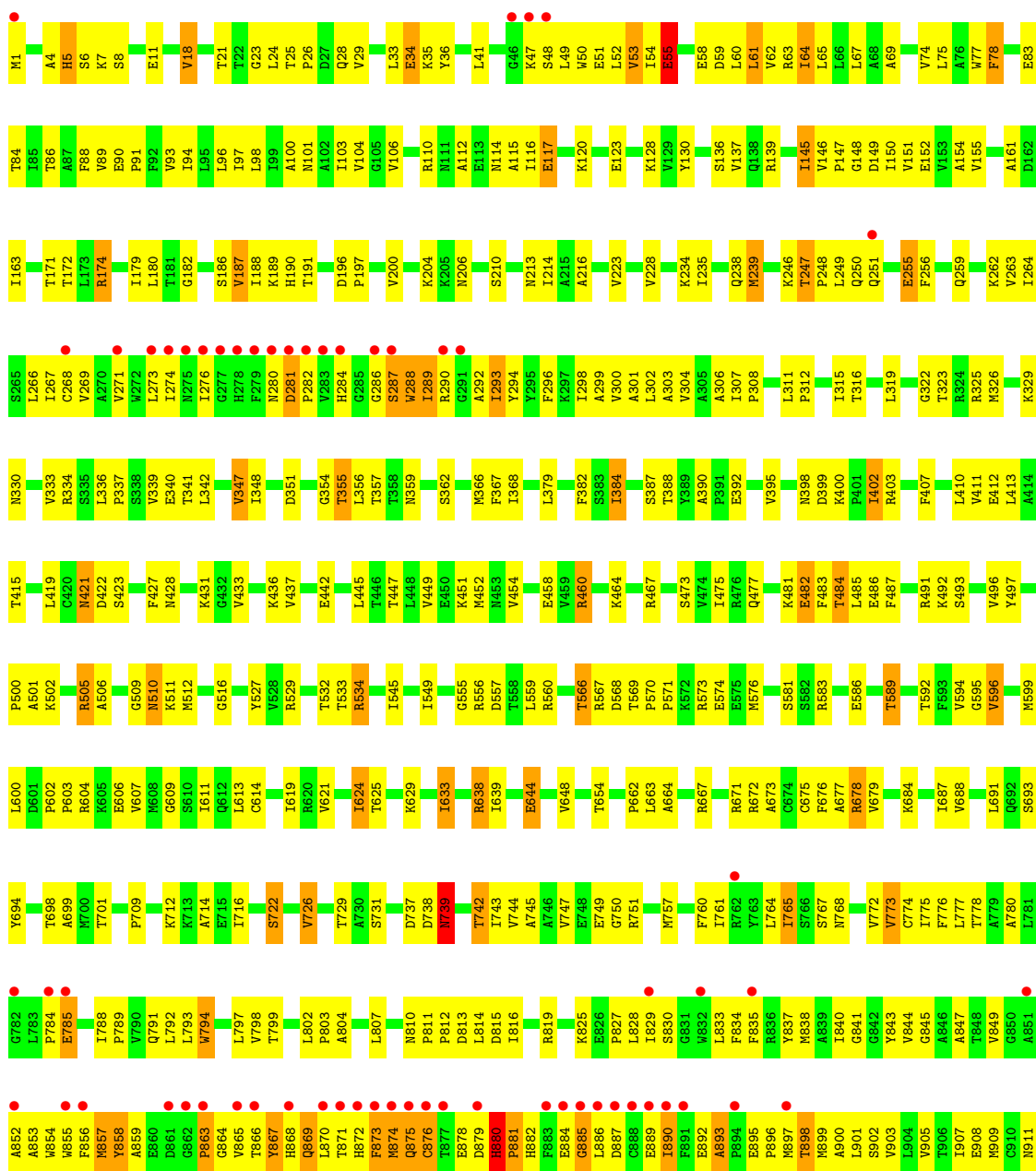
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

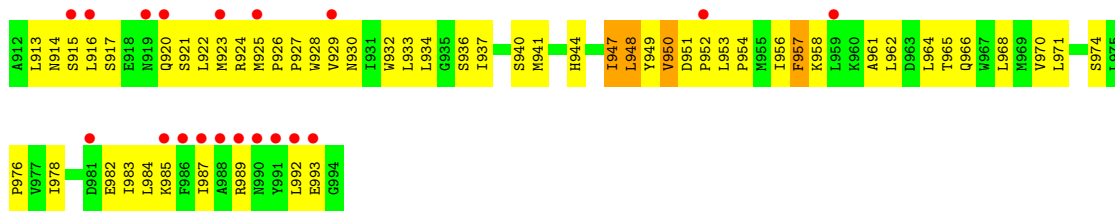




● Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.98Å 94.43Å 136.18Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 47.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.99-3.00) 99.5 (47.21-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 3.01Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.185 , 0.235 0.187 , 0.234	Depositor DCC
$R_{free}$ test set	1039 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 102.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, K, 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	0.60	0/7812	0.80	1/10592 (0.0%)
1	B	0.54	0/7812	0.74	1/10592 (0.0%)
All	All	0.57	0/15624	0.77	2/21184 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	A	162	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	55	GLU	Peptide

### 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	7762	486	0
1	B	7671	0	7762	480	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	14	2	0
5	B	31	0	14	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	15426	0	15552	967	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 31.

All (967) 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:B:50:TRP:O	1:B:53:VAL:HG12	1.43	1.16
1:B:264:ILE:HD11	1:B:306:ALA:HB3	1.30	1.12
1:A:953:LEU:HB2	1:A:954:PRO:HD2	1.23	1.12
1:A:951:ASP:HB3	1:A:952:PRO:HD2	1.38	1.04
1:A:951:ASP:HB3	1:A:952:PRO:CD	1.89	1.02
1:B:985:LYS:HB3	1:B:989:ARG:HH12	1.20	1.02
1:A:25:THR:H	1:A:28:GLN:HE21	1.05	1.02
1:B:678:ARG:HG3	1:B:678:ARG:HH11	1.24	1.01
1:B:855:TRP:HE1	1:B:899:MET:HG3	1.30	0.93
1:A:60:LEU:HD12	1:A:61:LEU:N	1.82	0.93
1:A:953:LEU:HB2	1:A:954:PRO:CD	1.98	0.93
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.51	0.92
1:B:171:THR:HG21	1:B:486:GLU:OE1	1.70	0.92
1:B:1:MET:HB2	1:B:36:TYR:CE1	2.06	0.91
1:B:65:LEU:HD21	1:B:307:ILE:HG13	1.52	0.90
1:B:481:LYS:HG3	1:B:496:VAL:CG1	2.02	0.90
1:A:951:ASP:CB	1:A:952:PRO:HD2	2.03	0.89
1:A:105:GLY:O	1:A:109:GLU:HG2	1.73	0.89
1:B:151:VAL:HG11	1:B:163:ILE:HD13	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:HIS:HA	1:A:282:PRO:HD2	1.55	0.88
1:B:556:ARG:HD2	1:B:644:GLU:O	1.75	0.87
1:B:869:GLN:HG3	1:B:872:HIS:ND1	1.90	0.86
1:A:49:LEU:HD13	1:A:51:GLU:HB2	1.59	0.85
1:A:436:LYS:HB2	1:A:443:THR:HG21	1.58	0.85
1:B:962:LEU:O	1:B:966:GLN:HB2	1.76	0.84
1:A:436:LYS:HE2	1:A:438:GLY:O	1.78	0.83
1:A:449:VAL:HG23	1:A:472:ASN:ND2	1.93	0.83
1:A:656:ARG:HG3	1:A:656:ARG:HH11	1.42	0.82
1:A:527:TYR:CG	1:A:534:ARG:HD3	2.14	0.82
1:B:187:VAL:HG22	1:B:189:LYS:HE2	1.60	0.82
1:A:865:VAL:HB	1:A:868:HIS:CD2	2.15	0.82
1:B:500:PRO:HD3	1:B:509:GLY:HA3	1.62	0.82
1:A:880:HIS:CD2	1:A:881:PRO:HD3	2.15	0.82
1:A:788:ILE:HG13	1:A:791:GLN:HG3	1.61	0.81
1:B:873:PHE:CE1	1:B:876:CYS:HA	2.15	0.81
1:A:869:GLN:HE21	1:A:871:THR:HG23	1.45	0.81
1:A:964:LEU:HD12	1:A:965:THR:HG23	1.61	0.80
1:B:964:LEU:HA	1:B:968:LEU:CD1	2.12	0.80
1:A:917:SER:OG	1:A:920:GLN:HB2	1.81	0.80
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.81	0.79
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.82	0.79
1:B:151:VAL:HG11	1:B:163:ILE:CD1	2.11	0.78
1:B:880:HIS:N	1:B:881:PRO:HD3	1.99	0.78
1:B:878:GLU:HB3	1:B:880:HIS:CD2	2.18	0.78
1:B:460:ARG:HH11	1:B:460:ARG:HB2	1.46	0.78
1:B:876:CYS:SG	1:B:882:HIS:HE1	2.05	0.78
1:A:950:VAL:HG21	1:A:953:LEU:HD12	1.65	0.78
1:B:739:ASN:HB3	1:B:742:THR:HG22	1.66	0.78
1:A:436:LYS:CB	1:A:443:THR:HG21	2.13	0.78
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.19	0.78
1:A:316:THR:O	1:A:316:THR:HG22	1.83	0.77
1:A:99:ILE:O	1:A:103:ILE:HG12	1.84	0.77
1:A:961:ALA:HB1	1:A:966:GLN:HB2	1.66	0.77
1:B:264:ILE:HD11	1:B:306:ALA:CB	2.11	0.77
1:B:855:TRP:NE1	1:B:899:MET:HG3	2.00	0.77
1:A:649:ALA:O	1:A:650:ASP:HB3	1.85	0.77
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.13	0.77
1:A:4:ALA:HB3	1:A:7:LYS:HG2	1.67	0.76
1:B:366:MET:HG2	1:B:384:ILE:HD11	1.66	0.76
1:A:922:LEU:HB3	1:A:927:PRO:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:O	1:A:297:LYS:HB2	1.86	0.76
1:B:964:LEU:HD12	1:B:964:LEU:O	1.85	0.76
1:A:155:VAL:HG12	1:A:216:ALA:HA	1.68	0.76
1:A:336:LEU:O	1:A:339:VAL:HG22	1.86	0.76
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.21	0.75
1:B:411:VAL:O	1:B:415:THR:HG23	1.86	0.75
1:B:922:LEU:HB3	1:B:927:PRO:HG3	1.66	0.75
1:B:51:GLU:O	1:B:54:ILE:HB	1.87	0.75
1:B:481:LYS:HG3	1:B:496:VAL:HG11	1.67	0.75
1:B:837:TYR:HA	1:B:840:ILE:HB	1.69	0.75
1:B:678:ARG:HH11	1:B:678:ARG:CG	1.99	0.74
1:B:930:ASN:O	1:B:934:LEU:HG	1.86	0.74
1:B:100:ALA:O	1:B:103:ILE:HG22	1.87	0.74
1:B:264:ILE:CD1	1:B:306:ALA:HB3	2.13	0.74
1:B:256:PHE:HZ	1:B:765:ILE:HD12	1.51	0.74
1:A:880:HIS:CG	1:A:881:PRO:HD3	2.23	0.74
1:B:765:ILE:HA	1:B:768:ASN:HB2	1.70	0.73
1:A:845:GLY:O	1:A:849:VAL:HG13	1.87	0.73
1:B:281:ASP:HB3	1:B:284:HIS:CD2	2.23	0.73
1:A:79:GLU:O	1:A:79:GLU:HG2	1.88	0.73
1:A:60:LEU:C	1:A:62:VAL:H	1.89	0.73
1:B:60:LEU:HA	1:B:63:ARG:HB3	1.70	0.73
1:B:101:ASN:O	1:B:104:VAL:HG22	1.88	0.73
1:B:985:LYS:HB3	1:B:989:ARG:NH1	2.00	0.72
1:A:60:LEU:HD13	1:A:307:ILE:HD12	1.70	0.72
1:A:953:LEU:C	1:A:955:MET:H	1.92	0.72
1:B:922:LEU:HD12	1:B:922:LEU:H	1.53	0.72
1:A:647:GLU:O	1:A:647:GLU:HG3	1.89	0.72
1:B:288:TRP:C	1:B:290:ARG:H	1.92	0.72
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.71	0.72
1:A:894:PRO:HB3	1:A:959:LEU:H	1.53	0.72
1:B:347:VAL:HG21	1:B:691:LEU:HD22	1.72	0.71
1:A:985:LYS:O	1:A:989:ARG:HG2	1.91	0.71
1:B:50:TRP:O	1:B:53:VAL:CG1	2.31	0.71
1:A:449:VAL:HG23	1:A:472:ASN:HD21	1.51	0.71
1:A:870:LEU:HB3	1:A:873:PHE:CZ	2.25	0.71
1:B:948:LEU:HD11	1:B:961:ALA:HB3	1.73	0.71
1:B:964:LEU:HA	1:B:968:LEU:HD12	1.73	0.71
1:A:947:ILE:O	1:A:954:PRO:HD3	1.91	0.71
1:A:947:ILE:HD13	1:A:953:LEU:HD13	1.73	0.71
1:A:948:LEU:O	1:A:954:PRO:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:VAL:HB	1:B:907:ILE:HG21	1.72	0.71
1:B:764:LEU:HD21	1:B:804:ALA:HB2	1.73	0.70
1:B:930:ASN:HB3	1:B:933:LEU:H	1.56	0.70
1:A:865:VAL:CA	1:A:868:HIS:HD2	2.04	0.70
1:B:859:ALA:HB3	1:B:864:GLY:CA	2.20	0.70
1:B:238:GLN:HG2	1:B:709:PRO:HB3	1.72	0.70
1:B:298:ILE:HD12	1:B:299:ALA:N	2.06	0.70
1:A:919:ASN:O	1:A:989:ARG:HD3	1.91	0.70
1:B:47:LYS:HG3	1:B:47:LYS:O	1.92	0.70
1:B:1:MET:HB2	1:B:36:TYR:HE1	1.52	0.70
1:B:249:LEU:HD11	1:B:340:GLU:HG2	1.74	0.70
1:A:903:VAL:HG23	1:A:970:VAL:HG22	1.73	0.69
1:B:876:CYS:SG	1:B:882:HIS:CE1	2.85	0.69
1:A:988:ALA:O	1:A:992:LEU:HB3	1.92	0.69
1:B:187:VAL:CG2	1:B:189:LYS:HE2	2.22	0.69
1:A:926:PRO:O	1:A:929:VAL:HG23	1.91	0.69
1:B:859:ALA:HB3	1:B:864:GLY:HA2	1.75	0.69
1:B:866:THR:HG22	1:B:867:TYR:CD1	2.28	0.69
1:A:765:ILE:HA	1:A:768:ASN:HD22	1.57	0.69
1:A:869:GLN:HG3	1:A:871:THR:OG1	1.93	0.69
1:A:813:ASP:O	1:A:816:ILE:HB	1.92	0.69
1:A:235:ILE:O	1:A:239:MET:HG2	1.93	0.68
1:A:473:SER:O	1:A:477:GLN:HG2	1.92	0.68
1:B:895:GLU:HA	1:B:898:THR:HG22	1.75	0.68
1:B:235:ILE:O	1:B:239:MET:HG3	1.93	0.68
1:A:961:ALA:HB1	1:A:966:GLN:CB	2.24	0.68
1:A:247:THR:HG23	1:A:250:GLN:HB3	1.76	0.68
1:A:981:ASP:O	1:A:985:LYS:HB2	1.93	0.67
1:A:828:LEU:HD12	1:A:829:ILE:HG12	1.75	0.67
1:A:662:PRO:HG2	1:A:665:GLU:HB2	1.77	0.67
1:B:814:LEU:HD12	1:B:815:ASP:N	2.08	0.67
1:A:72:SER:O	1:A:91:PRO:HG3	1.94	0.67
1:A:189:LYS:HE3	1:A:207:MET:O	1.94	0.67
1:A:775:ILE:HA	1:A:778:THR:HG22	1.77	0.67
1:B:481:LYS:HG3	1:B:496:VAL:HG13	1.77	0.67
1:A:278:HIS:HA	1:A:282:PRO:CD	2.24	0.67
1:A:832:TRP:CH2	1:A:988:ALA:HB2	2.30	0.66
1:B:899:MET:CE	1:B:966:GLN:HB3	2.25	0.66
1:B:648:VAL:HG12	1:B:648:VAL:O	1.95	0.66
1:A:424:SER:HB3	1:A:437:VAL:HG22	1.77	0.66
1:A:833:LEU:HD12	1:A:836:ARG:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HG22	1:B:293:ILE:O	1.96	0.66
1:B:560:ARG:HH12	5:B:998:ACP:H2'	1.61	0.66
1:A:893:ALA:O	1:A:896:PRO:HD2	1.96	0.66
1:B:917:SER:OG	1:B:920:GLN:HB2	1.96	0.66
1:B:483:PHE:HZ	1:B:576:MET:HE1	1.60	0.66
1:B:573:ARG:HA	1:B:576:MET:HE2	1.77	0.66
1:A:281:ASP:CG	1:A:282:PRO:HD3	2.16	0.66
1:B:950:VAL:O	1:B:954:PRO:HD2	1.96	0.66
1:A:869:GLN:HE21	1:A:871:THR:CG2	2.10	0.65
1:B:743:ILE:O	1:B:747:VAL:HG23	1.95	0.65
1:A:95:LEU:O	1:A:99:ILE:HG12	1.96	0.65
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.76	0.65
1:A:870:LEU:HB3	1:A:873:PHE:CE1	2.31	0.65
1:A:953:LEU:CB	1:A:954:PRO:CD	2.74	0.65
1:B:500:PRO:CD	1:B:509:GLY:HA3	2.26	0.65
1:A:292:ALA:O	1:A:296:PHE:HB2	1.96	0.65
1:A:683:HIS:O	1:A:687:ILE:HG13	1.97	0.65
1:B:256:PHE:CZ	1:B:765:ILE:HD12	2.32	0.65
1:A:889:GLU:O	1:A:889:GLU:HG2	1.95	0.65
1:B:624:ILE:HD11	1:B:687:ILE:HG21	1.77	0.65
1:A:656:ARG:HG3	1:A:656:ARG:NH1	2.06	0.65
1:A:832:TRP:CZ3	1:A:836:ARG:HD2	2.32	0.65
1:B:256:PHE:HZ	1:B:765:ILE:CD1	2.09	0.65
1:A:294:TYR:O	1:A:298:ILE:HG13	1.97	0.64
1:A:316:THR:O	1:A:316:THR:CG2	2.44	0.64
1:A:953:LEU:O	1:A:955:MET:N	2.29	0.64
1:B:751:ARG:HB3	1:B:816:ILE:HD11	1.80	0.64
1:B:856:PHE:HE1	1:B:896:PRO:HG2	1.62	0.64
1:A:249:LEU:HD12	1:A:250:GLN:N	2.12	0.64
1:A:717:GLY:O	1:A:731:SER:HB2	1.97	0.64
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.16	0.64
1:A:963:ASP:OD1	1:A:964:LEU:N	2.30	0.64
1:B:106:VAL:O	1:B:110:ARG:HB2	1.97	0.64
1:B:916:LEU:HD13	1:B:933:LEU:CD2	2.28	0.64
1:A:25:THR:H	1:A:28:GLN:NE2	1.88	0.64
1:A:899:MET:SD	1:A:970:VAL:HG23	2.38	0.64
1:A:859:ALA:HB3	1:A:864:GLY:CA	2.28	0.64
1:B:342:LEU:HD13	1:B:716:ILE:HD13	1.80	0.63
1:B:828:LEU:O	1:B:829:ILE:HD13	1.97	0.63
1:B:844:VAL:HB	1:B:907:ILE:HD13	1.80	0.63
1:A:62:VAL:HG12	1:A:63:ARG:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ILE:HG23	1:A:817:MET:HG2	1.80	0.63
1:A:247:THR:HG23	1:A:250:GLN:CB	2.28	0.63
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.78	0.63
1:B:52:LEU:O	1:B:55:GLU:HB2	1.99	0.63
1:B:280:ASN:C	1:B:282:PRO:HD2	2.18	0.63
1:A:716:ILE:HD12	1:A:716:ILE:N	2.13	0.63
1:B:266:LEU:O	1:B:269:VAL:HG22	1.99	0.63
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.81	0.63
1:B:916:LEU:HD13	1:B:933:LEU:HD22	1.79	0.63
1:B:246:LYS:HD2	1:B:250:GLN:HE22	1.64	0.63
1:A:171:THR:HG21	1:A:486:GLU:OE1	1.97	0.63
1:B:428:ASN:ND2	1:B:431:LYS:HD2	2.13	0.62
1:A:53:VAL:HG13	1:A:106:VAL:HG21	1.79	0.62
1:A:720:MET:CE	1:A:735:LEU:HD12	2.29	0.62
1:B:174:ARG:HD3	1:B:188:ILE:HD13	1.81	0.62
1:B:964:LEU:O	1:B:965:THR:HB	1.99	0.62
1:A:270:ALA:HA	1:A:273:LEU:HD23	1.81	0.62
1:B:145:ILE:HD11	1:B:223:VAL:HG21	1.82	0.62
1:B:775:ILE:HA	1:B:778:THR:HG22	1.82	0.62
1:A:774:CYS:O	1:A:778:THR:HB	2.00	0.62
1:A:975:LEU:HB2	1:A:976:PRO:HD3	1.81	0.62
1:B:857:MET:SD	1:B:867:TYR:HA	2.39	0.62
1:B:941:MET:HA	1:B:944:HIS:HB3	1.81	0.62
1:A:94:ILE:O	1:A:98:LEU:HB2	2.00	0.62
1:A:264:ILE:HD11	1:A:306:ALA:HB3	1.80	0.62
1:B:174:ARG:HG3	1:B:216:ALA:HB3	1.82	0.62
1:B:624:ILE:HD13	1:B:687:ILE:HD13	1.80	0.62
1:A:743:ILE:O	1:A:747:VAL:HG12	2.00	0.62
1:A:865:VAL:C	1:A:868:HIS:HD2	2.02	0.62
1:A:51:GLU:HB3	1:A:54:ILE:HG13	1.80	0.62
1:A:90:GLU:O	1:A:94:ILE:HG12	1.99	0.62
1:A:484:THR:HB	1:A:496:VAL:HG23	1.81	0.62
1:B:247:THR:HB	1:B:248:PRO:HD2	1.82	0.62
1:B:529:ARG:NH2	1:B:592:THR:HG21	2.15	0.62
1:B:239:MET:O	1:B:712:LYS:HE3	2.00	0.61
1:A:846:ALA:O	1:A:849:VAL:HG22	2.00	0.61
1:B:77:TRP:HD1	1:B:78:PHE:CD1	2.18	0.61
1:A:951:ASP:CB	1:A:952:PRO:CD	2.64	0.61
1:B:447:THR:HG22	1:B:451:LYS:HE3	1.82	0.61
1:B:844:VAL:CB	1:B:907:ILE:HG21	2.30	0.61
1:A:927:PRO:HD2	1:A:928:TRP:CZ3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.80	0.61
1:B:671:ARG:HH21	1:B:694:TYR:HB3	1.65	0.61
1:A:556:ARG:HH11	1:A:644:GLU:HB3	1.66	0.61
1:B:905:VAL:O	1:B:909:MET:HG2	2.00	0.61
1:A:992:LEU:HG	1:A:993:GLU:N	2.15	0.61
1:A:413:LEU:HD11	1:A:564:LEU:HD12	1.83	0.61
1:B:483:PHE:HZ	1:B:576:MET:CE	2.14	0.61
1:B:784:PRO:HD3	1:B:870:LEU:HD22	1.82	0.61
1:A:333:VAL:HG21	1:A:339:VAL:CG1	2.31	0.61
1:A:765:ILE:HD13	1:A:837:TYR:CE1	2.36	0.60
1:B:60:LEU:CA	1:B:63:ARG:HB3	2.30	0.60
1:B:84:THR:HG22	1:B:86:THR:H	1.65	0.60
1:A:198:ARG:HH21	1:A:659:ASP:HB3	1.64	0.60
1:B:607:VAL:O	1:B:611:ILE:HG12	2.01	0.60
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.82	0.60
1:A:767:SER:HB3	1:A:908:GLU:CD	2.22	0.60
1:A:784:PRO:HD3	1:A:873:PHE:CZ	2.36	0.60
1:B:484:THR:HB	1:B:496:VAL:HG22	1.84	0.60
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.01	0.60
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.00	0.60
1:B:567:ARG:NH1	1:B:571:PRO:HD3	2.16	0.60
1:B:629:LYS:O	1:B:633:ILE:HG13	2.01	0.60
1:B:803:PRO:O	1:B:807:LEU:HG	2.01	0.60
1:A:412:GLU:OE2	1:A:566:THR:CG2	2.49	0.60
1:A:865:VAL:O	1:A:868:HIS:HB2	2.02	0.60
1:A:963:ASP:O	1:A:964:LEU:HG	2.02	0.60
1:B:920:GLN:HB3	1:B:925:MET:HB2	1.83	0.60
1:B:722:SER:OG	1:B:738:ASP:OD1	2.20	0.60
1:B:964:LEU:HA	1:B:968:LEU:HD11	1.84	0.60
1:B:5:HIS:CD2	1:B:6:SER:N	2.69	0.59
1:A:815:ASP:CG	1:A:815:ASP:O	2.39	0.59
1:A:932:TRP:HA	1:A:932:TRP:CE3	2.37	0.59
1:B:869:GLN:HE21	1:B:872:HIS:CE1	2.21	0.59
1:A:484:THR:HB	1:A:496:VAL:CG2	2.32	0.59
1:B:62:VAL:HG13	1:B:98:LEU:HD22	1.83	0.59
1:A:649:ALA:O	1:A:650:ASP:CB	2.50	0.59
1:B:304:VAL:HG13	1:B:792:LEU:HD12	1.84	0.59
1:B:625:THR:HA	2:B:995:ALF:F1	1.93	0.59
1:B:843:TYR:OH	1:B:976:PRO:HB2	2.02	0.59
1:B:844:VAL:CG1	1:B:907:ILE:HG21	2.32	0.59
1:A:13:LEU:HD21	1:A:20:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.38	0.59
1:A:256:PHE:HA	1:A:259:GLN:HG2	1.85	0.59
1:A:450:GLU:OE2	1:A:467:ARG:NH2	2.36	0.59
1:A:720:MET:HE1	1:A:735:LEU:HD12	1.85	0.59
1:A:778:THR:OG1	1:A:785:GLU:HA	2.02	0.59
1:A:951:ASP:O	1:A:953:LEU:N	2.35	0.59
1:A:829:ILE:HD12	1:A:837:TYR:HE2	1.67	0.59
1:B:909:MET:SD	1:B:937:ILE:HG23	2.43	0.59
1:A:912:ALA:O	1:A:933:LEU:HD21	2.03	0.58
1:B:567:ARG:CZ	1:B:571:PRO:HD3	2.33	0.58
1:B:992:LEU:O	1:B:992:LEU:HG	2.03	0.58
1:B:128:LYS:HB3	1:B:137:VAL:CG2	2.33	0.58
1:B:413:LEU:HD12	1:B:595:GLY:HA3	1.84	0.58
1:B:445:LEU:O	1:B:449:VAL:HG13	2.02	0.58
1:B:987:ILE:O	1:B:987:ILE:HG22	2.03	0.58
1:A:505:ARG:O	1:A:506:ALA:HB3	2.02	0.58
1:A:960:LYS:HD2	1:A:960:LYS:O	2.03	0.58
1:B:25:THR:OG1	1:B:28:GLN:HG3	2.02	0.58
1:B:322:GLY:HA2	1:B:325:ARG:HB2	1.84	0.58
1:A:298:ILE:C	1:A:298:ILE:HD12	2.24	0.58
1:A:880:HIS:CE1	1:A:881:PRO:HG3	2.38	0.58
1:A:947:ILE:CD1	1:A:953:LEU:HD13	2.33	0.58
1:B:161:ALA:HA	1:B:210:SER:HB2	1.85	0.58
1:B:921:SER:HB2	1:B:982:GLU:OE1	2.03	0.58
1:B:501:ALA:O	1:B:502:LYS:HG2	2.04	0.58
1:B:874:MET:HG2	1:B:874:MET:O	2.02	0.58
1:B:916:LEU:HD11	1:B:930:ASN:ND2	2.19	0.58
1:A:47:LYS:HE2	1:A:242:THR:HG23	1.86	0.58
1:A:60:LEU:O	1:A:62:VAL:N	2.37	0.58
1:A:267:ILE:O	1:A:271:VAL:HG13	2.04	0.58
1:B:390:ALA:C	1:B:392:GLU:H	2.07	0.58
1:A:355:THR:O	1:A:604:ARG:HD2	2.03	0.58
1:B:161:ALA:CA	1:B:210:SER:HB2	2.34	0.58
1:B:334:ARG:HD3	1:B:731:SER:O	2.04	0.58
1:B:791:GLN:HB3	1:B:901:LEU:HD12	1.86	0.58
1:A:145:ILE:CD1	1:A:223:VAL:HG21	2.34	0.57
1:B:600:LEU:O	1:B:602:PRO:HD3	2.03	0.57
1:A:115:ALA:HA	1:A:729:THR:HG21	1.85	0.57
1:A:384:ILE:HG23	1:A:395:VAL:HG22	1.85	0.57
1:A:930:ASN:HB3	1:A:933:LEU:H	1.68	0.57
1:B:333:VAL:HG11	1:B:339:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:ASN:HB3	1:B:811:PRO:HD2	1.85	0.57
1:B:340:GLU:HA	1:B:750:GLY:HA2	1.85	0.57
1:B:856:PHE:HD2	1:B:870:LEU:HD11	1.69	0.57
1:B:120:LYS:HA	1:B:123:GLU:HG3	1.84	0.57
1:A:791:GLN:O	1:A:795:VAL:HG23	2.05	0.57
1:A:799:THR:HG22	1:A:909:MET:HE3	1.86	0.57
1:A:905:VAL:O	1:A:909:MET:HG2	2.04	0.57
1:A:52:LEU:HD22	1:A:106:VAL:HG22	1.85	0.57
1:A:60:LEU:C	1:A:62:VAL:N	2.58	0.57
1:A:832:TRP:CH2	1:A:836:ARG:HD2	2.38	0.57
1:A:988:ALA:HB1	1:A:992:LEU:HD22	1.86	0.57
1:B:319:LEU:HB3	1:B:336:LEU:HB3	1.87	0.57
1:A:79:GLU:HG3	1:A:87:ALA:HB2	1.86	0.57
1:A:539:GLY:N	1:A:540:PRO:HD2	2.20	0.57
1:B:965:THR:H	1:B:968:LEU:HD12	1.69	0.57
1:A:872:HIS:CE1	1:A:874:MET:HB3	2.39	0.57
1:B:911:ASN:HA	1:B:914:ASN:HB2	1.87	0.57
1:A:8:SER:OG	1:A:11:GLU:HG3	2.04	0.57
1:A:101:ASN:O	1:A:104:VAL:HG22	2.05	0.57
1:B:4:ALA:HB1	1:B:6:SER:OG	2.05	0.57
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.86	0.56
1:A:863:PRO:HB2	1:A:890:ILE:HG21	1.86	0.56
1:B:830:SER:H	1:B:833:LEU:HB3	1.70	0.56
1:A:255:GLU:HA	1:A:258:GLU:HB3	1.88	0.56
1:B:5:HIS:HD2	1:B:6:SER:N	2.03	0.56
1:B:301:ALA:HA	1:B:789:PRO:HG3	1.88	0.56
1:B:926:PRO:O	1:B:929:VAL:HG23	2.04	0.56
1:A:436:LYS:HB2	1:A:443:THR:CG2	2.34	0.56
1:A:722:SER:OG	1:A:738:ASP:OD1	2.24	0.56
1:A:901:LEU:CD2	1:A:944:HIS:HE1	2.18	0.56
1:B:288:TRP:C	1:B:290:ARG:N	2.59	0.56
1:B:354:GLY:N	1:B:359:ASN:HB2	2.20	0.56
1:B:609:GLY:O	1:B:613:LEU:HD13	2.06	0.56
1:A:936:SER:O	1:A:940:SER:HB2	2.06	0.56
1:B:248:PRO:HD2	1:B:341:THR:HG22	1.85	0.56
1:B:965:THR:HG22	1:B:965:THR:O	2.06	0.56
1:A:775:ILE:HA	1:A:778:THR:CG2	2.36	0.56
1:B:624:ILE:HD13	1:B:687:ILE:CD1	2.36	0.56
1:A:803:PRO:O	1:A:807:LEU:HG	2.06	0.56
1:A:828:LEU:CD1	1:A:829:ILE:HG12	2.36	0.56
1:B:834:PHE:O	1:B:838:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:C	1:A:360:GLN:HG2	2.27	0.56
1:B:8:SER:OG	1:B:11:GLU:HG3	2.04	0.56
1:A:44:GLU:HB2	1:A:116:ILE:HD12	1.88	0.56
1:A:52:LEU:C	1:A:52:LEU:HD23	2.26	0.56
1:A:296:PHE:O	1:A:300:VAL:HG13	2.06	0.56
1:A:767:SER:HB3	1:A:908:GLU:OE1	2.06	0.56
1:A:863:PRO:CB	1:A:890:ILE:HG21	2.35	0.55
1:A:79:GLU:HG3	1:A:87:ALA:CB	2.36	0.55
1:A:183:GLU:OE2	1:A:627:ASP:HB2	2.06	0.55
1:B:251:GLN:O	1:B:255:GLU:HG3	2.05	0.55
1:A:4:ALA:HB1	1:A:6:SER:H	1.72	0.55
1:A:946:LEU:O	1:A:950:VAL:CG2	2.55	0.55
1:B:24:LEU:CD1	1:B:149:ASP:HB3	2.37	0.55
1:A:739:ASN:O	1:A:742:THR:HG23	2.07	0.55
1:A:927:PRO:HD2	1:A:928:TRP:CE3	2.41	0.55
1:A:248:PRO:HG2	1:A:341:THR:HG22	1.89	0.55
1:A:865:VAL:O	1:A:865:VAL:HG23	2.06	0.55
1:B:24:LEU:HD12	1:B:149:ASP:HB3	1.88	0.55
1:B:34:GLU:OE1	1:B:34:GLU:HA	2.06	0.55
1:A:744:VAL:O	1:A:747:VAL:HG13	2.07	0.55
1:A:953:LEU:C	1:A:955:MET:N	2.59	0.55
1:B:974:SER:C	1:B:976:PRO:HD2	2.27	0.55
1:B:292:ALA:O	1:B:296:PHE:HB2	2.07	0.55
1:A:901:LEU:HD21	1:A:944:HIS:CE1	2.41	0.55
1:B:329:LYS:O	1:B:330:ASN:HB2	2.06	0.55
1:A:4:ALA:HB1	1:A:6:SER:OG	2.07	0.54
1:A:303:ALA:O	1:A:307:ILE:HG12	2.07	0.54
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.23	0.54
1:B:262:LYS:O	1:B:266:LEU:HB2	2.07	0.54
1:B:739:ASN:O	1:B:742:THR:HG22	2.07	0.54
1:B:930:ASN:HB2	1:B:933:LEU:HB3	1.90	0.54
1:B:855:TRP:HE1	1:B:899:MET:CG	2.13	0.54
1:B:947:ILE:O	1:B:947:ILE:HG13	2.08	0.54
1:A:395:VAL:C	1:A:396:LEU:HD23	2.27	0.54
1:B:354:GLY:O	1:B:604:ARG:NH1	2.40	0.54
1:B:613:LEU:HD23	1:B:744:VAL:HG11	1.88	0.54
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.89	0.54
1:B:100:ALA:O	1:B:104:VAL:HG13	2.08	0.54
1:B:286:GLY:O	1:B:287:SER:C	2.46	0.54
1:B:325:ARG:HD2	1:B:749:GLU:OE1	2.07	0.54
1:A:295:TYR:O	1:A:299:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:PHE:CD1	1:B:676:PHE:N	2.76	0.54
1:A:259:GLN:O	1:A:263:VAL:HG23	2.07	0.54
1:B:151:VAL:CG1	1:B:163:ILE:HD13	2.32	0.54
1:B:256:PHE:HA	1:B:259:GLN:HG2	1.90	0.54
1:B:411:VAL:HG22	1:B:454:VAL:HB	1.90	0.54
1:A:607:VAL:O	1:A:611:ILE:HG12	2.08	0.54
1:B:342:LEU:O	1:B:747:VAL:HG13	2.07	0.54
1:B:951:ASP:HB2	1:B:952:PRO:HD3	1.90	0.54
1:B:301:ALA:HA	1:B:304:VAL:HG12	1.90	0.53
1:A:109:GLU:C	1:A:111:ASN:H	2.10	0.53
1:B:18:VAL:HG11	1:B:148:GLY:O	2.08	0.53
1:B:852:ALA:HB2	1:B:900:ALA:HB2	1.91	0.53
1:B:930:ASN:CB	1:B:933:LEU:HB3	2.38	0.53
1:A:90:GLU:OE2	1:A:789:PRO:HB2	2.09	0.53
1:A:524:ARG:HH21	1:A:588:GLU:CB	2.21	0.53
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.08	0.53
1:B:281:ASP:HB3	1:B:284:HIS:NE2	2.22	0.53
1:A:859:ALA:HB3	1:A:864:GLY:HA3	1.90	0.53
1:B:47:LYS:O	1:B:47:LYS:CG	2.56	0.53
1:B:325:ARG:NH1	1:B:749:GLU:OE2	2.41	0.53
1:A:352:LYS:HD2	1:A:635:ILE:HG13	1.90	0.53
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.44	0.53
1:B:263:VAL:O	1:B:267:ILE:HB	2.09	0.53
1:B:288:TRP:O	1:B:289:ILE:HB	2.09	0.53
1:A:703:ASP:HB2	1:A:723:GLY:HA3	1.90	0.53
1:B:50:TRP:NE1	1:B:51:GLU:HG3	2.24	0.53
1:B:174:ARG:HB3	1:B:186:SER:HB3	1.91	0.53
1:B:415:THR:HA	1:B:475:ILE:HG21	1.91	0.53
1:A:413:LEU:HD11	1:A:564:LEU:CD1	2.38	0.52
1:B:336:LEU:N	1:B:337:PRO:HD2	2.24	0.52
1:A:648:VAL:O	1:A:649:ALA:C	2.46	0.52
1:B:899:MET:HE3	1:B:966:GLN:HB3	1.92	0.52
1:A:25:THR:N	1:A:28:GLN:HE21	1.89	0.52
1:B:410:LEU:HB3	1:B:452:MET:CE	2.40	0.52
1:B:739:ASN:HB3	1:B:742:THR:CG2	2.38	0.52
1:B:866:THR:HG22	1:B:867:TYR:HD1	1.73	0.52
1:A:33:LEU:O	1:A:33:LEU:HD23	2.09	0.52
1:A:51:GLU:O	1:A:52:LEU:C	2.48	0.52
1:A:395:VAL:HG12	1:A:402:ILE:CD1	2.39	0.52
1:B:74:VAL:HG13	1:B:75:LEU:HD12	1.91	0.52
1:B:294:TYR:O	1:B:298:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PHE:O	1:B:300:VAL:HG13	2.09	0.52
1:A:16:PHE:CD1	1:A:222:ILE:HD11	2.45	0.52
1:A:169:LYS:HD3	1:A:169:LYS:N	2.24	0.52
1:A:898:THR:HG21	1:A:961:ALA:HB2	1.91	0.52
1:B:825:LYS:O	1:B:827:PRO:HD3	2.10	0.52
1:A:863:PRO:HG2	1:A:890:ILE:HD12	1.92	0.52
1:A:901:LEU:CD2	1:A:944:HIS:CE1	2.93	0.52
1:B:235:ILE:O	1:B:239:MET:CG	2.58	0.52
1:B:511:LYS:HZ2	1:B:568:ASP:HA	1.75	0.52
1:A:194:VAL:HG23	1:A:206:ASN:ND2	2.24	0.52
1:A:760:PHE:CD1	1:A:760:PHE:C	2.83	0.52
1:A:865:VAL:C	1:A:868:HIS:CD2	2.83	0.52
1:A:330:ASN:HB3	1:A:736:ALA:HB3	1.92	0.52
5:A:998:ACP:O2B	5:A:998:ACP:H5'2	2.09	0.52
1:A:114:ASN:OD1	1:A:117:GLU:HB2	2.10	0.51
1:A:778:THR:HG23	1:A:778:THR:O	2.10	0.51
1:B:382:PHE:CE1	1:B:410:LEU:HD21	2.45	0.51
1:B:452:MET:HE2	1:B:454:VAL:CG1	2.40	0.51
1:B:500:PRO:HD3	1:B:509:GLY:CA	2.38	0.51
1:B:847:ALA:O	1:B:903:VAL:HG11	2.10	0.51
1:B:865:VAL:HB	1:B:868:HIS:CG	2.45	0.51
1:A:758:LYS:O	1:A:762:ARG:HG3	2.10	0.51
1:B:460:ARG:HB2	1:B:460:ARG:NH1	2.22	0.51
1:A:387:SER:HB2	1:A:602:PRO:HG2	1.92	0.51
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.91	0.51
1:B:96:LEU:HD23	1:B:96:LEU:O	2.10	0.51
1:A:23:GLY:HA3	1:A:130:TYR:O	2.10	0.51
1:A:51:GLU:O	1:A:53:VAL:N	2.44	0.51
1:A:290:ARG:HD2	1:A:874:MET:HE2	1.92	0.51
1:A:666:GLN:NE2	1:A:690:TYR:OH	2.44	0.51
1:B:268:CYS:HB3	1:B:302:LEU:CD2	2.41	0.51
1:B:855:TRP:CZ2	1:B:966:GLN:HG3	2.45	0.51
1:B:873:PHE:CZ	1:B:881:PRO:HG2	2.46	0.51
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.40	0.51
1:A:264:ILE:HD11	1:A:306:ALA:CB	2.40	0.51
1:A:678:ARG:O	1:A:678:ARG:HG2	2.11	0.51
1:A:957:PHE:O	1:A:958:LYS:HD3	2.10	0.51
1:B:115:ALA:HA	1:B:729:THR:HG21	1.93	0.51
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.92	0.51
1:B:323:THR:OG1	1:B:336:LEU:HD22	2.10	0.51
1:B:893:ALA:O	1:B:896:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:ASP:OD1	1:B:819:ARG:NH2	2.44	0.51
1:A:969:MET:O	1:A:973:ILE:HG13	2.10	0.51
1:B:97:ILE:O	1:B:101:ASN:HB2	2.10	0.51
1:B:757:MET:HG2	1:B:760:PHE:CZ	2.45	0.51
1:B:880:HIS:N	1:B:881:PRO:CD	2.69	0.51
1:B:881:PRO:HD2	1:B:882:HIS:H	1.76	0.51
1:A:857:MET:SD	1:A:867:TYR:HA	2.51	0.51
1:A:948:LEU:O	1:A:954:PRO:CG	2.59	0.51
1:B:247:THR:HB	1:B:248:PRO:CD	2.40	0.51
1:A:79:GLU:O	1:A:79:GLU:CG	2.56	0.51
1:A:688:VAL:O	1:A:692:GLN:HG3	2.11	0.50
1:A:859:ALA:HB3	1:A:864:GLY:HA2	1.93	0.50
1:B:5:HIS:CD2	1:B:6:SER:HB3	2.46	0.50
1:B:281:ASP:N	1:B:282:PRO:CD	2.74	0.50
1:B:878:GLU:CB	1:B:880:HIS:CD2	2.92	0.50
1:A:777:LEU:C	1:A:779:ALA:H	2.14	0.50
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.92	0.50
1:B:89:VAL:HG21	1:B:956:ILE:HG21	1.92	0.50
1:B:844:VAL:HG11	1:B:907:ILE:HG21	1.93	0.50
1:A:30:LYS:O	1:A:34:GLU:HB2	2.11	0.50
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.94	0.50
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.92	0.50
1:A:865:VAL:CB	1:A:868:HIS:CD2	2.91	0.50
1:A:946:LEU:O	1:A:950:VAL:HG21	2.11	0.50
1:B:354:GLY:CA	1:B:359:ASN:HB2	2.42	0.50
1:A:472:ASN:O	1:A:476:ARG:HG2	2.10	0.50
1:B:89:VAL:HG21	1:B:956:ILE:CG2	2.41	0.50
1:B:410:LEU:HB3	1:B:452:MET:HE1	1.93	0.50
1:A:768:ASN:O	1:A:772:VAL:HG23	2.12	0.50
1:B:897:MET:SD	1:B:958:LYS:HE2	2.51	0.50
1:A:262:LYS:O	1:A:266:LEU:HB2	2.11	0.50
1:B:154:ALA:O	1:B:214:ILE:HB	2.11	0.50
1:B:950:VAL:HB	1:B:953:LEU:HD12	1.92	0.50
1:A:60:LEU:HD12	1:A:61:LEU:H	1.72	0.50
1:A:188:ILE:HD13	1:A:487:PHE:CE2	2.46	0.50
1:A:449:VAL:CG2	1:A:472:ASN:HD21	2.22	0.50
1:A:300:VAL:O	1:A:300:VAL:HG23	2.10	0.50
1:B:322:GLY:O	1:B:326:MET:HG2	2.12	0.50
1:B:25:THR:HB	1:B:26:PRO:CD	2.42	0.49
1:B:83:GLU:CD	1:B:83:GLU:H	2.14	0.49
1:B:859:ALA:HB3	1:B:864:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:ILE:O	1:B:982:GLU:HB2	2.12	0.49
1:A:198:ARG:NH2	1:A:659:ASP:HB3	2.28	0.49
1:B:757:MET:O	1:B:761:ILE:HG13	2.12	0.49
1:A:114:ASN:OD1	1:A:117:GLU:CB	2.61	0.49
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.93	0.49
1:B:146:VAL:O	1:B:147:PRO:C	2.49	0.49
1:A:947:ILE:HD12	1:A:957:PHE:CE1	2.47	0.49
1:A:325:ARG:NH1	1:A:749:GLU:OE2	2.45	0.49
1:A:793:LEU:HD23	1:A:793:LEU:N	2.27	0.49
1:B:505:ARG:HG3	1:B:506:ALA:HA	1.95	0.49
1:B:23:GLY:HA3	1:B:130:TYR:O	2.12	0.49
1:A:878:GLU:HG3	1:A:878:GLU:O	2.12	0.49
1:B:421:ASN:HD22	1:B:422:ASP:H	1.61	0.49
1:A:4:ALA:CB	1:A:7:LYS:HG2	2.39	0.49
1:A:67:LEU:O	1:A:69:ALA:N	2.45	0.49
1:B:487:PHE:CE1	1:B:492:LYS:HA	2.47	0.49
1:B:948:LEU:HD22	1:B:949:TYR:CE1	2.47	0.49
1:A:200:VAL:O	1:A:203:ASP:HB2	2.12	0.49
1:B:65:LEU:HB2	1:B:98:LEU:HD21	1.94	0.49
1:B:172:THR:HG21	1:B:174:ARG:HH21	1.78	0.49
1:A:716:ILE:HD12	1:A:716:ILE:H	1.78	0.49
1:A:880:HIS:CG	1:A:881:PRO:CD	2.94	0.49
1:B:51:GLU:HG2	1:B:54:ILE:HD12	1.94	0.48
1:B:493:SER:HB3	1:B:516:GLY:HA3	1.95	0.48
1:A:625:THR:HA	2:A:995:ALF:F3	2.03	0.48
1:A:357:THR:HA	1:A:603:PRO:HA	1.94	0.48
1:B:773:VAL:CG1	1:B:845:GLY:HA3	2.43	0.48
1:B:873:PHE:HB2	1:B:875:GLN:HG3	1.96	0.48
1:A:57:PHE:HA	1:A:62:VAL:HG21	1.95	0.48
1:B:624:ILE:CD1	1:B:687:ILE:HG21	2.43	0.48
1:B:932:TRP:O	1:B:936:SER:HB3	2.12	0.48
1:A:315:ILE:C	1:A:317:THR:H	2.17	0.48
1:A:424:SER:HB3	1:A:437:VAL:CG2	2.42	0.48
1:A:518:PRO:O	1:A:522:ILE:HG13	2.14	0.48
1:A:762:ARG:HD3	1:A:833:LEU:HD21	1.95	0.48
1:A:898:THR:CG2	1:A:961:ALA:HB2	2.42	0.48
1:B:23:GLY:HA2	1:B:150:ILE:HG12	1.95	0.48
1:B:65:LEU:HD21	1:B:307:ILE:CG1	2.35	0.48
1:B:863:PRO:HB2	1:B:890:ILE:HD11	1.96	0.48
1:B:884:GLU:O	1:B:886:LEU:N	2.47	0.48
1:A:83:GLU:HG2	1:A:83:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:CD2	1:A:600:LEU:HD13	2.44	0.48
1:A:856:PHE:HB3	1:A:865:VAL:HG22	1.94	0.48
1:A:858:TYR:O	1:A:860:GLU:N	2.46	0.48
1:B:362:SER:O	1:B:599:MET:HA	2.14	0.48
1:A:505:ARG:O	1:A:506:ALA:CB	2.62	0.48
1:A:884:GLU:HB3	1:A:887:ASP:OD2	2.13	0.48
1:A:894:PRO:CB	1:A:959:LEU:H	2.24	0.48
1:B:351:ASP:OD2	1:B:355:THR:CG2	2.61	0.48
1:B:654:THR:HA	1:B:677:ALA:O	2.14	0.48
1:A:25:THR:O	1:A:29:VAL:HG23	2.14	0.48
1:A:840:ILE:HG22	1:A:841:GLY:N	2.28	0.48
1:B:421:ASN:HD22	1:B:422:ASP:N	2.10	0.48
1:B:671:ARG:HH21	1:B:694:TYR:CB	2.26	0.48
1:B:921:SER:HB3	1:B:989:ARG:NH2	2.29	0.48
1:B:948:LEU:HD11	1:B:961:ALA:CB	2.42	0.48
1:A:487:PHE:HA	1:A:493:SER:O	2.14	0.48
1:A:839:ALA:HB3	1:A:984:LEU:HD11	1.96	0.48
1:A:964:LEU:HA	1:A:968:LEU:HD21	1.95	0.48
1:B:303:ALA:O	1:B:307:ILE:HG12	2.14	0.47
1:B:606:GLU:HG3	1:B:739:ASN:ND2	2.29	0.47
1:A:930:ASN:HB2	1:A:933:LEU:HB3	1.96	0.47
1:B:51:GLU:HA	1:B:54:ILE:HG13	1.96	0.47
1:B:529:ARG:NH2	1:B:568:ASP:OD2	2.47	0.47
1:A:508:VAL:HG23	1:A:508:VAL:O	2.14	0.47
1:A:524:ARG:HH21	1:A:588:GLU:HB2	1.79	0.47
1:B:59:ASP:C	1:B:61:LEU:H	2.17	0.47
1:B:93:VAL:HG12	1:B:793:LEU:HD13	1.97	0.47
1:B:315:ILE:HG22	1:B:316:THR:N	2.28	0.47
1:B:773:VAL:HG13	1:B:845:GLY:HA3	1.95	0.47
1:A:719:ALA:HB3	1:A:734:VAL:HG22	1.97	0.47
1:A:739:ASN:C	1:A:739:ASN:HD22	2.17	0.47
1:A:895:GLU:N	1:A:896:PRO:CD	2.77	0.47
1:B:190:HIS:O	1:B:206:ASN:HA	2.14	0.47
1:B:775:ILE:O	1:B:775:ILE:HG22	2.15	0.47
1:B:268:CYS:O	1:B:271:VAL:HG22	2.15	0.47
1:B:844:VAL:CB	1:B:907:ILE:HD13	2.45	0.47
1:A:52:LEU:HD23	1:A:53:VAL:N	2.29	0.47
1:A:61:LEU:HD21	1:A:312:PRO:CG	2.45	0.47
1:A:74:VAL:HG22	1:A:78:PHE:HE2	1.78	0.47
1:A:430:THR:HG22	1:A:431:LYS:N	2.29	0.47
1:A:865:VAL:CB	1:A:868:HIS:HD2	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG13	1:B:54:ILE:N	2.30	0.47
1:B:86:THR:O	1:B:89:VAL:HG12	2.14	0.47
1:B:304:VAL:HG11	1:B:789:PRO:HB3	1.97	0.47
1:B:402:ILE:HG12	1:B:403:ARG:N	2.29	0.47
1:B:678:ARG:HG3	1:B:678:ARG:NH1	2.05	0.47
1:B:828:LEU:HD12	1:B:829:ILE:HG12	1.96	0.47
1:B:882:HIS:CD2	1:B:885:GLY:HA3	2.49	0.47
1:A:421:ASN:HD22	1:A:423:SER:H	1.61	0.47
1:B:58:GLU:O	1:B:60:LEU:HG	2.15	0.47
1:B:248:PRO:HD2	1:B:341:THR:CG2	2.44	0.47
1:B:667:ARG:NH2	1:B:693:SER:O	2.48	0.47
1:B:971:LEU:HD23	1:B:971:LEU:O	2.15	0.47
1:A:612:GLN:HA	1:A:612:GLN:OE1	2.14	0.47
1:A:829:ILE:CG2	1:A:834:PHE:HB2	2.44	0.47
1:A:865:VAL:HG23	1:A:868:HIS:HB2	1.97	0.47
1:A:903:VAL:O	1:A:907:ILE:HG13	2.14	0.47
1:B:25:THR:HB	1:B:26:PRO:HD2	1.97	0.47
1:A:83:GLU:HB2	1:A:86:THR:HG22	1.97	0.47
1:A:496:VAL:O	1:A:512:MET:HA	2.15	0.47
1:B:5:HIS:ND1	1:B:204:LYS:HG2	2.30	0.47
1:B:672:ARG:HG3	1:B:673:ALA:N	2.30	0.47
1:B:678:ARG:CG	1:B:678:ARG:NH1	2.68	0.47
1:A:342:LEU:HD13	1:A:716:ILE:HG21	1.96	0.46
1:B:69:ALA:HB2	1:B:94:ILE:HG21	1.96	0.46
1:B:151:VAL:HG13	1:B:152:GLU:N	2.30	0.46
1:B:483:PHE:HE2	1:B:485:LEU:HD21	1.81	0.46
1:B:873:PHE:HD1	1:B:875:GLN:CD	2.18	0.46
1:B:901:LEU:HD23	1:B:901:LEU:O	2.14	0.46
1:B:948:LEU:HD21	1:B:961:ALA:H	1.80	0.46
1:A:353:THR:HA	1:A:357:THR:OG1	2.16	0.46
1:A:145:ILE:HD11	1:A:223:VAL:HG21	1.97	0.46
1:A:392:GLU:O	1:A:451:LYS:HE2	2.15	0.46
1:A:921:SER:HB2	1:A:989:ARG:NE	2.31	0.46
1:B:300:VAL:O	1:B:304:VAL:HG12	2.16	0.46
1:B:671:ARG:HA	1:B:671:ARG:HD3	1.80	0.46
1:B:899:MET:HE1	1:B:966:GLN:HB3	1.97	0.46
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.61	0.46
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.98	0.46
1:B:128:LYS:HB3	1:B:137:VAL:HG22	1.98	0.46
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.45	0.46
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:PHE:O	1:B:91:PRO:HD2	2.15	0.46
1:A:71:ILE:O	1:A:75:LEU:HG	2.16	0.46
1:A:275:ASN:O	1:A:277:GLY:N	2.48	0.46
1:A:921:SER:HA	1:A:985:LYS:HD2	1.98	0.46
1:B:171:THR:HG21	1:B:486:GLU:CG	2.46	0.46
1:B:356:LEU:O	1:B:604:ARG:HG3	2.16	0.46
1:B:557:ASP:HA	1:B:638:ARG:NH2	2.31	0.46
1:B:965:THR:N	1:B:968:LEU:HD12	2.31	0.46
1:A:306:ALA:O	1:A:768:ASN:HB3	2.16	0.46
1:B:699:ALA:CB	1:B:716:ILE:HG23	2.45	0.46
1:B:760:PHE:HB3	1:B:807:LEU:HB2	1.96	0.46
1:B:921:SER:HB3	1:B:989:ARG:CZ	2.46	0.46
1:A:90:GLU:HG3	1:A:790:VAL:HG23	1.96	0.46
1:A:290:ARG:HD2	1:A:874:MET:CE	2.45	0.46
1:A:334:ARG:HD3	1:A:731:SER:O	2.15	0.46
1:A:762:ARG:CD	1:A:833:LEU:HD21	2.46	0.46
1:A:834:PHE:O	1:A:838:MET:HB2	2.15	0.46
1:B:477:GLN:O	1:B:501:ALA:HB3	2.15	0.46
1:B:936:SER:O	1:B:940:SER:HB2	2.16	0.46
1:A:60:LEU:CD2	1:A:257:GLY:HA2	2.45	0.46
1:B:89:VAL:HG13	1:B:90:GLU:N	2.31	0.46
1:B:509:GLY:O	1:B:510:ASN:C	2.54	0.46
1:B:684:LYS:O	1:B:688:VAL:HG23	2.16	0.46
1:A:36:TYR:CD2	1:A:147:PRO:HG2	2.51	0.46
1:A:57:PHE:HD1	1:A:62:VAL:HG13	1.81	0.46
1:A:258:GLU:O	1:A:262:LYS:HD3	2.16	0.46
1:A:387:SER:HB2	1:A:602:PRO:CG	2.45	0.46
1:B:25:THR:O	1:B:29:VAL:HG23	2.16	0.46
1:B:354:GLY:HA2	1:B:359:ASN:HB2	1.98	0.46
1:B:500:PRO:CG	1:B:509:GLY:HA3	2.46	0.46
1:B:853:ALA:C	1:B:854:TRP:CD1	2.89	0.46
1:A:140:ILE:HD11	1:A:145:ILE:HG22	1.98	0.45
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.16	0.45
1:A:963:ASP:C	1:A:965:THR:H	2.19	0.45
1:B:292:ALA:C	1:B:294:TYR:H	2.18	0.45
1:A:59:ASP:N	1:A:59:ASP:OD1	2.46	0.45
1:A:174:ARG:HG3	1:A:174:ARG:HH11	1.81	0.45
1:A:600:LEU:O	1:A:602:PRO:HD3	2.16	0.45
1:A:773:VAL:HG21	1:A:842:GLY:HA2	1.99	0.45
1:A:947:ILE:HD13	1:A:947:ILE:HA	1.72	0.45
1:B:64:ILE:HG22	1:B:65:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ASN:HD21	1:B:442:GLU:HB3	1.82	0.45
1:B:481:LYS:CG	1:B:496:VAL:HG13	2.46	0.45
1:B:892:GLU:O	1:B:893:ALA:C	2.54	0.45
1:B:915:SER:C	1:B:917:SER:H	2.19	0.45
1:B:933:LEU:O	1:B:933:LEU:HG	2.16	0.45
1:B:785:GLU:O	1:B:897:MET:HG2	2.16	0.45
1:B:921:SER:HB2	1:B:982:GLU:CD	2.36	0.45
1:A:61:LEU:HD21	1:A:312:PRO:HG2	1.98	0.45
1:A:142:ALA:O	1:A:145:ILE:HG23	2.15	0.45
1:A:720:MET:HE2	1:A:735:LEU:HD12	1.99	0.45
1:A:760:PHE:C	1:A:760:PHE:HD1	2.20	0.45
1:B:48:SER:O	1:B:49:LEU:C	2.55	0.45
1:B:97:ILE:CD1	1:B:797:LEU:HD22	2.46	0.45
1:B:326:MET:HE3	1:B:326:MET:HA	1.99	0.45
1:B:944:HIS:O	1:B:944:HIS:CD2	2.70	0.45
1:A:79:GLU:OE1	1:A:79:GLU:N	2.50	0.45
1:A:840:ILE:HD11	1:A:980:LEU:HB2	1.99	0.45
1:B:281:ASP:N	1:B:282:PRO:HD2	2.31	0.45
1:B:473:SER:O	1:B:477:GLN:HG2	2.16	0.45
1:B:555:GLY:C	1:B:557:ASP:N	2.69	0.45
1:B:933:LEU:O	1:B:937:ILE:HG12	2.17	0.45
1:B:873:PHE:HD1	1:B:875:GLN:NE2	2.15	0.45
1:A:869:GLN:NE2	1:A:871:THR:HG23	2.25	0.45
1:A:913:LEU:O	1:A:922:LEU:HD21	2.17	0.45
1:B:4:ALA:HB1	1:B:6:SER:H	1.82	0.45
1:B:114:ASN:OD1	1:B:117:GLU:HB2	2.16	0.45
1:B:302:LEU:HD12	1:B:772:VAL:HG13	1.98	0.45
1:B:348:ILE:HB	1:B:621:VAL:HG22	1.99	0.45
1:B:351:ASP:OD2	1:B:355:THR:HG23	2.16	0.45
1:B:625:THR:O	1:B:679:VAL:HG22	2.16	0.45
1:A:165:ILE:HG13	1:A:206:ASN:O	2.16	0.45
1:A:396:LEU:HD23	1:A:396:LEU:N	2.32	0.45
1:A:543:GLU:O	1:A:547:SER:HB3	2.17	0.45
1:B:629:LYS:HA	1:B:677:ALA:CB	2.47	0.45
1:B:889:GLU:O	1:B:889:GLU:HG3	2.17	0.45
1:A:115:ALA:CA	1:A:729:THR:HG21	2.46	0.44
1:A:155:VAL:HG23	1:A:155:VAL:O	2.17	0.44
1:A:978:ILE:O	1:A:982:GLU:HG2	2.17	0.44
1:A:988:ALA:HA	1:A:992:LEU:CB	2.33	0.44
1:B:583:ARG:O	1:B:586:GLU:HG2	2.17	0.44
1:A:179:ILE:CG2	1:A:212:THR:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASN:HA	1:A:442:GLU:OE2	2.18	0.44
1:B:110:ARG:NH2	1:B:112:ALA:HB2	2.33	0.44
1:B:794:TRP:O	1:B:798:VAL:HB	2.17	0.44
1:B:951:ASP:O	1:B:953:LEU:N	2.51	0.44
1:A:311:LEU:HG	1:A:315:ILE:HD12	1.98	0.44
1:A:342:LEU:HD23	1:A:746:ALA:HB3	1.98	0.44
1:A:642:PHE:CZ	1:A:648:VAL:HG13	2.52	0.44
1:A:922:LEU:HA	1:A:925:MET:O	2.18	0.44
1:B:983:ILE:O	1:B:987:ILE:HG13	2.18	0.44
1:A:358:THR:O	1:A:359:ASN:HB3	2.18	0.44
1:A:359:ASN:O	1:A:360:GLN:HG2	2.17	0.44
1:A:508:VAL:C	1:A:510:ASN:H	2.19	0.44
1:B:264:ILE:HA	1:B:267:ILE:HG22	2.00	0.44
1:B:500:PRO:HG3	1:B:509:GLY:HA3	1.98	0.44
1:A:79:GLU:O	1:A:81:GLY:N	2.48	0.44
1:A:174:ARG:HG3	1:A:174:ARG:NH1	2.32	0.44
1:A:793:LEU:HD23	1:A:793:LEU:H	1.83	0.44
1:B:55:GLU:OE1	1:B:58:GLU:HB3	2.18	0.44
1:B:423:SER:HB2	1:B:437:VAL:O	2.18	0.44
1:B:776:PHE:O	1:B:780:ALA:HB3	2.17	0.44
1:A:418:ALA:HB3	1:A:475:ILE:HG21	2.00	0.44
1:A:962:LEU:HB3	1:A:965:THR:OG1	2.18	0.44
1:B:863:PRO:CB	1:B:890:ILE:HD11	2.48	0.44
1:A:23:GLY:HA2	1:A:150:ILE:HG12	2.00	0.44
1:B:50:TRP:CD1	1:B:51:GLU:HG3	2.52	0.44
1:B:182:GLY:HA3	2:B:995:ALF:F3	2.08	0.44
1:B:407:PHE:N	1:B:407:PHE:CD2	2.85	0.44
1:B:964:LEU:O	1:B:965:THR:CB	2.64	0.44
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.79	0.44
1:A:567:ARG:HG3	1:A:591:LEU:HD23	2.00	0.44
1:A:672:ARG:NH1	1:A:672:ARG:HG2	2.33	0.44
1:B:35:LYS:HD3	1:B:36:TYR:CZ	2.53	0.44
1:B:799:THR:HG21	1:B:905:VAL:HG22	2.00	0.44
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.62	0.43
1:A:189:LYS:HD2	1:A:205:LYS:O	2.18	0.43
1:A:492:LYS:HB3	1:A:517:ALA:HB2	2.00	0.43
1:B:276:ILE:HG22	1:B:276:ILE:O	2.18	0.43
1:B:527:TYR:CE2	1:B:534:ARG:NH1	2.86	0.43
1:B:555:GLY:C	1:B:557:ASP:H	2.21	0.43
1:B:923:MET:HE3	1:B:924:ARG:HD2	2.00	0.43
1:A:179:ILE:O	1:A:705:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:LEU:HB3	1:A:873:PHE:HZ	1.79	0.43
1:B:298:ILE:O	1:B:302:LEU:HB2	2.18	0.43
1:A:302:LEU:HD22	1:A:772:VAL:HG13	1.99	0.43
1:A:333:VAL:HG21	1:A:339:VAL:HG12	1.99	0.43
1:A:444:ALA:HB3	1:A:599:MET:HE2	2.00	0.43
1:A:557:ASP:O	1:A:557:ASP:OD1	2.37	0.43
1:B:41:LEU:HG	1:B:123:GLU:OE1	2.19	0.43
1:B:856:PHE:CE1	1:B:896:PRO:HG2	2.48	0.43
1:A:276:ILE:HD12	1:A:278:HIS:CE1	2.53	0.43
1:A:368:ILE:HD12	1:A:409:GLY:HA3	2.00	0.43
1:A:672:ARG:HG2	1:A:672:ARG:HH11	1.82	0.43
1:A:764:LEU:O	1:A:768:ASN:ND2	2.51	0.43
1:A:932:TRP:HA	1:A:932:TRP:HE3	1.81	0.43
1:B:23:GLY:HA2	1:B:150:ILE:CG1	2.48	0.43
1:B:614:CYS:O	1:B:619:ILE:HB	2.18	0.43
1:B:807:LEU:HA	1:B:810:ASN:ND2	2.34	0.43
1:A:179:ILE:HD12	1:A:179:ILE:HG21	1.86	0.43
1:A:679:VAL:HB	1:A:683:HIS:HB2	2.01	0.43
1:A:948:LEU:HD12	1:A:948:LEU:HA	1.88	0.43
1:A:972:LYS:HA	1:A:972:LYS:HD2	1.76	0.43
1:B:529:ARG:HH22	1:B:568:ASP:CG	2.22	0.43
1:B:814:LEU:HD12	1:B:815:ASP:HB3	2.01	0.43
1:B:992:LEU:O	1:B:993:GLU:HB2	2.18	0.43
1:A:7:LYS:HB3	1:A:11:GLU:HB2	2.01	0.43
1:A:13:LEU:CD2	1:A:20:GLU:HB2	2.47	0.43
1:A:57:PHE:CA	1:A:62:VAL:HG11	2.48	0.43
1:A:610:SER:OG	1:A:741:SER:HA	2.18	0.43
1:B:234:LYS:O	1:B:238:GLN:HB2	2.19	0.43
1:B:482:GLU:HB3	1:B:483:PHE:H	1.72	0.43
1:B:767:SER:HB3	1:B:908:GLU:CD	2.39	0.43
1:B:913:LEU:HD23	1:B:933:LEU:HD21	2.00	0.43
1:B:923:MET:CE	1:B:924:ARG:HD2	2.48	0.43
1:A:559:LEU:HD23	1:A:600:LEU:HD13	2.00	0.43
1:B:648:VAL:O	1:B:648:VAL:CG1	2.63	0.43
1:B:761:ILE:O	1:B:761:ILE:CG2	2.67	0.43
1:A:45:GLU:O	1:A:46:GLY:C	2.57	0.43
1:A:88:PHE:O	1:A:88:PHE:CD1	2.72	0.43
1:A:398:ASN:C	1:A:400:LYS:H	2.22	0.43
1:A:441:THR:HG22	1:A:599:MET:SD	2.59	0.43
1:B:926:PRO:HB3	1:B:928:TRP:NE1	2.34	0.43
1:B:948:LEU:HD22	1:B:949:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:VAL:HG11	1:A:845:GLY:HA3	1.95	0.43
1:B:895:GLU:H	1:B:896:PRO:HD2	1.83	0.43
1:A:53:VAL:O	1:A:55:GLU:N	2.52	0.43
1:A:298:ILE:C	1:A:298:ILE:CD1	2.87	0.43
1:B:246:LYS:HD2	1:B:250:GLN:NE2	2.31	0.43
1:B:496:VAL:O	1:B:512:MET:HA	2.19	0.43
1:B:662:PRO:O	1:B:664:ALA:N	2.52	0.43
1:B:893:ALA:HB3	1:B:896:PRO:HG2	2.01	0.43
1:A:16:PHE:HD1	1:A:222:ILE:HD11	1.84	0.42
1:A:75:LEU:HD22	1:A:293:ILE:HD13	2.00	0.42
1:A:901:LEU:HD21	1:A:944:HIS:HE1	1.82	0.42
1:A:933:LEU:O	1:A:937:ILE:HG13	2.18	0.42
1:A:958:LYS:HD3	1:A:958:LYS:HA	1.87	0.42
1:B:368:ILE:HG23	1:B:410:LEU:HD23	2.00	0.42
1:B:873:PHE:CE2	1:B:881:PRO:HG2	2.54	0.42
1:B:913:LEU:HD23	1:B:933:LEU:CD2	2.49	0.42
1:A:268:CYS:O	1:A:271:VAL:HG22	2.18	0.42
1:A:305:ALA:HB3	1:A:772:VAL:HG22	2.01	0.42
1:B:329:LYS:NZ	1:B:745:ALA:HB1	2.33	0.42
1:B:777:LEU:HD12	1:B:849:VAL:HG21	2.01	0.42
1:A:74:VAL:HG13	1:A:75:LEU:N	2.34	0.42
1:A:275:ASN:C	1:A:277:GLY:H	2.22	0.42
1:A:642:PHE:CE2	1:A:648:VAL:HG13	2.54	0.42
1:A:789:PRO:O	1:A:793:LEU:HG	2.19	0.42
1:A:886:LEU:O	1:A:886:LEU:HG	2.19	0.42
1:B:497:TYR:CD2	1:B:576:MET:HE1	2.55	0.42
1:B:556:ARG:NH1	1:B:644:GLU:HB3	2.34	0.42
1:A:177:GLN:HA	1:A:212:THR:HG22	2.00	0.42
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.55	0.42
1:A:948:LEU:C	1:A:954:PRO:HG3	2.39	0.42
1:B:51:GLU:O	1:B:54:ILE:CB	2.65	0.42
1:A:120:LYS:HB3	1:A:120:LYS:HE2	1.79	0.42
1:A:247:THR:HG23	1:A:250:GLN:HB2	1.99	0.42
1:B:477:GLN:HA	1:B:477:GLN:OE1	2.20	0.42
1:A:63:ARG:HD2	1:A:63:ARG:HA	1.71	0.42
1:A:298:ILE:HD12	1:A:299:ALA:N	2.35	0.42
1:A:333:VAL:HG11	1:A:339:VAL:HG13	2.02	0.42
1:B:196:ASP:HA	1:B:197:PRO:HD3	1.87	0.42
1:B:785:GLU:HG3	1:B:897:MET:CE	2.49	0.42
1:A:342:LEU:HD23	1:A:746:ALA:CB	2.49	0.42
1:A:947:ILE:HD13	1:A:953:LEU:CD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ASN:OD1	1:B:428:ASN:C	2.58	0.42
1:B:567:ARG:NH1	1:B:569:THR:O	2.52	0.42
1:B:761:ILE:O	1:B:761:ILE:HG22	2.20	0.42
1:B:840:ILE:CG2	1:B:911:ASN:HD21	2.33	0.42
1:B:844:VAL:HG11	1:B:907:ILE:CG2	2.49	0.42
1:A:67:LEU:C	1:A:69:ALA:H	2.23	0.42
1:A:539:GLY:N	1:A:540:PRO:CD	2.83	0.42
1:B:5:HIS:CD2	1:B:5:HIS:C	2.93	0.42
1:B:77:TRP:CD1	1:B:78:PHE:CE1	3.03	0.42
1:B:357:THR:HA	1:B:603:PRO:HA	2.01	0.42
1:B:421:ASN:ND2	1:B:423:SER:H	2.18	0.42
1:B:511:LYS:HZ2	1:B:568:ASP:CA	2.33	0.42
1:B:726:VAL:O	1:B:726:VAL:CG2	2.68	0.42
1:A:1:MET:HB2	1:A:36:TYR:OH	2.20	0.42
1:A:53:VAL:C	1:A:55:GLU:N	2.73	0.42
1:A:310:GLY:O	1:A:314:VAL:HG23	2.19	0.42
1:B:67:LEU:HD12	1:B:67:LEU:HA	1.84	0.42
1:B:412:GLU:HG2	1:B:594:VAL:HG11	2.01	0.42
1:B:840:ILE:HD12	1:B:911:ASN:HD21	1.83	0.42
1:A:596:VAL:CG1	1:A:597:VAL:N	2.83	0.42
1:A:611:ILE:HG23	1:A:621:VAL:HG21	2.02	0.42
1:A:961:ALA:HB1	1:A:966:GLN:HB3	2.02	0.42
1:B:307:ILE:HA	1:B:308:PRO:HD3	1.77	0.42
1:B:773:VAL:HG11	1:B:841:GLY:O	2.20	0.42
1:B:840:ILE:O	1:B:844:VAL:HG13	2.20	0.42
1:B:965:THR:O	1:B:965:THR:CG2	2.68	0.42
1:A:97:ILE:HD12	1:A:797:LEU:HD22	2.02	0.41
1:A:421:ASN:ND2	1:A:423:SER:H	2.18	0.41
1:A:828:LEU:HG	1:A:829:ILE:H	1.84	0.41
1:B:304:VAL:HG11	1:B:789:PRO:CB	2.50	0.41
1:B:774:CYS:C	1:B:776:PHE:H	2.23	0.41
1:B:898:THR:O	1:B:898:THR:HG23	2.20	0.41
1:A:249:LEU:HD12	1:A:250:GLN:H	1.84	0.41
1:A:276:ILE:HD12	1:A:276:ILE:HA	1.89	0.41
1:A:652:ALA:HA	1:A:675:CYS:O	2.19	0.41
1:B:501:ALA:O	1:B:502:LYS:CG	2.66	0.41
1:B:778:THR:HG23	1:B:778:THR:O	2.20	0.41
1:A:103:ILE:O	1:A:103:ILE:HG22	2.20	0.41
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.72	0.41
1:A:524:ARG:HH21	1:A:588:GLU:HB3	1.84	0.41
1:A:527:TYR:CB	1:A:534:ARG:HD3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:N	1:B:337:PRO:CD	2.82	0.41
1:B:920:GLN:O	1:B:921:SER:C	2.58	0.41
1:A:162:ASP:OD1	1:A:230:THR:HB	2.20	0.41
1:A:916:LEU:HD13	1:A:933:LEU:CD2	2.50	0.41
1:A:917:SER:OG	1:A:918:GLU:N	2.50	0.41
1:B:726:VAL:O	1:B:726:VAL:HG23	2.19	0.41
1:B:793:LEU:HD23	1:B:793:LEU:HA	1.82	0.41
1:A:872:HIS:O	1:A:873:PHE:CD1	2.74	0.41
1:B:4:ALA:HB3	1:B:7:LYS:HG2	2.02	0.41
1:B:549:ILE:HD11	1:B:596:VAL:HG21	2.03	0.41
1:B:586:GLU:O	1:B:589:THR:HG22	2.21	0.41
1:A:276:ILE:O	1:A:279:PHE:CD2	2.74	0.41
1:A:814:LEU:HG	1:A:815:ASP:N	2.35	0.41
1:B:78:PHE:CD1	1:B:78:PHE:N	2.88	0.41
1:B:965:THR:H	1:B:968:LEU:HB2	1.86	0.41
1:A:53:VAL:C	1:A:55:GLU:H	2.24	0.41
1:A:56:GLN:NE2	1:A:102:ALA:HA	2.35	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	0.41
1:A:545:ILE:HG21	1:A:545:ILE:HD13	1.81	0.41
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.90	0.41
1:B:452:MET:HE2	1:B:454:VAL:HG12	2.03	0.41
1:B:483:PHE:CZ	1:B:576:MET:CE	3.00	0.41
1:B:957:PHE:O	1:B:958:LYS:HD3	2.19	0.41
1:A:44:GLU:OE1	1:A:114:ASN:HB3	2.21	0.41
1:A:857:MET:HA	1:A:866:THR:HA	2.02	0.41
1:A:902:SER:HB2	1:A:970:VAL:HG21	2.03	0.41
1:A:917:SER:CB	1:A:920:GLN:HB2	2.50	0.41
1:B:422:ASP:HB2	1:B:442:GLU:OE1	2.21	0.41
1:B:788:ILE:HG12	1:B:791:GLN:NE2	2.36	0.41
1:B:878:GLU:CB	1:B:880:HIS:NE2	2.83	0.41
1:B:902:SER:O	1:B:970:VAL:HG13	2.20	0.41
1:A:67:LEU:O	1:A:71:ILE:N	2.43	0.41
1:A:413:LEU:CD1	1:A:564:LEU:CD1	2.99	0.41
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.91	0.41
1:A:581:SER:HA	1:A:584:PHE:CD1	2.56	0.41
1:A:716:ILE:N	1:A:716:ILE:CD1	2.80	0.41
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.82	0.41
1:B:145:ILE:HD11	1:B:223:VAL:CG2	2.49	0.41
1:B:246:LYS:HB3	1:B:250:GLN:HB2	2.03	0.41
1:B:274:ILE:HG21	1:B:780:ALA:HA	2.03	0.41
1:B:336:LEU:HB2	1:B:337:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:ASP:OD2	1:B:739:ASN:HB2	2.21	0.41
1:B:855:TRP:HB2	1:B:896:PRO:HG3	2.03	0.41
1:B:873:PHE:CZ	1:B:881:PRO:CG	3.04	0.41
1:A:279:PHE:CD1	1:A:279:PHE:C	2.94	0.41
1:A:945:PHE:CZ	1:A:967:TRP:CZ2	3.09	0.41
1:B:200:VAL:O	1:B:204:LYS:HD2	2.21	0.41
1:B:699:ALA:HB2	1:B:716:ILE:HG23	2.02	0.41
1:B:737:ASP:O	1:B:738:ASP:HB2	2.21	0.41
1:B:948:LEU:HD23	1:B:948:LEU:C	2.41	0.41
1:A:1:MET:HB2	1:A:36:TYR:CZ	2.56	0.40
1:A:49:LEU:CD1	1:A:52:LEU:N	2.84	0.40
1:A:116:ILE:O	1:A:120:LYS:HG3	2.21	0.40
1:A:953:LEU:HA	1:A:956:ILE:HG13	2.02	0.40
1:B:814:LEU:HD12	1:B:815:ASP:CA	2.52	0.40
1:B:857:MET:O	1:B:858:TYR:CD2	2.74	0.40
1:A:67:LEU:C	1:A:69:ALA:N	2.75	0.40
1:A:410:LEU:HB3	1:A:452:MET:CE	2.51	0.40
1:A:624:ILE:HG22	1:A:684:LYS:HG2	2.03	0.40
1:A:934:LEU:HD23	1:A:934:LEU:HA	1.77	0.40
1:B:171:THR:HG21	1:B:486:GLU:CD	2.36	0.40
1:B:267:ILE:HG23	1:B:302:LEU:HD21	2.02	0.40
1:B:419:LEU:O	1:B:481:LYS:HE2	2.21	0.40
1:B:566:THR:HG23	1:B:594:VAL:HG21	2.03	0.40
1:A:739:ASN:HB3	1:A:742:THR:HG22	2.03	0.40
1:A:921:SER:HA	1:A:985:LYS:CD	2.52	0.40
1:A:925:MET:HA	1:A:926:PRO:HD3	1.97	0.40
1:B:319:LEU:HA	1:B:319:LEU:HD23	1.83	0.40
1:B:398:ASN:O	1:B:399:ASP:HB2	2.20	0.40
1:B:427:PHE:CZ	1:B:464:LYS:HD3	2.56	0.40
1:A:24:LEU:HB2	1:A:149:ASP:HB3	2.03	0.40
1:A:49:LEU:C	1:A:51:GLU:N	2.73	0.40
1:A:51:GLU:OE1	1:A:54:ILE:HG13	2.22	0.40
1:A:57:PHE:HA	1:A:62:VAL:HG11	2.02	0.40
1:A:516:GLY:HA2	5:A:998:ACP:N3	2.36	0.40
1:A:861:ASP:CG	1:A:862:GLY:N	2.74	0.40
1:A:894:PRO:O	1:A:958:LYS:HB3	2.22	0.40
1:B:5:HIS:HD2	1:B:6:SER:CA	2.35	0.40
1:B:545:ILE:HD13	1:B:545:ILE:HG21	1.84	0.40
1:B:624:ILE:HG22	1:B:679:VAL:HG21	2.03	0.40
1:B:879:ASP:C	1:B:881:PRO:HD3	2.42	0.40
1:A:179:ILE:HG22	1:A:212:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:LEU:O	1:A:965:THR:OG1	2.29	0.40
1:A:992:LEU:CG	1:A:993:GLU:N	2.85	0.40
1:B:340:GLU:HA	1:B:750:GLY:CA	2.51	0.40
1:B:483:PHE:CZ	1:B:576:MET:HE1	2.48	0.40
1:B:835:PHE:HE2	1:B:984:LEU:HD21	1.86	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%)	858 (86%)	106 (11%)	28 (3%)	5	25
1	B	992/994 (100%)	853 (86%)	110 (11%)	29 (3%)	4	24
All	All	1984/1988 (100%)	1711 (86%)	216 (11%)	57 (3%)	4	24

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	571	PRO
1	A	859	ALA
1	A	863	PRO
1	A	883	PHE
1	A	952	PRO
1	A	953	LEU
1	A	954	PRO
1	B	288	TRP
1	B	289	ILE
1	B	881	PRO
1	A	46	GLY
1	A	54	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	62	VAL
1	A	68	ALA
1	A	869	GLN
1	B	55	GLU
1	B	287	SER
1	B	785	GLU
1	B	813	ASP
1	B	863	PRO
1	B	867	TYR
1	B	876	CYS
1	B	885	GLY
1	A	61	LEU
1	A	275	ASN
1	A	276	ILE
1	A	770	GLY
1	A	888	CYS
1	B	644	GLU
1	B	663	LEU
1	B	714	ALA
1	B	887	ASP
1	B	948	LEU
1	B	957	PHE
1	A	80	GLU
1	A	287	SER
1	A	465	VAL
1	B	858	TYR
1	B	893	ALA
1	A	44	GLU
1	A	59	ASP
1	A	281	ASP
1	A	316	THR
1	B	510	ASN
1	B	638	ARG
1	B	739	ASN
1	B	880	HIS
1	A	87	ALA
1	B	281	ASP
1	B	293	ILE
1	B	950	VAL
1	A	951	ASP
1	B	812	PRO
1	B	247	THR

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Mol	Chain	Res	Type
1	A	880	HIS
1	B	947	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/840 (100%)	764 (91%)	76 (9%)	9 35
1	B	840/840 (100%)	764 (91%)	76 (9%)	9 35
All	All	1680/1680 (100%)	1528 (91%)	152 (9%)	9 35

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	24	LEU
1	A	34	GLU
1	A	48	SER
1	A	49	LEU
1	A	60	LEU
1	A	66	LEU
1	A	79	GLU
1	A	82	GLU
1	A	117	GLU
1	A	145	ILE
1	A	170	SER
1	A	171	THR
1	A	177	GLN
1	A	179	ILE
1	A	185	VAL
1	A	187	VAL
1	A	191	THR
1	A	236	ARG
1	A	238	GLN
1	A	247	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	254	ASP
1	A	255	GLU
1	A	315	ILE
1	A	347	VAL
1	A	360	GLN
1	A	384	ILE
1	A	401	PRO
1	A	402	ILE
1	A	421	ASN
1	A	426	ASP
1	A	437	VAL
1	A	441	THR
1	A	465	VAL
1	A	476	ARG
1	A	484	THR
1	A	494	MET
1	A	496	VAL
1	A	510	ASN
1	A	532	THR
1	A	547	SER
1	A	556	ARG
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	582	SER
1	A	619	ILE
1	A	647	GLU
1	A	671	ARG
1	A	682	SER
1	A	691	LEU
1	A	705	VAL
1	A	716	ILE
1	A	722	SER
1	A	726	VAL
1	A	739	ASN
1	A	742	THR
1	A	747	VAL
1	A	760	PHE
1	A	761	ILE
1	A	764	LEU
1	A	765	ILE
1	A	778	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	802	LEU
1	A	805	THR
1	A	815	ASP
1	A	830	SER
1	A	840	ILE
1	A	857	MET
1	A	872	HIS
1	A	932	TRP
1	A	940	SER
1	A	948	LEU
1	A	956	ILE
1	A	960	LYS
1	A	986	PHE
1	B	5	HIS
1	B	18	VAL
1	B	21	THR
1	B	33	LEU
1	B	34	GLU
1	B	61	LEU
1	B	64	ILE
1	B	78	PHE
1	B	116	ILE
1	B	117	GLU
1	B	136	SER
1	B	139	ARG
1	B	145	ILE
1	B	155	VAL
1	B	174	ARG
1	B	179	ILE
1	B	180	LEU
1	B	187	VAL
1	B	191	THR
1	B	213	ASN
1	B	228	VAL
1	B	239	MET
1	B	255	GLU
1	B	273	LEU
1	B	347	VAL
1	B	355	THR
1	B	367	PHE
1	B	379	LEU
1	B	384	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	387	SER
1	B	388	THR
1	B	395	VAL
1	B	400	LYS
1	B	402	ILE
1	B	421	ASN
1	B	433	VAL
1	B	436	LYS
1	B	458	GLU
1	B	460	ARG
1	B	467	ARG
1	B	482	GLU
1	B	484	THR
1	B	491	ARG
1	B	505	ARG
1	B	532	THR
1	B	533	THR
1	B	534	ARG
1	B	559	LEU
1	B	566	THR
1	B	574	GLU
1	B	581	SER
1	B	589	THR
1	B	596	VAL
1	B	624	ILE
1	B	633	ILE
1	B	639	ILE
1	B	675	CYS
1	B	678	ARG
1	B	698	THR
1	B	701	THR
1	B	722	SER
1	B	726	VAL
1	B	739	ASN
1	B	742	THR
1	B	765	ILE
1	B	773	VAL
1	B	794	TRP
1	B	857	MET
1	B	869	GLN
1	B	871	THR
1	B	873	PHE

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Mol	Chain	Res	Type
1	B	874	MET
1	B	875	GLN
1	B	880	HIS
1	B	890	ILE
1	B	898	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	56	GLN
1	A	177	GLN
1	A	250	GLN
1	A	421	ASN
1	A	472	ASN
1	A	510	ASN
1	A	666	GLN
1	A	739	ASN
1	A	759	GLN
1	A	768	ASN
1	A	868	HIS
1	A	869	GLN
1	A	872	HIS
1	A	930	ASN
1	B	5	HIS
1	B	238	GLN
1	B	259	GLN
1	B	275	ASN
1	B	278	HIS
1	B	421	ASN
1	B	666	GLN
1	B	739	ASN
1	B	759	GLN
1	B	810	ASN
1	B	872	HIS
1	B	875	GLN
1	B	882	HIS
1	B	911	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ACP	A	998	-	27,33,33	2.05	9 (33%)	32,52,52	2.52	8 (25%)
2	ALF	A	995	-	0,4,4	-	-	-	-	-
5	ACP	B	998	-	27,33,33	2.18	8 (29%)	32,52,52	2.73	10 (31%)
2	ALF	B	995	-	0,4,4	-	-	-	-	-

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	ACP	A	998	-	-	5/15/38/38	0/3/3/3
5	ACP	B	998	-	-	4/15/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	998	ACP	PB-O3A	6.45	1.65	1.58
5	B	998	ACP	PG-O1G	4.86	1.60	1.50
5	A	998	ACP	PG-O1G	4.86	1.60	1.50
5	A	998	ACP	PG-O3G	-4.23	1.45	1.54
5	B	998	ACP	PG-O3G	-4.09	1.45	1.54
5	A	998	ACP	PB-O3A	3.99	1.62	1.58
5	A	998	ACP	O4'-C1'	3.38	1.45	1.41
5	A	998	ACP	C2'-C1'	2.88	1.58	1.53
5	B	998	ACP	C2'-C1'	2.77	1.58	1.53
5	B	998	ACP	O4'-C1'	2.33	1.44	1.41
5	A	998	ACP	C5-C4	2.32	1.47	1.40
5	B	998	ACP	C2-N3	2.30	1.35	1.32
5	B	998	ACP	PG-O2G	2.20	1.59	1.54
5	B	998	ACP	PB-O1B	-2.17	1.46	1.51
5	A	998	ACP	PB-O2B	2.15	1.61	1.56
5	A	998	ACP	PB-O1B	-2.15	1.46	1.51
5	A	998	ACP	PG-O2G	2.04	1.59	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	ACP	O4'-C1'-C2'	-9.64	92.84	106.93
5	A	998	ACP	O4'-C1'-C2'	-8.60	94.36	106.93
5	B	998	ACP	O4'-C4'-C3'	-5.79	93.66	105.11
5	B	998	ACP	O3'-C3'-C4'	5.42	126.71	111.05
5	A	998	ACP	O4'-C4'-C3'	-5.17	94.87	105.11
5	A	998	ACP	O3'-C3'-C4'	5.11	125.83	111.05
5	A	998	ACP	O2G-PG-O1G	-4.87	99.52	112.39
5	B	998	ACP	PB-O3A-PA	4.31	146.22	132.56
5	B	998	ACP	O2G-PG-O1G	-3.50	103.14	112.39
5	B	998	ACP	C3'-C2'-C1'	2.96	105.43	100.98
5	A	998	ACP	O3G-PG-C3B	2.87	113.37	106.40
5	A	998	ACP	O4'-C4'-C5'	-2.84	100.02	109.37
5	B	998	ACP	O3G-PG-O2G	2.79	116.23	108.08
5	A	998	ACP	O3G-PG-O2G	2.75	116.12	108.08
5	B	998	ACP	O3G-PG-C3B	2.46	112.36	106.40
5	B	998	ACP	O4'-C4'-C5'	-2.34	101.68	109.37
5	B	998	ACP	O3G-PG-O1G	-2.10	106.83	112.39
5	A	998	ACP	C2'-C3'-C4'	2.06	106.65	102.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

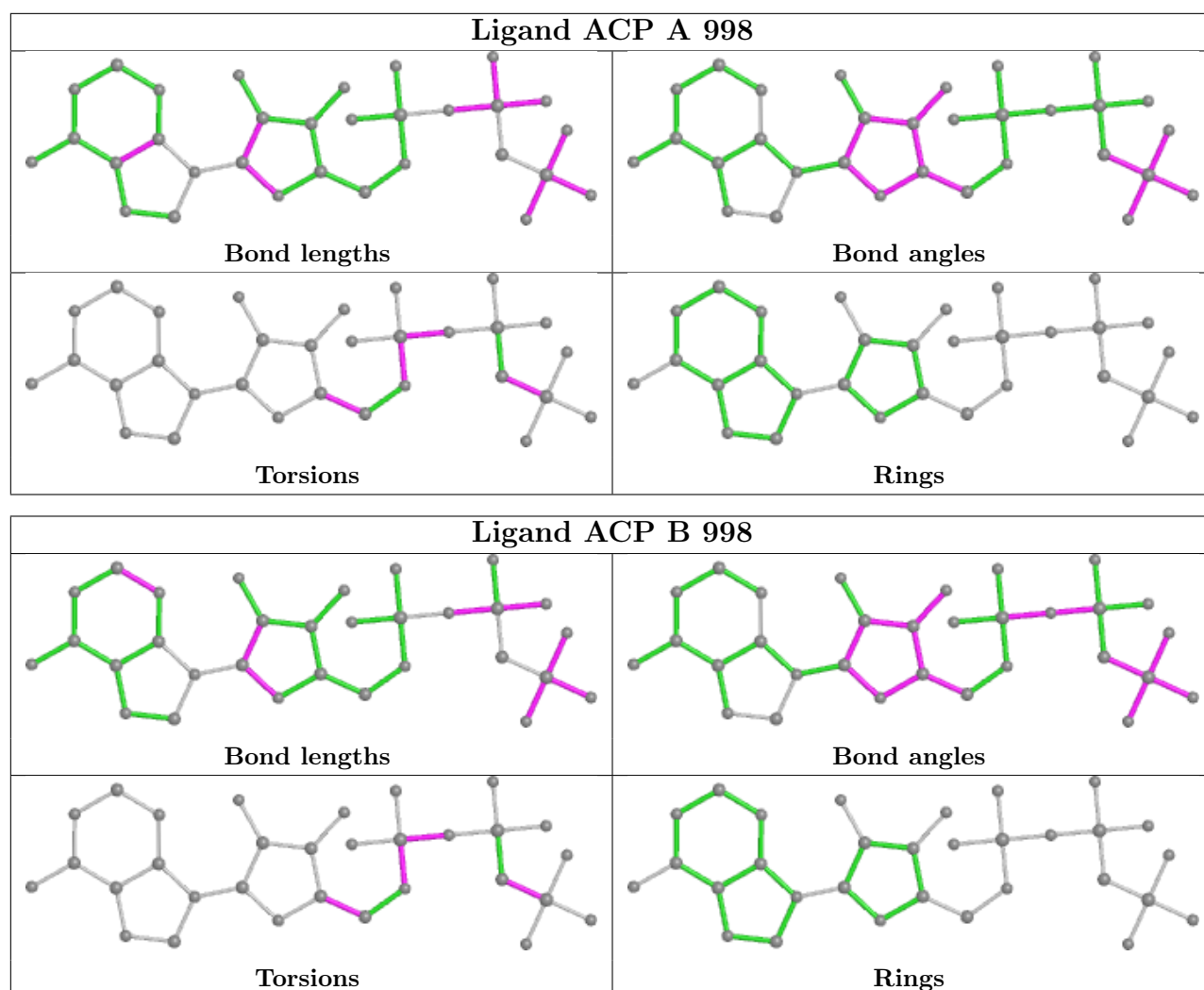
Mol	Chain	Res	Type	Atoms
5	A	998	ACP	C5'-O5'-PA-O1A
5	A	998	ACP	O4'-C4'-C5'-O5'
5	B	998	ACP	PB-C3B-PG-O2G
5	B	998	ACP	C5'-O5'-PA-O1A
5	B	998	ACP	O4'-C4'-C5'-O5'
5	A	998	ACP	C3'-C4'-C5'-O5'
5	A	998	ACP	PB-O3A-PA-O5'
5	B	998	ACP	PB-O3A-PA-O5'
5	A	998	ACP	PB-C3B-PG-O1G

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	998	ACP	2	0
2	A	995	ALF	1	0
5	B	998	ACP	1	0
2	B	995	ALF	2	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	994/994 (100%)	-0.06	47 (4%) 31 11	36, 86, 210, 329	0
1	B	994/994 (100%)	0.15	79 (7%) 12 4	47, 108, 222, 298	0
All	All	1988/1988 (100%)	0.05	126 (6%) 20 6	36, 97, 216, 329	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	861	ASP	11.9
1	B	991	TYR	11.1
1	B	280	ASN	8.8
1	B	275	ASN	7.9
1	A	281	ASP	7.5
1	B	990	ASN	7.4
1	B	852	ALA	6.9
1	B	276	ILE	6.7
1	A	286	GLY	6.1
1	B	785	GLU	6.0
1	B	894	PRO	5.8
1	B	277	GLY	5.8
1	A	55	GLU	5.7
1	B	281	ASP	5.6
1	B	284	HIS	5.5
1	A	885	GLY	5.5
1	A	284	HIS	4.9
1	B	286	GLY	4.6
1	B	782	GLY	4.6
1	B	891	PHE	4.6
1	B	871	THR	4.5
1	B	959	LEU	4.5
1	B	883	PHE	4.5
1	A	882	HIS	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	855	TRP	4.4
1	A	279	PHE	4.4
1	B	865	VAL	4.3
1	B	877	THR	4.3
1	B	876	CYS	4.3
1	B	889	GLU	4.3
1	A	994	GLY	4.3
1	A	278	HIS	4.3
1	B	784	PRO	4.3
1	A	283	VAL	4.3
1	B	278	HIS	4.2
1	B	868	HIS	4.2
1	B	832	TRP	4.1
1	A	504	SER	4.1
1	B	874	MET	4.1
1	A	48	SER	4.0
1	B	875	GLN	4.0
1	A	290	ARG	4.0
1	B	279	PHE	4.0
1	B	863	PRO	4.0
1	A	280	ASN	4.0
1	A	245	ASP	3.9
1	A	875	GLN	3.9
1	B	981	ASP	3.9
1	B	873	PHE	3.8
1	B	987	ILE	3.8
1	B	988	ALA	3.7
1	B	47	LYS	3.7
1	A	853	ALA	3.6
1	A	282	PRO	3.6
1	A	857	MET	3.5
1	A	891	PHE	3.5
1	A	886	LEU	3.3
1	A	285	GLY	3.2
1	B	862	GLY	3.2
1	A	57	PHE	3.2
1	A	829	ILE	3.2
1	B	282	PRO	3.2
1	B	887	ASP	3.2
1	A	50	TRP	3.2
1	A	276	ILE	3.1
1	B	884	GLU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	885	GLY	3.1
1	A	880	HIS	3.1
1	B	48	SER	3.1
1	B	872	HIS	3.1
1	B	915	SER	3.0
1	B	993	GLU	3.0
1	A	993	GLU	2.9
1	B	291	GLY	2.9
1	B	274	ILE	2.8
1	B	46	GLY	2.8
1	A	47	LYS	2.8
1	B	251	GLN	2.7
1	B	856	PHE	2.7
1	B	986	PHE	2.7
1	B	923	MET	2.7
1	A	924	ARG	2.7
1	B	283	VAL	2.7
1	A	111	ASN	2.7
1	B	851	ALA	2.7
1	B	879	ASP	2.6
1	B	1	MET	2.6
1	B	989	ARG	2.6
1	A	56	GLN	2.5
1	A	289	ILE	2.5
1	A	505	ARG	2.5
1	A	890	ILE	2.5
1	A	923	MET	2.4
1	B	762	ARG	2.4
1	B	271	VAL	2.4
1	B	287	SER	2.4
1	A	242	THR	2.4
1	B	829	ILE	2.4
1	B	866	THR	2.4
1	A	883	PHE	2.3
1	B	919	ASN	2.3
1	B	890	ILE	2.3
1	A	877	THR	2.3
1	A	983	ILE	2.3
1	B	920	GLN	2.3
1	B	835	PHE	2.2
1	B	929	VAL	2.2
1	A	964	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	273	LEU	2.2
1	B	870	LEU	2.2
1	A	874	MET	2.2
1	A	786	ALA	2.2
1	B	952	PRO	2.2
1	B	916	LEU	2.2
1	B	888	CYS	2.1
1	A	871	THR	2.1
1	B	992	LEU	2.1
1	A	966	GLN	2.1
1	B	268	CYS	2.1
1	B	897	MET	2.1
1	B	290	ARG	2.1
1	B	886	LEU	2.1
1	A	45	GLU	2.1
1	B	985	LYS	2.0
1	A	984	LEU	2.0
1	B	925	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

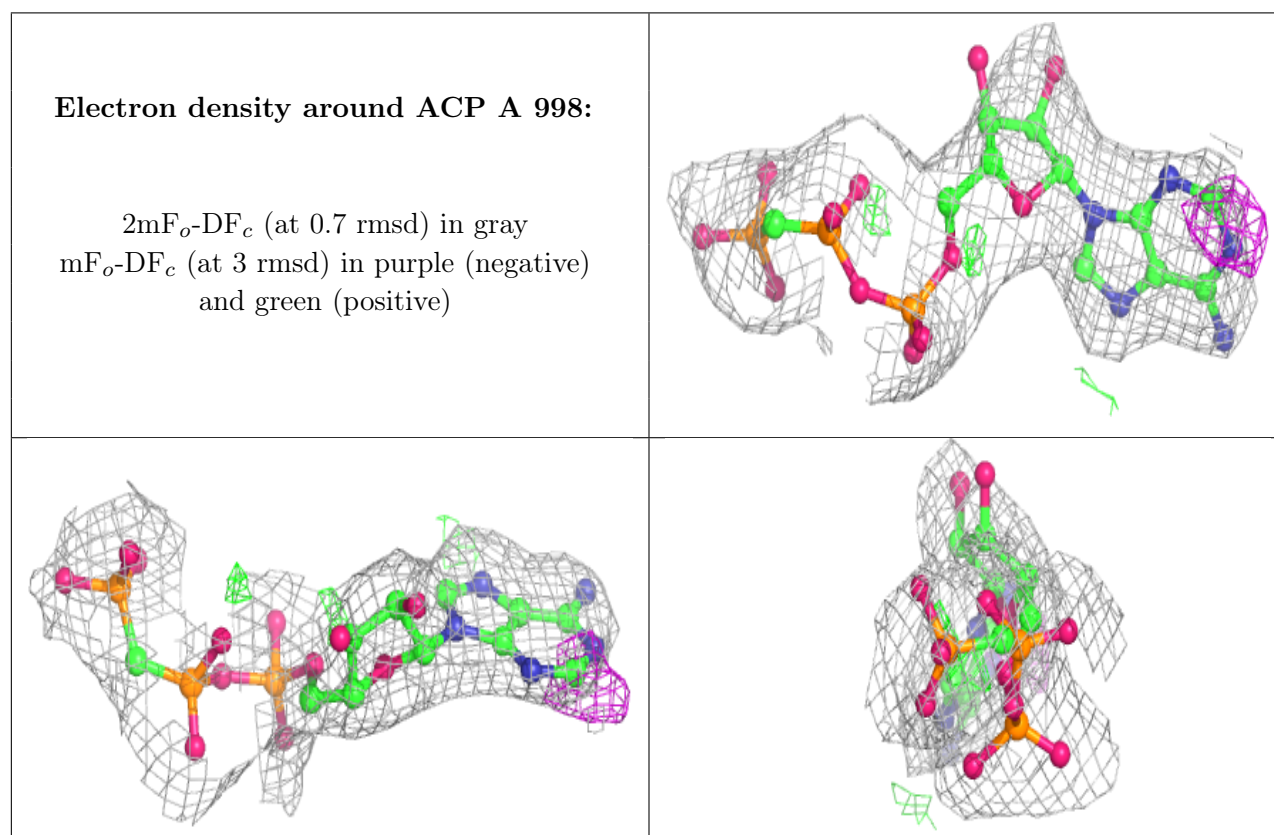
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACP	A	998	31/31	0.91	0.24	63,113,171,279	0
5	ACP	B	998	31/31	0.92	0.21	55,101,210,335	0
4	K	A	997	1/1	0.96	0.20	78,78,78,78	0
3	MG	B	996	1/1	0.99	0.18	43,43,43,43	0
4	K	B	997	1/1	0.99	0.12	99,99,99,99	0

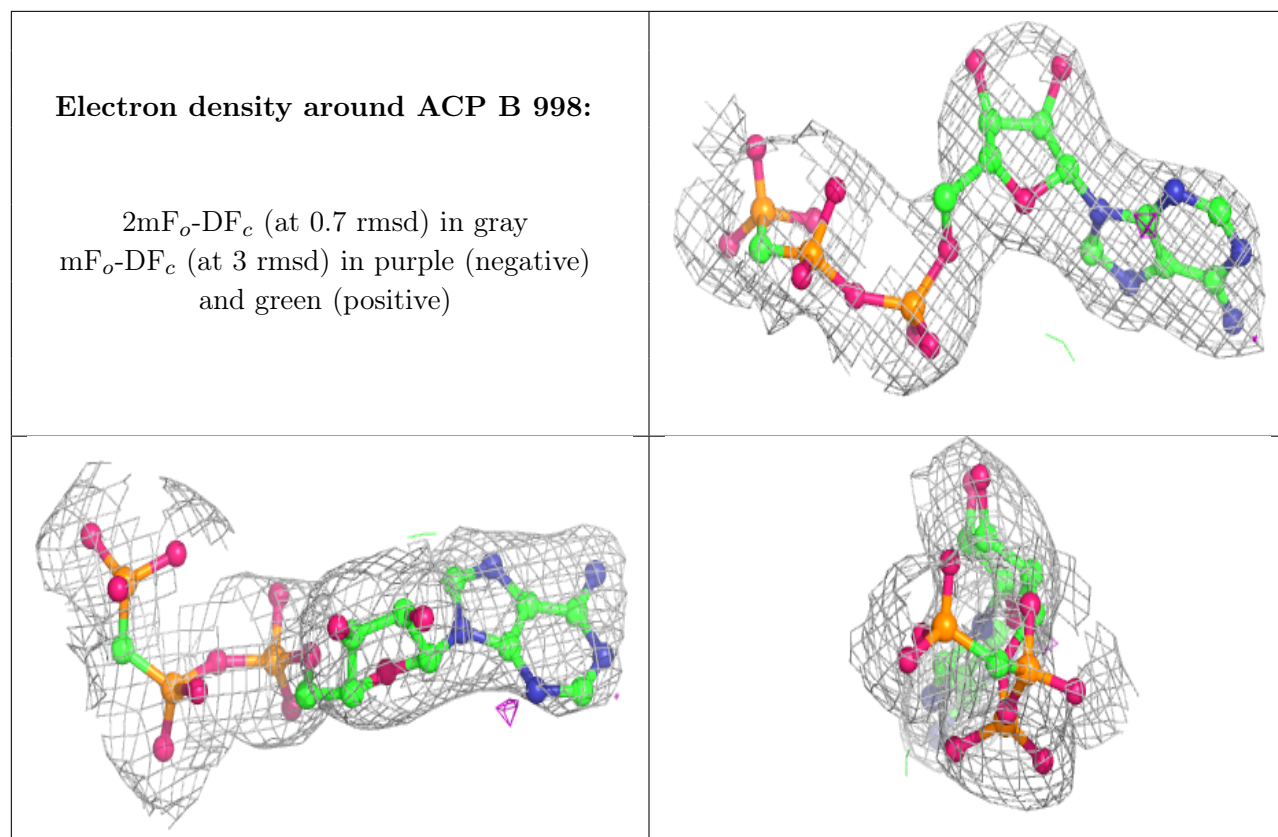
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	996	1/1	1.00	0.23	23,23,23,23	0
2	ALF	A	995	5/5	1.00	0.20	18,47,49,50	0
2	ALF	B	995	5/5	1.00	0.20	42,50,61,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.