



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 12:31 AM EST

PDB ID : 1XP5
Title : Structure Of The (Sr)Ca²⁺-ATPase E2-A1F4- Form
Authors : Olesen, C.; Sorensen, T.L.S.; Nielsen, R.C.; Moller, J.V.; Nissen, P.
Deposited on : 2004-10-08
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

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>.

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

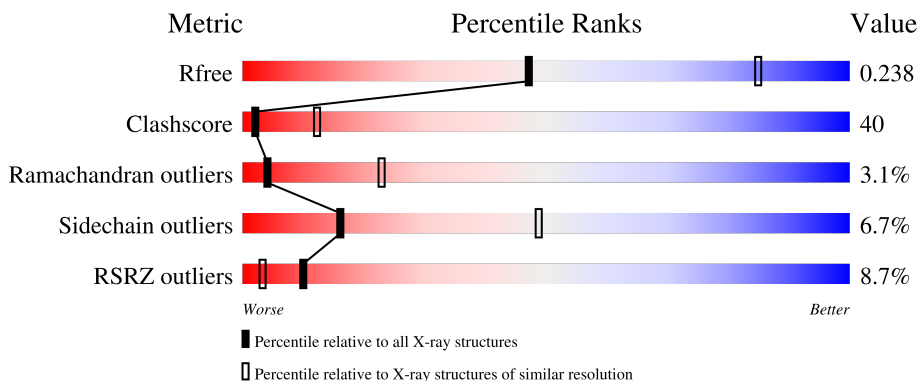
1 Overall quality at a glance i

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 ≥ 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	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="margin-top: 5px;">9% 43% 52% 5%</p>

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
5	TG1	A	999	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7727 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

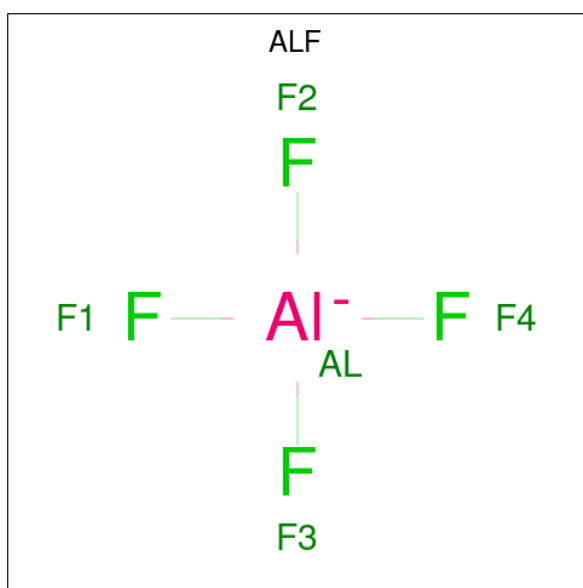
There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).

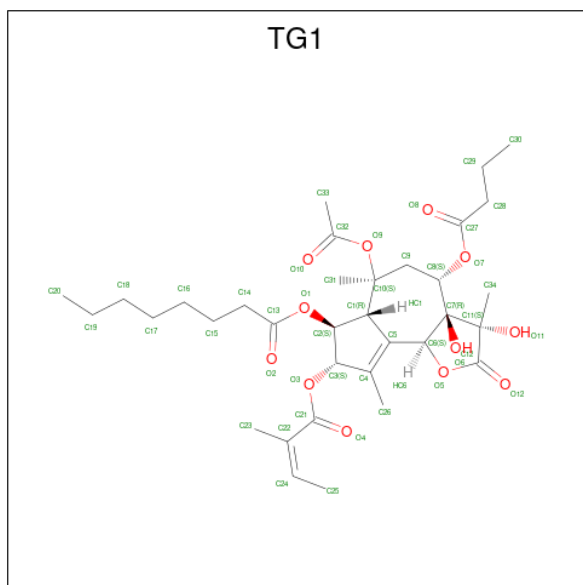


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		

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

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

- Molecule 5 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C₃₄H₅₀O₁₂).



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

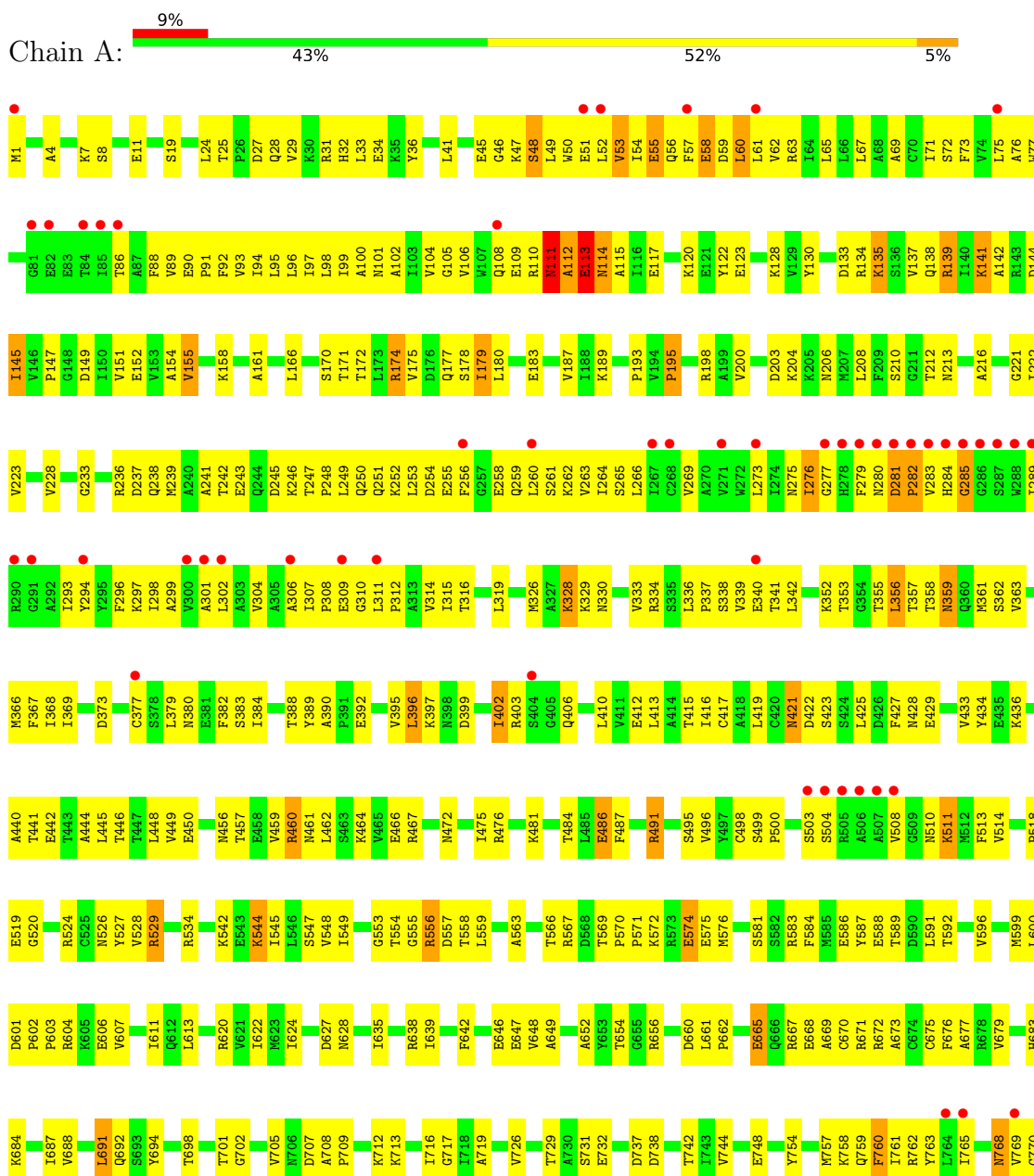
- Molecule 6 is water.

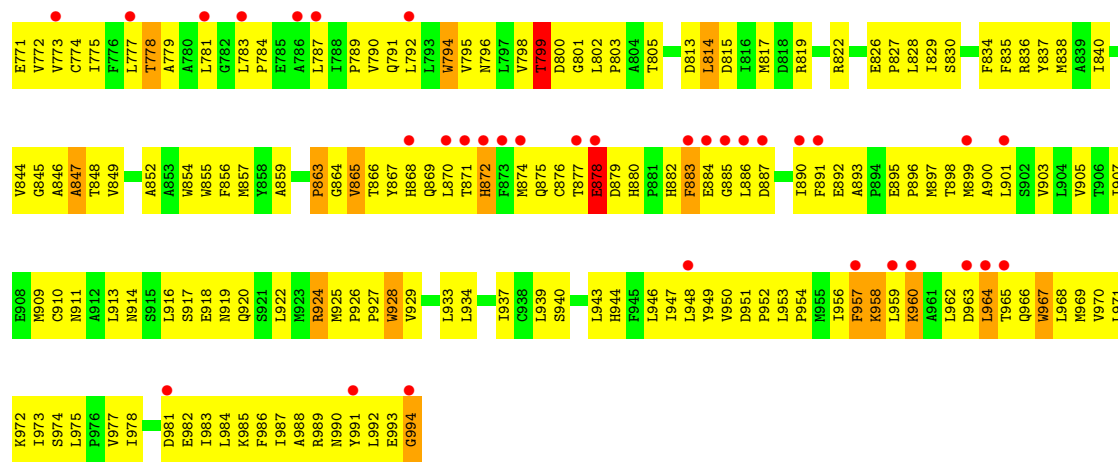
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		

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





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.51Å 119.27Å 142.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 3.00 142.26 – 2.86	Depositor EDS
% Data completeness (in resolution range)	92.5 (80.00-3.00) 98.3 (142.26-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.86Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.265 0.237 , 0.238	Depositor DCC
R_{free} test set	1732 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtrriage
Anisotropy	0.109	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7727	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: K, TG1, MG, ALF

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	0.44	2/7812 (0.0%)	0.72	9/10592 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	994	GLY	C-OXT	9.99	1.42	1.23
1	A	957	PHE	CB-CG	-5.58	1.41	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	960	LYS	N-CA-C	7.41	131.00	111.00
1	A	113	GLU	N-CA-C	7.39	130.95	111.00
1	A	373	ASP	N-CA-C	-6.92	92.32	111.00
1	A	878	GLU	N-CA-C	-6.34	93.87	111.00
1	A	111	ASN	N-CA-C	-6.12	94.46	111.00
1	A	48	SER	N-CA-C	-5.51	96.12	111.00
1	A	959	LEU	N-CA-C	5.21	125.08	111.00
1	A	504	SER	N-CA-C	5.21	125.07	111.00
1	A	285	GLY	N-CA-C	5.21	126.12	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	7766	623	1
2	A	1	0	0	0	0
3	A	5	0	0	1	0
4	A	1	0	0	0	0
5	A	46	0	50	11	0
6	A	3	0	0	1	0
All	All	7727	0	7816	623	1

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 40.

All (623) 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:260:LEU:HD11	1:A:306:ALA:HB1	1.31	1.11
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.29	1.10
1:A:283:VAL:HG12	1:A:284:HIS:H	1.02	1.09
1:A:51:GLU:HG3	1:A:54:ILE:HD11	1.16	1.08
1:A:108:GLN:OE1	1:A:336:LEU:HG	1.58	1.03
1:A:179:ILE:H	1:A:179:ILE:HD12	1.25	1.02
1:A:869:GLN:HB3	1:A:872:HIS:HB2	1.38	1.01
1:A:854:TRP:HH2	1:A:966:GLN:HG2	1.20	1.00
1:A:984:LEU:HA	1:A:987:ILE:HD12	1.47	0.97
1:A:111:ASN:HD22	1:A:111:ASN:C	1.69	0.95
1:A:108:GLN:HE22	1:A:336:LEU:HD11	1.29	0.95
1:A:854:TRP:CH2	1:A:966:GLN:HG2	2.04	0.92
1:A:863:PRO:HG2	1:A:890:ILE:HG21	1.49	0.92
1:A:51:GLU:CG	1:A:54:ILE:HD11	2.00	0.92
1:A:878:GLU:OE1	1:A:880:HIS:CD2	2.23	0.91
1:A:1:MET:HB2	1:A:36:TYR:CE1	2.06	0.91
1:A:283:VAL:HG12	1:A:284:HIS:N	1.84	0.90
1:A:859:ALA:HB3	1:A:864:GLY:HA2	1.56	0.88
1:A:283:VAL:CG1	1:A:284:HIS:H	1.84	0.88
1:A:179:ILE:HD13	1:A:212:THR:HG22	1.55	0.88
1:A:326:MET:HE1	1:A:339:VAL:HG22	1.55	0.88
1:A:108:GLN:NE2	1:A:336:LEU:HD11	1.90	0.87
1:A:145:ILE:CD1	1:A:223:VAL:HG21	2.05	0.85
1:A:957:PHE:C	1:A:958:LYS:HG2	1.98	0.84
1:A:247:THR:HG22	1:A:249:LEU:H	1.42	0.84
1:A:141:LYS:H	1:A:141:LYS:HD2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:HG21	1:A:472:ASN:OD1	1.79	0.83
1:A:174:ARG:HG3	1:A:216:ALA:HB3	1.59	0.83
1:A:403:ARG:HD3	1:A:456:ASN:HD21	1.42	0.82
1:A:50:TRP:O	1:A:54:ILE:CG2	2.27	0.81
1:A:355:THR:O	1:A:604:ARG:HD2	1.80	0.81
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.10	0.80
1:A:875:GLN:HG3	1:A:876:CYS:H	1.44	0.80
1:A:108:GLN:OE1	1:A:336:LEU:CG	2.30	0.80
1:A:879:ASP:OD2	1:A:885:GLY:HA3	1.80	0.80
1:A:51:GLU:HG3	1:A:54:ILE:CD1	2.08	0.79
1:A:449:VAL:HG21	1:A:472:ASN:CG	2.04	0.79
1:A:879:ASP:OD1	1:A:882:HIS:HB3	1.81	0.79
1:A:962:LEU:HB2	1:A:964:LEU:HG	1.65	0.79
1:A:759:GLN:HE22	1:A:762:ARG:HH21	1.31	0.78
1:A:781:LEU:HD12	1:A:783:LEU:HD11	1.64	0.78
1:A:111:ASN:O	1:A:113:GLU:N	2.18	0.77
1:A:51:GLU:HA	1:A:54:ILE:HG12	1.65	0.77
1:A:903:VAL:HG12	1:A:907:ILE:HD11	1.65	0.77
1:A:446:THR:O	1:A:449:VAL:HG22	1.85	0.76
1:A:481:LYS:HG3	1:A:496:VAL:HG13	1.68	0.76
1:A:556:ARG:H	1:A:556:ARG:HD3	1.51	0.75
1:A:293:ILE:HG22	1:A:297:LYS:HB2	1.69	0.75
1:A:950:VAL:O	1:A:954:PRO:HD2	1.86	0.75
1:A:798:VAL:O	1:A:801:GLY:N	2.20	0.75
1:A:50:TRP:O	1:A:54:ILE:HG21	1.87	0.74
1:A:183:GLU:OE2	6:A:2006:HOH:O	2.04	0.74
1:A:878:GLU:OE1	1:A:880:HIS:HD2	1.66	0.74
1:A:47:LYS:HB3	1:A:52:LEU:CD1	2.17	0.74
1:A:957:PHE:O	1:A:958:LYS:HG2	1.88	0.74
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.70	0.74
1:A:757:MET:O	1:A:761:ILE:HG13	1.89	0.73
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.69	0.73
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.03	0.73
1:A:75:LEU:HD21	1:A:296:PHE:HB3	1.70	0.72
1:A:247:THR:HG21	1:A:340:GLU:CD	2.09	0.72
1:A:476:ARG:NH1	1:A:476:ARG:HB2	2.03	0.72
1:A:844:VAL:HG12	1:A:907:ILE:HD13	1.71	0.72
1:A:58:GLU:OE2	1:A:58:GLU:HA	1.89	0.72
1:A:111:ASN:C	1:A:111:ASN:ND2	2.38	0.72
1:A:557:ASP:O	1:A:559:LEU:HG	1.89	0.72
1:A:96:LEU:HA	1:A:99:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:O	1:A:112:ALA:C	2.25	0.71
1:A:759:GLN:NE2	1:A:762:ARG:HH21	1.87	0.71
1:A:47:LYS:HD3	1:A:52:LEU:CD1	2.20	0.71
1:A:315:ILE:HG13	1:A:316:THR:N	2.04	0.71
1:A:863:PRO:HG2	1:A:890:ILE:CG2	2.21	0.70
1:A:397:LYS:H	1:A:402:ILE:HD12	1.57	0.70
1:A:950:VAL:HB	1:A:953:LEU:HD12	1.73	0.70
1:A:988:ALA:HB1	1:A:992:LEU:HD12	1.73	0.70
1:A:887:ASP:CG	1:A:890:ILE:HD11	2.12	0.70
1:A:67:LEU:O	1:A:71:ILE:HG12	1.91	0.70
1:A:277:GLY:HA2	1:A:281:ASP:OD2	1.90	0.70
1:A:926:PRO:HB3	1:A:928:TRP:NE1	2.07	0.70
1:A:47:LYS:CB	1:A:52:LEU:HD11	2.22	0.70
1:A:32:HIS:HD2	1:A:147:PRO:O	1.75	0.70
1:A:109:GLU:HA	1:A:109:GLU:OE1	1.90	0.70
1:A:174:ARG:CG	1:A:216:ALA:HB3	2.22	0.70
1:A:835:PHE:HA	1:A:838:MET:HB3	1.73	0.69
1:A:662:PRO:HD2	1:A:665:GLU:HB2	1.73	0.69
1:A:262:LYS:O	1:A:266:LEU:HD23	1.93	0.69
1:A:769:VAL:O	1:A:773:VAL:HG23	1.93	0.69
1:A:56:GLN:HE21	1:A:106:VAL:HG23	1.58	0.69
1:A:878:GLU:HB3	1:A:880:HIS:CD2	2.27	0.69
1:A:987:ILE:O	1:A:991:TYR:HB3	1.93	0.69
1:A:76:ALA:HB1	1:A:88:PHE:CE2	2.28	0.68
1:A:145:ILE:HD12	1:A:223:VAL:HG21	1.76	0.68
1:A:421:ASN:ND2	1:A:423:SER:H	1.90	0.68
1:A:903:VAL:O	1:A:907:ILE:HG13	1.93	0.68
1:A:56:GLN:NE2	1:A:106:VAL:N	2.40	0.68
1:A:705:VAL:HB	1:A:726:VAL:HG11	1.75	0.68
1:A:247:THR:HG23	1:A:248:PRO:HD2	1.74	0.68
1:A:758:LYS:CG	1:A:828:LEU:HD22	2.18	0.68
1:A:50:TRP:O	1:A:54:ILE:HG23	1.92	0.68
1:A:247:THR:HG22	1:A:249:LEU:N	2.08	0.68
1:A:768:ASN:N	1:A:768:ASN:HD22	1.90	0.68
1:A:155:VAL:HG12	1:A:216:ALA:HA	1.77	0.67
1:A:47:LYS:HB3	1:A:52:LEU:HD11	1.74	0.67
1:A:567:ARG:NH1	1:A:569:THR:O	2.27	0.67
1:A:500:PRO:HD2	1:A:510:ASN:ND2	2.09	0.67
1:A:836:ARG:O	1:A:840:ILE:HG12	1.94	0.67
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.76	0.67
1:A:179:ILE:H	1:A:179:ILE:CD1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HG	1:A:221:GLY:HA2	1.76	0.67
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.25	0.67
1:A:449:VAL:HG21	1:A:472:ASN:ND2	2.09	0.67
1:A:51:GLU:HA	1:A:54:ILE:CD1	2.25	0.66
1:A:836:ARG:NH1	1:A:985:LYS:HG2	2.10	0.66
1:A:905:VAL:HG21	1:A:944:HIS:CE1	2.31	0.66
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.75	0.66
1:A:114:ASN:HB3	1:A:117:GLU:HB3	1.76	0.66
1:A:134:ARG:HH11	1:A:138:GLN:HG2	1.58	0.66
1:A:56:GLN:HE22	1:A:106:VAL:N	1.94	0.66
1:A:47:LYS:CG	1:A:52:LEU:HD11	2.26	0.66
1:A:572:LYS:HB2	1:A:575:GLU:CG	2.26	0.66
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.78	0.66
1:A:51:GLU:HA	1:A:54:ILE:CG1	2.26	0.65
1:A:56:GLN:HE21	1:A:106:VAL:CG2	2.09	0.65
1:A:311:LEU:N	1:A:312:PRO:HD2	2.12	0.65
1:A:336:LEU:N	1:A:337:PRO:HD2	2.12	0.65
1:A:798:VAL:O	1:A:800:ASP:N	2.30	0.65
1:A:397:LYS:N	1:A:402:ILE:HD12	2.10	0.65
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.61	0.65
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.77	0.64
1:A:337:PRO:O	1:A:340:GLU:HG2	1.97	0.64
1:A:312:PRO:O	1:A:315:ILE:HG12	1.98	0.64
1:A:957:PHE:O	1:A:958:LYS:CG	2.46	0.64
1:A:572:LYS:HB2	1:A:575:GLU:HG3	1.77	0.64
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.62	0.64
1:A:909:MET:SD	1:A:937:ILE:HG23	2.38	0.64
1:A:895:GLU:HA	1:A:898:THR:HG22	1.79	0.64
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.79	0.64
1:A:491:ARG:HD2	1:A:588:GLU:OE2	1.98	0.63
1:A:983:ILE:O	1:A:987:ILE:HG13	1.98	0.63
1:A:769:VAL:HG21	5:A:999:TG1:H332	1.79	0.63
1:A:792:LEU:O	1:A:796:ASN:ND2	2.32	0.63
1:A:768:ASN:O	1:A:772:VAL:HG23	1.99	0.62
1:A:975:LEU:H	1:A:975:LEU:CD2	2.11	0.62
1:A:926:PRO:HB2	1:A:929:VAL:HG23	1.81	0.62
1:A:1:MET:HB2	1:A:36:TYR:HE1	1.63	0.62
1:A:72:SER:O	1:A:76:ALA:HB2	2.00	0.62
1:A:890:ILE:N	1:A:890:ILE:HD12	2.14	0.62
1:A:383:SER:C	1:A:384:ILE:HD13	2.19	0.62
1:A:369:ILE:HG13	1:A:528:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:PHE:O	1:A:958:LYS:CB	2.47	0.62
1:A:613:LEU:HD23	1:A:744:VAL:HG11	1.82	0.62
1:A:55:GLU:HA	1:A:55:GLU:OE1	1.97	0.61
1:A:95:LEU:HD22	1:A:99:ILE:HD11	1.82	0.61
1:A:449:VAL:HG23	1:A:450:GLU:N	2.15	0.61
1:A:88:PHE:O	1:A:92:PHE:HB2	2.01	0.61
1:A:769:VAL:HA	5:A:999:TG1:H231	1.83	0.61
1:A:924:ARG:HA	1:A:924:ARG:NE	2.15	0.61
1:A:113:GLU:OE2	1:A:334:ARG:NH2	2.34	0.60
1:A:795:VAL:HA	1:A:799:THR:CB	2.30	0.60
1:A:798:VAL:HG11	1:A:943:LEU:HD13	1.82	0.60
1:A:648:VAL:HG12	1:A:648:VAL:O	2.01	0.60
1:A:781:LEU:HB2	1:A:783:LEU:HG	1.81	0.60
1:A:384:ILE:HD12	1:A:395:VAL:HG22	1.83	0.60
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.82	0.60
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.31	0.60
1:A:895:GLU:O	1:A:898:THR:HG22	2.01	0.60
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.83	0.60
1:A:844:VAL:HG12	1:A:907:ILE:HG21	1.83	0.60
1:A:761:ILE:O	1:A:765:ILE:HG12	2.02	0.60
1:A:45:GLU:OE1	1:A:45:GLU:HA	2.01	0.60
1:A:496:VAL:HG12	1:A:498:CYS:SG	2.42	0.60
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.84	0.60
1:A:916:LEU:HB3	1:A:925:MET:SD	2.42	0.60
1:A:975:LEU:H	1:A:975:LEU:HD22	1.66	0.60
1:A:298:ILE:HD12	1:A:299:ALA:N	2.17	0.59
1:A:486:GLU:O	1:A:491:ARG:NH2	2.35	0.59
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.83	0.59
1:A:947:ILE:HA	1:A:953:LEU:HD13	1.83	0.59
1:A:795:VAL:HA	1:A:799:THR:HB	1.83	0.59
1:A:844:VAL:CG1	1:A:907:ILE:HG21	2.32	0.59
1:A:353:THR:HA	1:A:357:THR:OG1	2.03	0.59
1:A:298:ILE:HD12	1:A:298:ILE:C	2.22	0.59
1:A:544:LYS:HD3	1:A:544:LYS:C	2.22	0.59
1:A:671:ARG:HG3	1:A:694:TYR:CE2	2.37	0.59
1:A:688:VAL:O	1:A:692:GLN:HG3	2.03	0.59
1:A:984:LEU:HA	1:A:987:ILE:CD1	2.27	0.59
1:A:304:VAL:HG21	1:A:789:PRO:HB3	1.84	0.58
1:A:877:THR:O	1:A:877:THR:HG22	2.02	0.58
1:A:946:LEU:O	1:A:953:LEU:HD12	2.03	0.58
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:VAL:HA	1:A:799:THR:OG1	2.03	0.58
1:A:855:TRP:HZ3	1:A:966:GLN:NE2	2.02	0.58
1:A:606:GLU:H	1:A:606:GLU:CD	2.07	0.58
1:A:679:VAL:HB	1:A:683:HIS:HB2	1.84	0.58
1:A:988:ALA:CB	1:A:992:LEU:HD12	2.34	0.58
1:A:47:LYS:HB3	1:A:52:LEU:HD12	1.86	0.58
1:A:985:LYS:HB3	1:A:989:ARG:HH12	1.69	0.58
1:A:276:ILE:HG23	1:A:279:PHE:HB3	1.85	0.58
1:A:421:ASN:HD22	1:A:422:ASP:N	2.01	0.58
1:A:60:LEU:HA	1:A:63:ARG:HB2	1.85	0.58
1:A:314:VAL:HG22	1:A:805:THR:OG1	2.04	0.58
1:A:622:ILE:HD12	1:A:691:LEU:HD21	1.85	0.58
1:A:829:ILE:HD12	5:A:999:TG1:HC91	1.85	0.58
1:A:49:LEU:O	1:A:53:VAL:HG23	2.03	0.58
1:A:571:PRO:HG2	1:A:576:MET:SD	2.43	0.58
1:A:789:PRO:HA	1:A:792:LEU:HB2	1.84	0.58
1:A:247:THR:HG21	1:A:340:GLU:OE1	2.03	0.57
1:A:855:TRP:HZ3	1:A:966:GLN:HE22	1.52	0.57
1:A:27:ASP:OD1	1:A:31:ARG:NH1	2.37	0.57
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.85	0.57
1:A:926:PRO:HB3	1:A:928:TRP:HE1	1.67	0.57
1:A:293:ILE:HG22	1:A:293:ILE:O	2.05	0.57
1:A:342:LEU:HD13	1:A:716:ILE:HD13	1.85	0.57
1:A:383:SER:O	1:A:384:ILE:HD13	2.04	0.57
1:A:800:ASP:O	1:A:803:PRO:HD2	2.03	0.57
1:A:269:VAL:O	1:A:273:LEU:HG	2.05	0.57
1:A:763:TYR:HD1	1:A:911:ASN:ND2	2.02	0.57
1:A:247:THR:HB	1:A:250:GLN:HG3	1.86	0.57
1:A:355:THR:HG21	1:A:701:THR:HG22	1.86	0.57
1:A:968:LEU:HD12	1:A:968:LEU:H	1.70	0.57
1:A:41:LEU:O	1:A:120:LYS:HE2	2.05	0.56
1:A:484:THR:HG22	1:A:496:VAL:HG22	1.87	0.56
1:A:765:ILE:HD12	5:A:999:TG1:H313	1.86	0.56
1:A:427:PHE:HA	1:A:434:TYR:HA	1.87	0.56
1:A:966:GLN:O	1:A:969:MET:HB3	2.05	0.56
1:A:177:GLN:HB3	1:A:212:THR:HG21	1.87	0.56
1:A:968:LEU:HD12	1:A:968:LEU:N	2.20	0.56
1:A:193:PRO:O	1:A:195:PRO:HD3	2.05	0.56
1:A:248:PRO:HD2	1:A:341:THR:HG22	1.88	0.56
1:A:49:LEU:O	1:A:53:VAL:CG2	2.54	0.56
1:A:72:SER:CB	1:A:91:PRO:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:GLN:HE22	1:A:762:ARG:NH2	2.01	0.56
1:A:29:VAL:O	1:A:33:LEU:HB2	2.06	0.56
1:A:128:LYS:HG2	1:A:139:ARG:HD2	1.88	0.56
1:A:166:LEU:HD21	1:A:222:ILE:HG22	1.87	0.56
1:A:356:LEU:HB3	1:A:639:ILE:HD11	1.87	0.56
1:A:800:ASP:C	1:A:803:PRO:HD2	2.26	0.56
1:A:875:GLN:CG	1:A:876:CYS:H	2.17	0.56
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.69	0.55
1:A:51:GLU:O	1:A:51:GLU:HG2	2.06	0.55
1:A:111:ASN:C	1:A:113:GLU:N	2.59	0.55
1:A:342:LEU:CD1	1:A:716:ILE:HD13	2.36	0.55
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.88	0.55
1:A:762:ARG:HD2	1:A:829:ILE:HG12	1.89	0.55
1:A:762:ARG:HD3	1:A:828:LEU:O	2.06	0.55
1:A:421:ASN:HD22	1:A:421:ASN:C	2.09	0.55
1:A:484:THR:CG2	1:A:496:VAL:HG22	2.36	0.55
1:A:69:ALA:HB2	1:A:94:ILE:HG22	1.88	0.55
1:A:276:ILE:O	1:A:276:ILE:HG22	2.07	0.55
1:A:777:LEU:HD12	1:A:845:GLY:O	2.07	0.55
1:A:879:ASP:OD1	1:A:879:ASP:O	2.25	0.55
1:A:139:ARG:HH11	1:A:139:ARG:CG	2.19	0.55
1:A:627:ASP:OD2	1:A:628:ASN:N	2.37	0.55
1:A:971:LEU:C	1:A:973:ILE:H	2.09	0.55
1:A:390:ALA:C	1:A:392:GLU:H	2.11	0.55
1:A:926:PRO:HB3	1:A:928:TRP:CD1	2.42	0.55
1:A:273:LEU:O	1:A:276:ILE:HG13	2.08	0.54
1:A:854:TRP:HH2	1:A:966:GLN:CG	2.08	0.54
1:A:829:ILE:HB	5:A:999:TG1:HC92	1.88	0.54
1:A:76:ALA:O	1:A:88:PHE:HE2	1.91	0.54
1:A:86:THR:HG22	1:A:86:THR:O	2.07	0.54
1:A:108:GLN:OE1	1:A:336:LEU:CD1	2.54	0.54
1:A:248:PRO:CD	1:A:341:THR:HG22	2.38	0.54
1:A:358:THR:O	1:A:359:ASN:HB3	2.06	0.54
1:A:607:VAL:O	1:A:611:ILE:HG12	2.08	0.54
1:A:875:GLN:HG3	1:A:876:CYS:N	2.17	0.54
1:A:4:ALA:HB1	1:A:7:LYS:HG2	1.90	0.54
1:A:933:LEU:O	1:A:937:ILE:HG13	2.08	0.54
1:A:988:ALA:HA	1:A:992:LEU:HG	1.89	0.54
1:A:922:LEU:N	1:A:922:LEU:HD12	2.22	0.54
1:A:329:LYS:O	1:A:330:ASN:HB2	2.08	0.54
1:A:198:ARG:NH1	1:A:660:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:C	1:A:277:GLY:H	2.12	0.53
1:A:895:GLU:N	1:A:896:PRO:HD2	2.23	0.53
1:A:777:LEU:C	1:A:779:ALA:H	2.12	0.53
1:A:258:GLU:O	1:A:261:SER:HB3	2.08	0.53
1:A:544:LYS:HD3	1:A:544:LYS:O	2.09	0.53
1:A:774:CYS:O	1:A:778:THR:HG22	2.09	0.53
1:A:142:ALA:O	1:A:145:ILE:HG23	2.08	0.53
1:A:620:ARG:NH2	1:A:622:ILE:HD11	2.24	0.53
1:A:529:ARG:NH2	1:A:592:THR:HG21	2.23	0.53
1:A:684:LYS:NZ	1:A:707:ASP:OD1	2.39	0.53
1:A:847:ALA:HB1	1:A:973:ILE:CG2	2.39	0.53
1:A:252:LYS:O	1:A:255:GLU:HG2	2.09	0.53
1:A:719:ALA:HB2	1:A:731:SER:OG	2.09	0.53
1:A:304:VAL:HG21	1:A:789:PRO:CB	2.39	0.53
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.91	0.53
1:A:481:LYS:HG3	1:A:496:VAL:CG1	2.38	0.53
1:A:333:VAL:HG11	1:A:339:VAL:HG23	1.91	0.52
1:A:604:ARG:HH21	1:A:738:ASP:HB3	1.74	0.52
1:A:460:ARG:HG3	1:A:460:ARG:HH11	1.73	0.52
1:A:673:ALA:HB3	1:A:676:PHE:CZ	2.45	0.52
1:A:111:ASN:O	1:A:111:ASN:ND2	2.39	0.52
1:A:667:ARG:HH11	1:A:667:ARG:HG2	1.74	0.52
1:A:903:VAL:CG1	1:A:907:ILE:HD11	2.38	0.52
1:A:962:LEU:C	1:A:964:LEU:H	2.13	0.52
1:A:336:LEU:O	1:A:339:VAL:HB	2.10	0.52
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.40	0.52
1:A:315:ILE:CG1	1:A:316:THR:N	2.72	0.52
1:A:586:GLU:O	1:A:589:THR:HG22	2.10	0.52
1:A:48:SER:HB3	1:A:51:GLU:HB3	1.90	0.52
1:A:319:LEU:HD23	1:A:336:LEU:HB3	1.92	0.52
1:A:662:PRO:HD2	1:A:665:GLU:CB	2.38	0.52
1:A:72:SER:OG	1:A:91:PRO:HB3	2.10	0.52
1:A:338:SER:HA	1:A:341:THR:OG1	2.10	0.52
1:A:366:MET:CE	1:A:448:LEU:HD11	2.39	0.52
1:A:65:LEU:HD11	1:A:307:ILE:HG21	1.91	0.52
1:A:247:THR:HB	1:A:250:GLN:CG	2.40	0.52
1:A:757:MET:HA	1:A:760:PHE:CE2	2.45	0.52
1:A:965:THR:HA	1:A:968:LEU:HD13	1.91	0.52
1:A:72:SER:HB3	1:A:91:PRO:HB3	1.92	0.51
1:A:834:PHE:O	1:A:838:MET:HB2	2.10	0.51
1:A:281:ASP:HB2	1:A:282:PRO:HD3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.91	0.51
1:A:481:LYS:HD3	1:A:484:THR:CG2	2.40	0.51
1:A:611:ILE:HG13	1:A:639:ILE:HG23	1.92	0.51
1:A:134:ARG:HD2	1:A:138:GLN:CD	2.31	0.51
1:A:135:LYS:HZ2	1:A:135:LYS:HB3	1.75	0.51
1:A:366:MET:HA	1:A:596:VAL:O	2.11	0.51
1:A:879:ASP:O	1:A:882:HIS:O	2.29	0.51
1:A:255:GLU:HG3	1:A:256:PHE:N	2.26	0.51
1:A:768:ASN:N	1:A:768:ASN:ND2	2.57	0.51
1:A:366:MET:HE1	1:A:448:LEU:HD11	1.92	0.51
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.10	0.51
1:A:966:GLN:O	1:A:970:VAL:HG23	2.10	0.51
1:A:559:LEU:HD22	1:A:600:LEU:HB2	1.93	0.51
1:A:768:ASN:HB2	5:A:999:TG1:H251	1.92	0.51
1:A:857:MET:HA	1:A:866:THR:HA	1.92	0.51
1:A:866:THR:HG22	1:A:867:TYR:HD1	1.75	0.50
1:A:963:ASP:O	1:A:963:ASP:OD1	2.29	0.50
1:A:433:VAL:HG22	1:A:434:TYR:N	2.27	0.50
1:A:553:GLY:O	1:A:554:THR:HG23	2.11	0.50
1:A:717:GLY:N	1:A:732:GLU:OE1	2.38	0.50
1:A:775:ILE:HA	1:A:778:THR:HG22	1.93	0.50
1:A:260:LEU:CD2	1:A:307:ILE:HD13	2.41	0.50
1:A:567:ARG:HH11	1:A:570:PRO:HA	1.77	0.50
1:A:402:ILE:HG12	1:A:402:ILE:O	2.12	0.49
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.42	0.49
1:A:59:ASP:O	1:A:62:VAL:HG22	2.12	0.49
1:A:254:ASP:O	1:A:258:GLU:HG2	2.12	0.49
1:A:865:VAL:HB	1:A:868:HIS:CB	2.42	0.49
1:A:929:VAL:HG12	1:A:929:VAL:O	2.12	0.49
1:A:47:LYS:HE3	1:A:111:ASN:HD21	1.77	0.49
1:A:141:LYS:HD3	1:A:144:ASP:OD2	2.13	0.49
1:A:260:LEU:HD23	1:A:307:ILE:HD13	1.93	0.49
1:A:476:ARG:HB2	1:A:476:ARG:HH11	1.73	0.49
1:A:874:MET:HG3	1:A:891:PHE:CD2	2.47	0.49
1:A:58:GLU:OE2	1:A:58:GLU:CA	2.59	0.49
1:A:968:LEU:H	1:A:968:LEU:CD1	2.25	0.49
1:A:456:ASN:O	1:A:457:THR:C	2.51	0.49
1:A:141:LYS:HD2	1:A:141:LYS:N	2.19	0.49
1:A:646:GLU:O	1:A:648:VAL:HG23	2.13	0.49
1:A:802:LEU:N	1:A:802:LEU:HD22	2.28	0.49
1:A:102:ALA:O	1:A:106:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:SER:O	1:A:269:VAL:HG23	2.12	0.49
1:A:661:LEU:HB3	1:A:665:GLU:HB3	1.95	0.48
1:A:922:LEU:HD12	1:A:922:LEU:H	1.78	0.48
1:A:572:LYS:HB3	1:A:574:GLU:OE2	2.12	0.48
1:A:581:SER:HA	1:A:584:PHE:CZ	2.48	0.48
1:A:880:HIS:C	1:A:882:HIS:H	2.16	0.48
1:A:47:LYS:HD3	1:A:52:LEU:HD13	1.94	0.48
1:A:57:PHE:O	1:A:62:VAL:CG2	2.61	0.48
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.48	0.48
1:A:918:GLU:O	1:A:919:ASN:ND2	2.42	0.48
1:A:948:LEU:C	1:A:949:TYR:HD1	2.17	0.48
1:A:963:ASP:O	1:A:964:LEU:C	2.52	0.48
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.96	0.48
1:A:837:TYR:HB3	5:A:999:TG1:H331	1.96	0.48
1:A:326:MET:CE	1:A:333:VAL:HG21	2.44	0.48
1:A:362:SER:O	1:A:599:MET:HA	2.14	0.48
1:A:879:ASP:OD2	1:A:885:GLY:CA	2.55	0.48
1:A:396:LEU:HD13	1:A:399:ASP:HA	1.94	0.48
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.95	0.48
1:A:847:ALA:HB1	1:A:973:ILE:HG22	1.96	0.48
1:A:975:LEU:HD22	1:A:975:LEU:N	2.27	0.48
1:A:97:ILE:HG22	1:A:101:ASN:HD21	1.79	0.48
1:A:198:ARG:HB2	1:A:656:ARG:NH2	2.28	0.48
1:A:352:LYS:HD2	1:A:635:ILE:HG13	1.96	0.48
1:A:500:PRO:HD2	1:A:510:ASN:HD22	1.77	0.48
1:A:415:THR:HG22	1:A:419:LEU:HD12	1.95	0.48
1:A:837:TYR:CB	5:A:999:TG1:H331	2.44	0.48
1:A:897:MET:C	1:A:899:MET:H	2.17	0.48
1:A:326:MET:HE1	1:A:339:VAL:CG2	2.37	0.48
1:A:416:ILE:HG23	1:A:513:PHE:HB3	1.95	0.48
1:A:676:PHE:CD2	1:A:687:ILE:HD11	2.48	0.48
1:A:846:ALA:O	1:A:848:THR:N	2.46	0.48
1:A:957:PHE:O	1:A:958:LYS:HB2	2.14	0.48
1:A:249:LEU:HD13	1:A:754:TYR:HE1	1.79	0.47
1:A:442:GLU:HA	1:A:445:LEU:HD13	1.96	0.47
1:A:500:PRO:CD	1:A:510:ASN:HD22	2.27	0.47
1:A:519:GLU:HG2	1:A:520:GLY:H	1.78	0.47
1:A:887:ASP:OD1	1:A:890:ILE:HD11	2.13	0.47
1:A:403:ARG:HD3	1:A:456:ASN:ND2	2.20	0.47
1:A:460:ARG:HG3	1:A:460:ARG:NH1	2.28	0.47
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:HA	1:A:210:SER:HB2	1.97	0.47
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.96	0.47
1:A:600:LEU:O	1:A:602:PRO:HD3	2.14	0.47
1:A:869:GLN:OE1	1:A:872:HIS:HD2	1.98	0.47
1:A:248:PRO:O	1:A:252:LYS:HG2	2.14	0.47
1:A:315:ILE:HG13	1:A:316:THR:H	1.77	0.47
1:A:944:HIS:C	1:A:946:LEU:H	2.17	0.47
1:A:962:LEU:C	1:A:964:LEU:N	2.67	0.47
1:A:993:GLU:O	1:A:994:GLY:OXT	2.32	0.47
1:A:524:ARG:HB2	1:A:591:LEU:HD12	1.95	0.47
1:A:47:LYS:HG2	1:A:52:LEU:HD11	1.95	0.47
1:A:326:MET:HE1	1:A:333:VAL:HG21	1.97	0.47
1:A:421:ASN:ND2	1:A:421:ASN:C	2.67	0.47
1:A:939:LEU:O	1:A:943:LEU:HG	2.15	0.47
1:A:100:ALA:O	1:A:104:VAL:HG23	2.14	0.47
1:A:187:VAL:HG23	1:A:189:LYS:HE2	1.95	0.47
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.44	0.47
1:A:415:THR:HA	1:A:475:ILE:HD13	1.96	0.47
1:A:969:MET:O	1:A:973:ILE:HG13	2.15	0.47
1:A:115:ALA:HB1	1:A:239:MET:HE2	1.96	0.47
1:A:500:PRO:HG2	1:A:503:SER:OG	2.15	0.47
1:A:794:TRP:CH2	1:A:943:LEU:HB3	2.50	0.47
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.97	0.47
1:A:54:ILE:HG13	1:A:55:GLU:N	2.30	0.47
1:A:310:GLY:H	1:A:312:PRO:HD2	1.78	0.47
1:A:357:THR:HB	1:A:601:ASP:OD1	2.15	0.47
1:A:963:ASP:HA	1:A:967:TRP:HB2	1.97	0.47
1:A:8:SER:OG	1:A:11:GLU:HG3	2.15	0.46
1:A:429:GLU:CD	1:A:429:GLU:H	2.19	0.46
1:A:883:PHE:O	1:A:885:GLY:N	2.48	0.46
1:A:357:THR:O	1:A:604:ARG:NH1	2.48	0.46
1:A:57:PHE:O	1:A:62:VAL:HG23	2.15	0.46
1:A:558:THR:O	1:A:559:LEU:HD23	2.16	0.46
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.15	0.46
1:A:417:CYS:HB3	1:A:445:LEU:HB3	1.96	0.46
1:A:449:VAL:CG2	1:A:472:ASN:HD21	2.28	0.46
1:A:672:ARG:HG2	1:A:672:ARG:HH11	1.80	0.46
1:A:859:ALA:HB3	1:A:864:GLY:CA	2.37	0.46
1:A:953:LEU:O	1:A:956:ILE:HG12	2.16	0.46
1:A:89:VAL:O	1:A:93:VAL:HG23	2.16	0.46
1:A:957:PHE:C	1:A:958:LYS:CG	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:O	1:A:302:LEU:HB2	2.15	0.46
1:A:403:ARG:CZ	1:A:406:GLN:HB2	2.45	0.46
1:A:445:LEU:H	1:A:445:LEU:HD12	1.80	0.46
1:A:836:ARG:HG3	1:A:984:LEU:HD13	1.98	0.46
1:A:527:TYR:HB3	1:A:534:ARG:HD3	1.98	0.46
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.15	0.46
1:A:151:VAL:HG12	1:A:152:GLU:N	2.29	0.46
1:A:328:LYS:HE2	1:A:328:LYS:CA	2.43	0.46
1:A:380:ASN:O	1:A:382:PHE:CD1	2.69	0.46
1:A:569:THR:O	1:A:569:THR:HG22	2.16	0.46
1:A:813:ASP:OD2	1:A:819:ARG:NH1	2.49	0.46
1:A:459:VAL:HB	1:A:462:LEU:HD12	1.98	0.46
1:A:642:PHE:CE1	1:A:648:VAL:HG11	2.51	0.46
1:A:33:LEU:O	1:A:33:LEU:HD23	2.15	0.45
1:A:179:ILE:HD12	1:A:179:ILE:N	2.10	0.45
1:A:499:SER:HA	1:A:510:ASN:ND2	2.31	0.45
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.97	0.45
1:A:293:ILE:O	1:A:297:LYS:CB	2.64	0.45
1:A:311:LEU:N	1:A:312:PRO:CD	2.80	0.45
1:A:556:ARG:H	1:A:556:ARG:CD	2.18	0.45
1:A:760:PHE:CD1	1:A:760:PHE:C	2.90	0.45
1:A:41:LEU:HD21	1:A:233:GLY:HA2	1.99	0.45
1:A:135:LYS:N	1:A:135:LYS:HE2	2.31	0.45
1:A:526:ASN:HB2	1:A:527:TYR:CE2	2.52	0.45
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.57	0.45
1:A:781:LEU:O	1:A:871:THR:HG23	2.16	0.45
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.98	0.45
1:A:965:THR:O	1:A:965:THR:HG22	2.17	0.45
1:A:238:GLN:O	1:A:242:THR:HG23	2.16	0.45
1:A:366:MET:CE	1:A:384:ILE:HD11	2.47	0.45
1:A:903:VAL:HG12	1:A:907:ILE:CD1	2.39	0.45
1:A:917:SER:OG	1:A:920:GLN:HB2	2.17	0.45
1:A:927:PRO:O	1:A:934:LEU:HD21	2.17	0.45
1:A:984:LEU:HD23	1:A:987:ILE:HD12	1.98	0.45
1:A:389:TYR:OH	1:A:440:ALA:HB1	2.17	0.45
1:A:417:CYS:SG	1:A:445:LEU:HD23	2.57	0.45
1:A:581:SER:HA	1:A:584:PHE:CE1	2.52	0.45
1:A:822:ARG:HD2	1:A:826:GLU:OE2	2.17	0.45
1:A:870:LEU:HD23	1:A:891:PHE:HE2	1.81	0.45
1:A:51:GLU:HA	1:A:54:ILE:HD13	1.97	0.45
1:A:622:ILE:CD1	1:A:691:LEU:HD21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:MET:O	1:A:969:MET:HE3	2.17	0.45
1:A:120:LYS:O	1:A:123:GLU:HG2	2.17	0.45
1:A:251:GLN:HA	1:A:254:ASP:OD2	2.16	0.45
1:A:255:GLU:OE1	5:A:999:TG1:H341	2.17	0.45
1:A:402:ILE:HD13	1:A:402:ILE:H	1.82	0.45
1:A:306:ALA:O	1:A:308:PRO:HD3	2.17	0.44
1:A:652:ALA:HA	1:A:675:CYS:O	2.17	0.44
1:A:857:MET:CE	1:A:867:TYR:HA	2.47	0.44
1:A:890:ILE:HD12	1:A:890:ILE:H	1.79	0.44
1:A:977:VAL:HG13	1:A:978:ILE:N	2.31	0.44
1:A:59:ASP:O	1:A:61:LEU:N	2.51	0.44
1:A:177:GLN:HA	1:A:212:THR:HG22	1.98	0.44
1:A:748:GLU:OE1	1:A:817:MET:HG3	2.17	0.44
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.45	0.44
1:A:950:VAL:C	1:A:952:PRO:HD2	2.38	0.44
1:A:166:LEU:HD21	1:A:222:ILE:CG2	2.48	0.44
1:A:277:GLY:O	1:A:282:PRO:HD3	2.17	0.44
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.98	0.44
1:A:377:CYS:HB3	1:A:544:LYS:HG3	2.00	0.44
1:A:865:VAL:O	1:A:868:HIS:HB2	2.18	0.44
1:A:893:ALA:O	1:A:896:PRO:HD2	2.18	0.44
1:A:179:ILE:O	1:A:705:VAL:HG22	2.17	0.44
1:A:369:ILE:HG13	1:A:528:VAL:HG12	1.94	0.44
1:A:396:LEU:HA	1:A:402:ILE:CD1	2.48	0.44
1:A:527:TYR:CG	1:A:534:ARG:HD3	2.53	0.44
1:A:814:LEU:O	1:A:815:ASP:HB3	2.18	0.44
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.18	0.44
1:A:98:LEU:HA	1:A:101:ASN:HD22	1.82	0.44
1:A:133:ASP:O	1:A:134:ARG:HG3	2.18	0.44
1:A:476:ARG:HB2	1:A:476:ARG:CZ	2.47	0.44
1:A:527:TYR:CB	1:A:534:ARG:HD3	2.48	0.44
1:A:583:ARG:O	1:A:586:GLU:HG2	2.18	0.44
1:A:656:ARG:HG3	1:A:656:ARG:HH11	1.83	0.44
1:A:702:GLY:O	1:A:719:ALA:HA	2.18	0.44
1:A:798:VAL:O	1:A:799:THR:C	2.56	0.44
1:A:228:VAL:HG13	1:A:237:ASP:OD1	2.18	0.43
1:A:294:TYR:OH	1:A:779:ALA:HA	2.18	0.43
1:A:110:ARG:C	1:A:112:ALA:H	2.20	0.43
1:A:380:ASN:HB3	1:A:382:PHE:HE1	1.83	0.43
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.77	0.43
1:A:648:VAL:O	1:A:648:VAL:CG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:PRO:HG3	1:A:874:MET:SD	2.58	0.43
1:A:51:GLU:O	1:A:52:LEU:HD23	2.18	0.43
1:A:255:GLU:O	1:A:259:GLN:HG2	2.19	0.43
1:A:584:PHE:N	1:A:584:PHE:CD2	2.84	0.43
1:A:924:ARG:C	1:A:926:PRO:HD3	2.39	0.43
1:A:428:ASN:OD1	1:A:428:ASN:C	2.56	0.43
1:A:449:VAL:HG23	1:A:450:GLU:H	1.81	0.43
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.72	0.43
1:A:771:GLU:O	1:A:775:ILE:HG12	2.18	0.43
1:A:925:MET:SD	1:A:925:MET:O	2.76	0.43
1:A:75:LEU:HD12	1:A:75:LEU:N	2.33	0.43
1:A:4:ALA:CB	1:A:7:LYS:HG2	2.48	0.43
1:A:281:ASP:H	1:A:282:PRO:HD2	1.83	0.43
1:A:403:ARG:NH1	1:A:406:GLN:N	2.67	0.43
1:A:798:VAL:CG1	1:A:943:LEU:HD13	2.47	0.43
1:A:848:THR:O	1:A:900:ALA:HB2	2.18	0.43
1:A:253:LEU:HG	5:A:999:TG1:C30	2.48	0.43
1:A:333:VAL:HG11	1:A:339:VAL:CG2	2.48	0.43
1:A:956:ILE:HG13	1:A:957:PHE:CD1	2.54	0.43
1:A:115:ALA:HA	1:A:729:THR:HG21	2.01	0.43
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.86	0.43
1:A:259:GLN:O	1:A:262:LYS:N	2.52	0.43
1:A:656:ARG:HG3	1:A:656:ARG:NH1	2.34	0.43
1:A:897:MET:C	1:A:899:MET:N	2.71	0.43
1:A:855:TRP:HD1	1:A:856:PHE:CE1	2.37	0.43
1:A:491:ARG:HH11	1:A:588:GLU:CD	2.23	0.42
1:A:828:LEU:HD12	5:A:999:TG1:H291	2.00	0.42
1:A:868:HIS:CG	1:A:868:HIS:O	2.72	0.42
1:A:916:LEU:HB3	1:A:925:MET:HE2	2.01	0.42
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.91	0.42
1:A:791:GLN:NE2	1:A:901:LEU:HD22	2.34	0.42
1:A:145:ILE:HD11	1:A:223:VAL:HG21	1.95	0.42
1:A:246:LYS:HB2	1:A:246:LYS:HE3	1.89	0.42
1:A:302:LEU:HD13	1:A:302:LEU:O	2.19	0.42
1:A:511:LYS:HA	1:A:570:PRO:HD3	2.01	0.42
1:A:737:ASP:OD1	1:A:742:THR:HG21	2.18	0.42
1:A:890:ILE:C	1:A:892:GLU:H	2.21	0.42
1:A:895:GLU:HA	1:A:898:THR:CG2	2.49	0.42
1:A:250:GLN:O	1:A:254:ASP:OD2	2.38	0.42
1:A:369:ILE:HD13	1:A:379:LEU:CD2	2.49	0.42
1:A:527:TYR:O	1:A:592:THR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:O	1:A:158:LYS:HD3	2.19	0.42
1:A:654:THR:HA	1:A:677:ALA:O	2.20	0.42
1:A:794:TRP:HH2	1:A:943:LEU:HB3	1.84	0.42
1:A:154:ALA:O	1:A:155:VAL:C	2.58	0.42
1:A:402:ILE:HD13	1:A:402:ILE:N	2.35	0.42
1:A:264:ILE:HG23	1:A:302:LEU:HD12	2.02	0.42
1:A:380:ASN:O	1:A:382:PHE:CE1	2.72	0.42
1:A:849:VAL:O	1:A:852:ALA:HB3	2.20	0.42
1:A:880:HIS:C	1:A:882:HIS:N	2.73	0.42
1:A:974:SER:O	1:A:977:VAL:HG12	2.19	0.42
1:A:236:ARG:HD3	1:A:236:ARG:C	2.40	0.42
1:A:242:THR:OG1	1:A:712:LYS:HE3	2.20	0.42
1:A:668:GLU:HG3	1:A:672:ARG:NH1	2.35	0.42
1:A:446:THR:O	1:A:449:VAL:CG2	2.64	0.42
1:A:903:VAL:HA	1:A:970:VAL:HG13	2.00	0.42
1:A:460:ARG:HG2	1:A:461:ASN:N	2.35	0.41
1:A:775:ILE:HA	1:A:778:THR:CG2	2.50	0.41
1:A:879:ASP:CG	1:A:885:GLY:HA3	2.40	0.41
1:A:47:LYS:CD	1:A:52:LEU:CD1	2.95	0.41
1:A:200:VAL:O	1:A:203:ASP:HB2	2.20	0.41
1:A:611:ILE:HG13	1:A:639:ILE:CG2	2.50	0.41
1:A:781:LEU:CD1	1:A:783:LEU:HD11	2.41	0.41
1:A:885:GLY:O	1:A:886:LEU:HG	2.20	0.41
1:A:947:ILE:HA	1:A:953:LEU:CD1	2.50	0.41
1:A:255:GLU:CG	1:A:256:PHE:N	2.84	0.41
1:A:366:MET:HE3	1:A:384:ILE:HD11	2.02	0.41
1:A:909:MET:SD	1:A:940:SER:HB3	2.60	0.41
1:A:950:VAL:HB	1:A:953:LEU:CD1	2.47	0.41
1:A:135:LYS:H	1:A:135:LYS:HG2	1.49	0.41
1:A:301:ALA:CB	1:A:789:PRO:HD3	2.50	0.41
1:A:353:THR:HB	3:A:2002:ALF:F3	2.10	0.41
1:A:56:GLN:HE22	1:A:105:GLY:C	2.23	0.41
1:A:158:LYS:HE3	1:A:158:LYS:HB2	1.75	0.41
1:A:315:ILE:CG1	1:A:316:THR:H	2.33	0.41
1:A:459:VAL:HA	1:A:462:LEU:CD1	2.50	0.41
1:A:487:PHE:CD2	1:A:487:PHE:C	2.94	0.41
1:A:688:VAL:CG1	1:A:713:LYS:HG3	2.51	0.41
1:A:827:PRO:HG2	1:A:830:SER:OG	2.20	0.41
1:A:916:LEU:HD23	1:A:925:MET:HG2	2.02	0.41
1:A:763:TYR:CD1	1:A:911:ASN:ND2	2.86	0.41
1:A:901:LEU:O	1:A:905:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:C	1:A:206:ASN:H	2.24	0.41
1:A:557:ASP:O	1:A:558:THR:C	2.59	0.41
1:A:576:MET:HG2	1:A:587:TYR:CE1	2.56	0.41
1:A:813:ASP:OD2	1:A:819:ARG:CZ	2.69	0.41
1:A:878:GLU:OE1	1:A:880:HIS:NE2	2.52	0.41
1:A:178:SER:HB3	1:A:183:GLU:C	2.41	0.41
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.03	0.40
1:A:802:LEU:N	1:A:802:LEU:CD2	2.84	0.40
1:A:907:ILE:O	1:A:910:CYS:HB2	2.21	0.40
1:A:151:VAL:CG1	1:A:152:GLU:N	2.84	0.40
1:A:846:ALA:C	1:A:848:THR:H	2.23	0.40
1:A:367:PHE:CD2	1:A:367:PHE:C	2.94	0.40
1:A:836:ARG:HH12	1:A:985:LYS:HG2	1.86	0.40
1:A:869:GLN:OE1	1:A:872:HIS:CD2	2.75	0.40
1:A:73:PHE:HA	1:A:76:ALA:HB3	2.03	0.40
1:A:669:ALA:HA	1:A:672:ARG:NH1	2.36	0.40
1:A:679:VAL:HB	1:A:683:HIS:CB	2.51	0.40
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.80	0.40
1:A:47:LYS:CG	1:A:52:LEU:CD1	2.98	0.40
1:A:175:VAL:HG21	1:A:208:LEU:CD2	2.51	0.40
1:A:298:ILE:C	1:A:298:ILE:CD1	2.90	0.40
1:A:464:LYS:HD2	1:A:464:LYS:HA	1.96	0.40
1:A:986:PHE:CD1	1:A:990:ASN:ND2	2.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH1	1:A:647:GLU:OE2[4_555]	2.18	0.02

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%)	835 (84%)	126 (13%)	31 (3%)	4 23

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLY
1	A	486	GLU
1	A	799	THR
1	A	960	LYS
1	A	964	LEU
1	A	60	LEU
1	A	112	ALA
1	A	155	VAL
1	A	285	GLY
1	A	555	GLY
1	A	649	ALA
1	A	778	THR
1	A	847	ALA
1	A	883	PHE
1	A	958	LYS
1	A	241	ALA
1	A	309	GLU
1	A	865	VAL
1	A	884	GLU
1	A	972	LYS
1	A	280	ASN
1	A	281	ASP
1	A	863	PRO
1	A	878	GLU
1	A	951	ASP
1	A	276	ILE
1	A	282	PRO
1	A	872	HIS
1	A	195	PRO
1	A	289	ILE
1	A	263	VAL

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%)	784 (93%)	56 (7%)	16 49

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	34	GLU
1	A	53	VAL
1	A	55	GLU
1	A	58	GLU
1	A	77	TRP
1	A	111	ASN
1	A	113	GLU
1	A	114	ASN
1	A	135	LYS
1	A	139	ARG
1	A	141	LYS
1	A	145	ILE
1	A	170	SER
1	A	171	THR
1	A	172	THR
1	A	174	ARG
1	A	179	ILE
1	A	180	LEU
1	A	213	ASN
1	A	243	GLU
1	A	245	ASP
1	A	328	LYS
1	A	356	LEU
1	A	359	ASN
1	A	388	THR
1	A	396	LEU
1	A	402	ILE
1	A	413	LEU
1	A	421	ASN
1	A	436	LYS
1	A	441	THR
1	A	460	ARG
1	A	466	GLU
1	A	467	ARG

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Mol	Chain	Res	Type
1	A	491	ARG
1	A	508	VAL
1	A	511	LYS
1	A	529	ARG
1	A	542	LYS
1	A	544	LYS
1	A	547	SER
1	A	556	ARG
1	A	566	THR
1	A	574	GLU
1	A	665	GLU
1	A	691	LEU
1	A	760	PHE
1	A	768	ASN
1	A	794	TRP
1	A	799	THR
1	A	814	LEU
1	A	924	ARG
1	A	928	TRP
1	A	967	TRP
1	A	982	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	56	GLN
1	A	101	ASN
1	A	111	ASN
1	A	114	ASN
1	A	213	ASN
1	A	250	GLN
1	A	251	GLN
1	A	275	ASN
1	A	280	ASN
1	A	359	ASN
1	A	421	ASN
1	A	456	ASN
1	A	469	ASN
1	A	510	ASN
1	A	666	GLN
1	A	759	GLN

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Mol	Chain	Res	Type
1	A	796	ASN
1	A	872	HIS
1	A	875	GLN
1	A	880	HIS
1	A	911	ASN
1	A	914	ASN
1	A	919	ASN
1	A	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ALF	A	2002	1,2,6	0,4,4	-	-	-		
5	TG1	A	999	-	43,48,48	2.27	14 (32%)	44,72,72	2.09	13 (29%)

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	TG1	A	999	-	-	13/33/99/99	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	TG1	O4-C21	5.78	1.33	1.21
5	A	999	TG1	C4-C5	4.53	1.38	1.34
5	A	999	TG1	O1-C13	4.39	1.46	1.34
5	A	999	TG1	C9-C8	4.12	1.57	1.52
5	A	999	TG1	C11-C7	4.10	1.60	1.55
5	A	999	TG1	O3-C3	3.96	1.52	1.44
5	A	999	TG1	O6-C7	3.79	1.49	1.43
5	A	999	TG1	C34-C11	3.59	1.58	1.53
5	A	999	TG1	O7-C27	3.29	1.43	1.34
5	A	999	TG1	C9-C10	3.18	1.59	1.54
5	A	999	TG1	C31-C10	2.91	1.58	1.52
5	A	999	TG1	C21-C22	2.83	1.59	1.50
5	A	999	TG1	O11-C11	2.38	1.47	1.42
5	A	999	TG1	O7-C8	2.35	1.50	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	TG1	C10-O9-C32	7.51	139.35	121.53
5	A	999	TG1	O12-C12-C11	-4.08	124.18	128.28
5	A	999	TG1	C7-C6-C5	3.54	124.48	115.41
5	A	999	TG1	C11-C7-C6	-3.34	96.60	103.03
5	A	999	TG1	C24-C22-C21	3.22	133.51	120.78
5	A	999	TG1	O5-C12-O12	2.88	125.44	121.62
5	A	999	TG1	C31-C10-C9	-2.70	104.81	110.29
5	A	999	TG1	C23-C22-C21	-2.67	109.41	116.09
5	A	999	TG1	C3-O3-C21	2.37	122.11	117.07
5	A	999	TG1	C8-O7-C27	2.35	122.35	117.92
5	A	999	TG1	C26-C4-C3	-2.23	117.66	121.27
5	A	999	TG1	O11-C11-C12	-2.20	98.88	106.32
5	A	999	TG1	O7-C27-O8	2.09	128.76	123.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

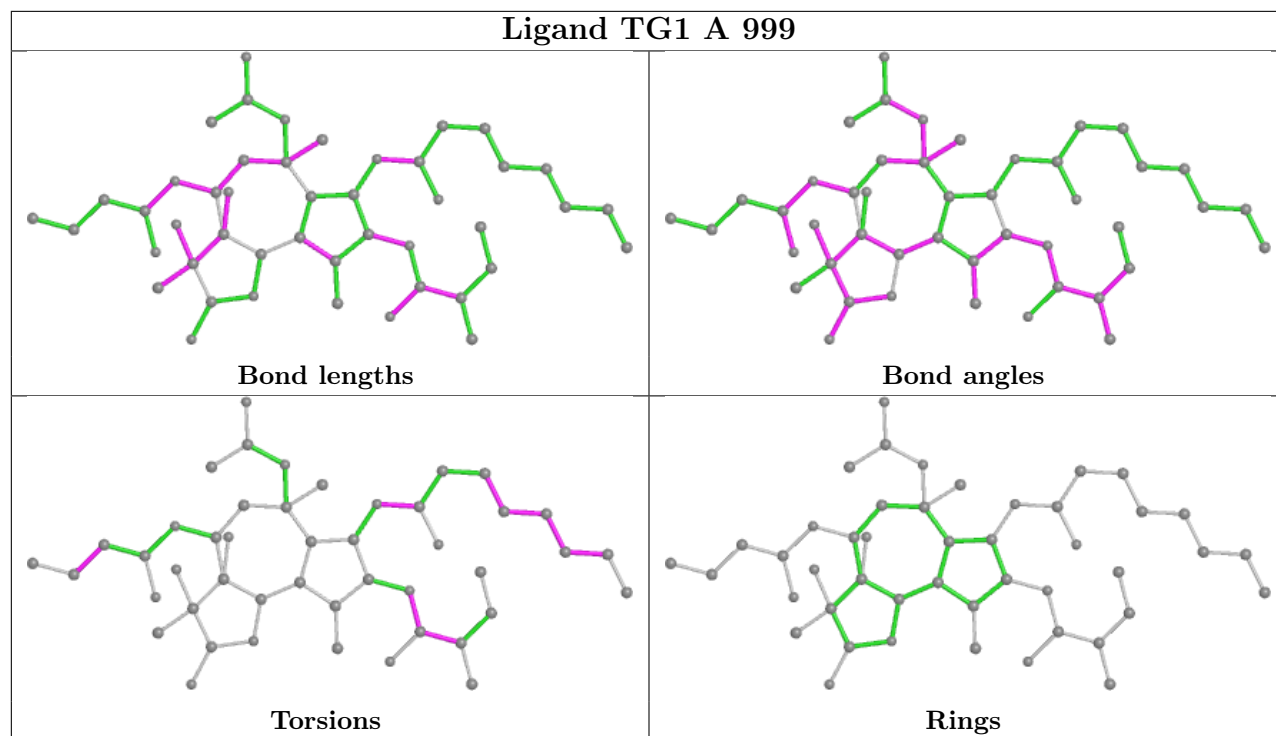
Mol	Chain	Res	Type	Atoms
5	A	999	TG1	O3-C21-C22-C23
5	A	999	TG1	O3-C21-C22-C24
5	A	999	TG1	O4-C21-C22-C23
5	A	999	TG1	O4-C21-C22-C24
5	A	999	TG1	C22-C21-O3-C3
5	A	999	TG1	C14-C13-O1-C2
5	A	999	TG1	O4-C21-O3-C3
5	A	999	TG1	O2-C13-O1-C2
5	A	999	TG1	C15-C16-C17-C18
5	A	999	TG1	C16-C17-C18-C19
5	A	999	TG1	C27-C28-C29-C30
5	A	999	TG1	C17-C18-C19-C20
5	A	999	TG1	C14-C15-C16-C17

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2002	ALF	1	0
5	A	999	TG1	11	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, 95th 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 ²)	Q<0.9
1	A	994/994 (100%)	0.53	86 (8%) 10 3	27, 72, 163, 197	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	THR	11.2
1	A	504	SER	10.9
1	A	506	ALA	10.5
1	A	507	ALA	9.5
1	A	877	THR	9.3
1	A	873	PHE	9.3
1	A	886	LEU	6.9
1	A	290	ARG	6.9
1	A	871	THR	6.6
1	A	959	LEU	6.4
1	A	287	SER	6.4
1	A	285	GLY	6.3
1	A	994	GLY	6.2
1	A	284	HIS	6.2
1	A	508	VAL	6.0
1	A	891	PHE	5.9
1	A	280	ASN	5.8
1	A	286	GLY	5.8
1	A	294	TYR	5.8
1	A	279	PHE	5.7
1	A	277	GLY	5.6
1	A	278	HIS	5.3
1	A	300	VAL	5.3
1	A	260	LEU	5.2
1	A	890	ILE	5.2
1	A	85	ILE	5.1
1	A	309	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	965	THR	4.6
1	A	75	LEU	4.5
1	A	872	HIS	4.5
1	A	786	ALA	4.5
1	A	787	LEU	4.4
1	A	963	ASP	4.2
1	A	964	LEU	4.2
1	A	81	GLY	4.1
1	A	82	GLU	4.1
1	A	291	GLY	4.0
1	A	289	ILE	4.0
1	A	282	PRO	3.8
1	A	505	ARG	3.8
1	A	887	ASP	3.7
1	A	311	LEU	3.7
1	A	874	MET	3.6
1	A	108	GLN	3.6
1	A	281	ASP	3.5
1	A	1	MET	3.5
1	A	960	LYS	3.5
1	A	781	LEU	3.4
1	A	51	GLU	3.4
1	A	256	PHE	3.3
1	A	868	HIS	3.3
1	A	957	PHE	3.3
1	A	503	SER	3.2
1	A	302	LEU	3.2
1	A	268	CYS	3.0
1	A	885	GLY	3.0
1	A	301	ALA	3.0
1	A	271	VAL	2.9
1	A	57	PHE	2.8
1	A	899	MET	2.7
1	A	870	LEU	2.7
1	A	884	GLU	2.7
1	A	765	ILE	2.6
1	A	86	THR	2.5
1	A	61	LEU	2.5
1	A	283	VAL	2.5
1	A	901	LEU	2.4
1	A	306	ALA	2.4
1	A	273	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	773	VAL	2.3
1	A	288	TRP	2.3
1	A	377	CYS	2.3
1	A	878	GLU	2.3
1	A	783	LEU	2.3
1	A	883	PHE	2.2
1	A	792	LEU	2.2
1	A	948	LEU	2.2
1	A	267	ILE	2.2
1	A	991	TYR	2.2
1	A	52	LEU	2.1
1	A	340	GLU	2.1
1	A	777	LEU	2.1
1	A	769	VAL	2.1
1	A	764	LEU	2.0
1	A	404	SER	2.0
1	A	981	ASP	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.

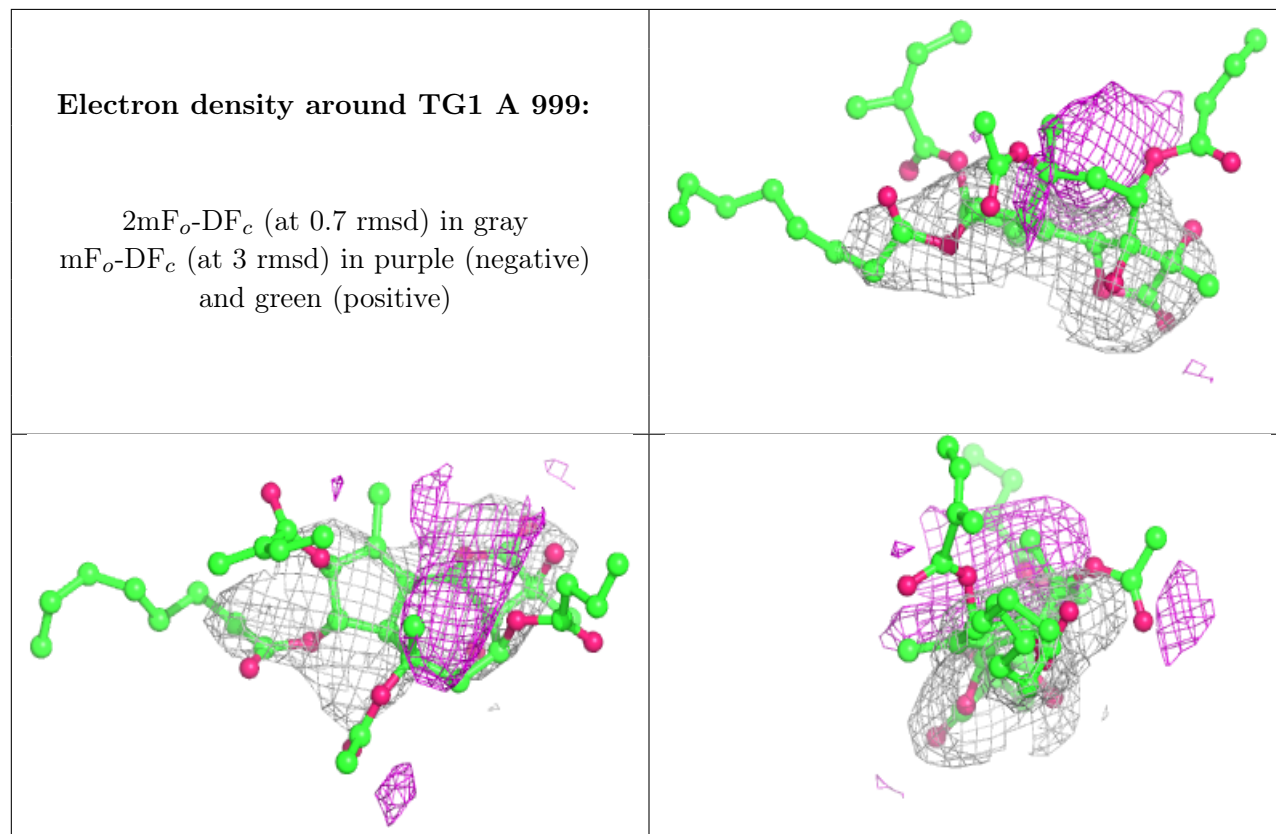
6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
5	TG1	A	999	46/46	0.77	0.90	107,139,152,155	0
4	K	A	2003	1/1	0.95	0.20	67,67,67,67	0
2	MG	A	2001	1/1	0.97	0.24	33,33,33,33	0
3	ALF	A	2002	5/5	0.99	0.20	41,56,58,63	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.