



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:05 PM UTC

PDB ID : 1XP5 / pdb_00001xp5
Title : Structure Of The (Sr)Ca²⁺-ATPase E2-AlF₄- 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

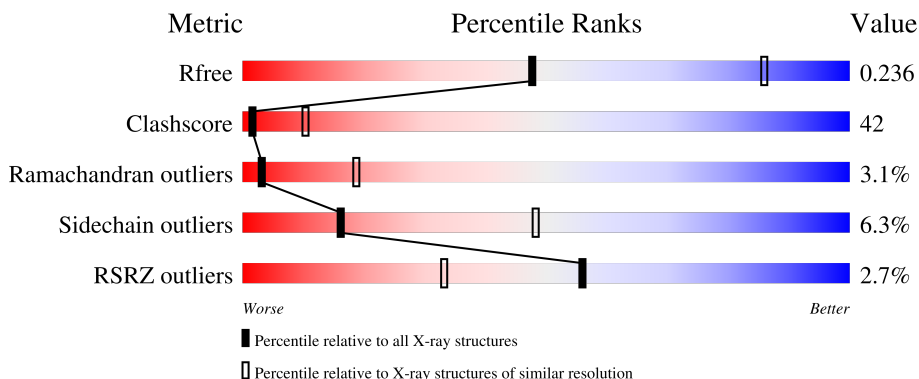
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

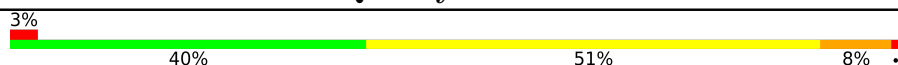
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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	

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
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

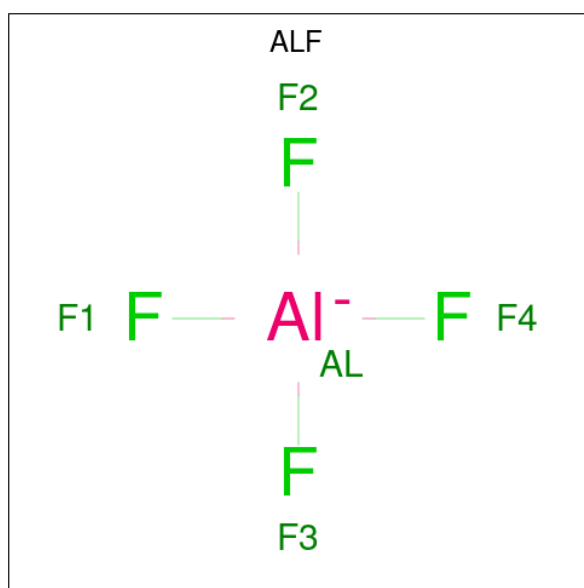
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

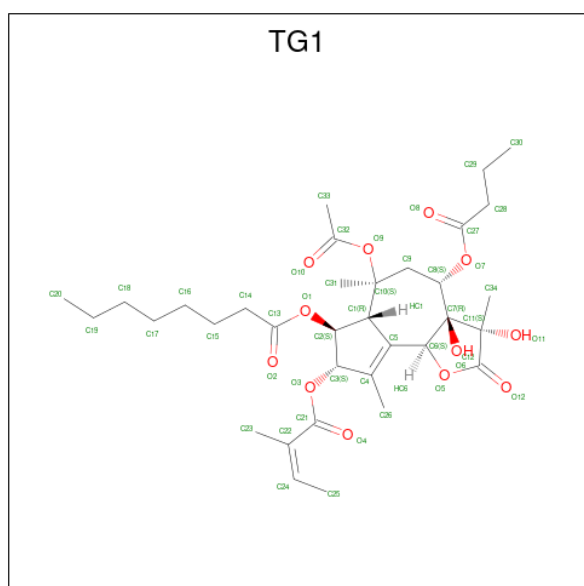


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is POTASSIUM ION (CCD ID: 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), 9BETA]]-6-(ACETYLOXY)-2,3,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



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

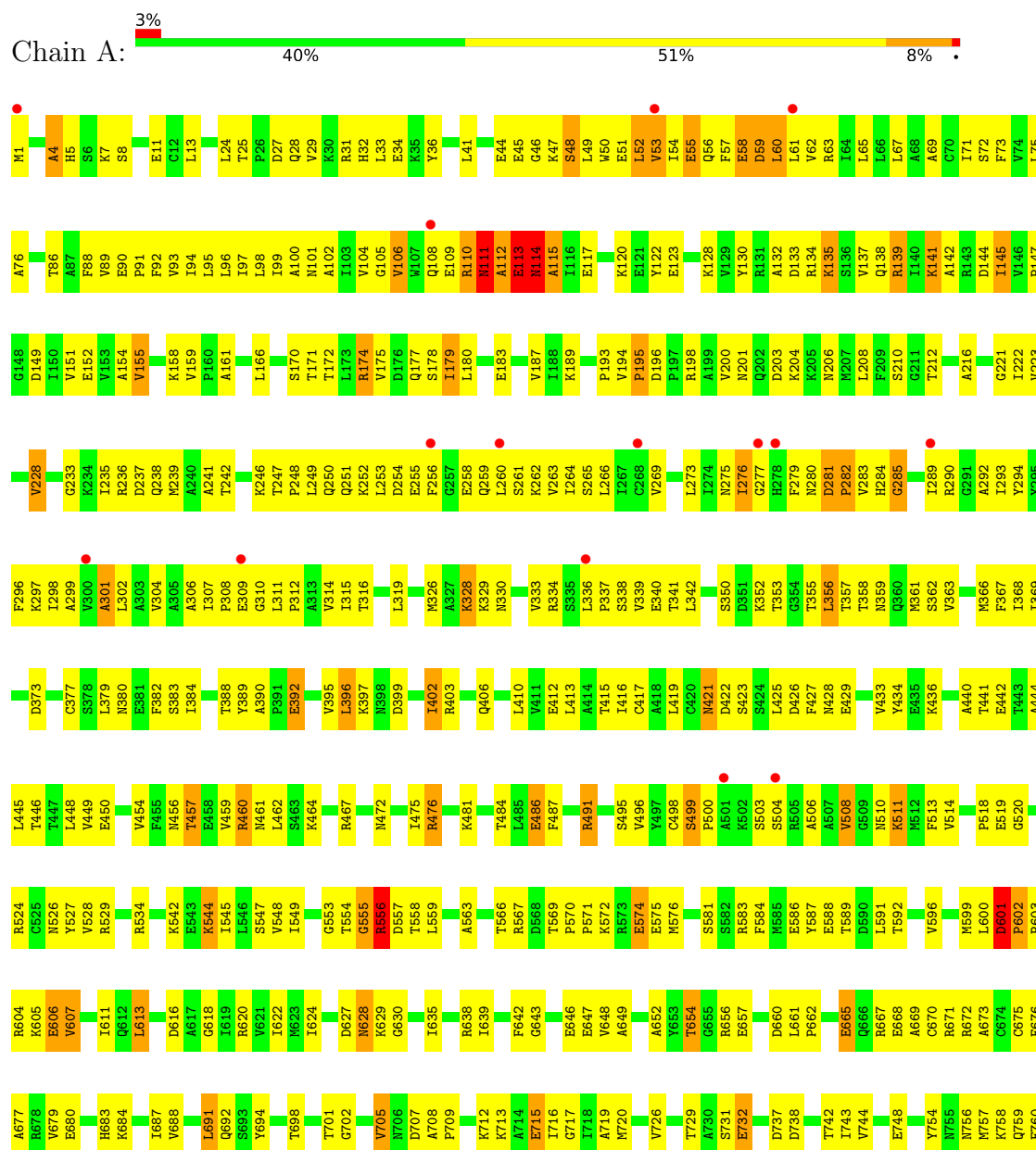
- Molecule 6 is water.

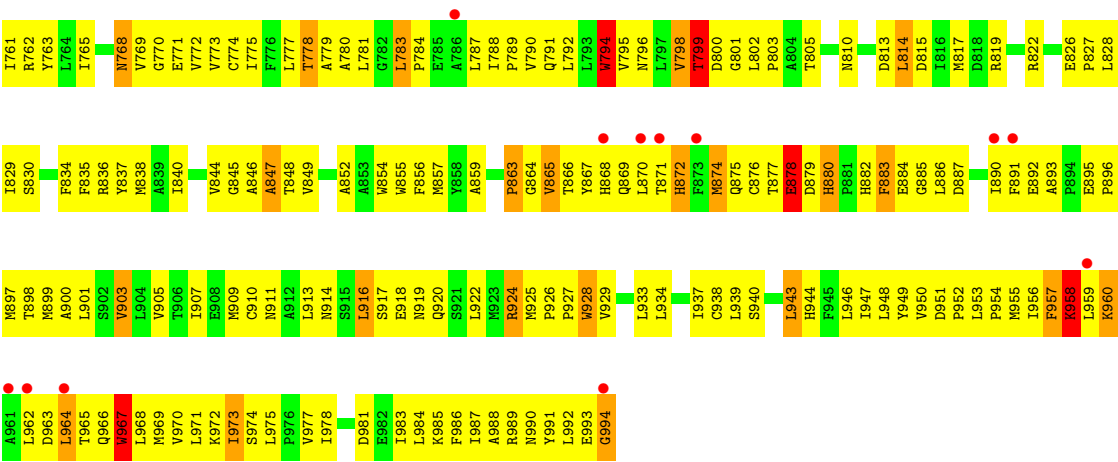
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		

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

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 80.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (80.00-3.00) 99.8 (80.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.265 0.235 , 0.236	Depositor DCC
R_{free} test set	1732 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: ALF, K, TG1, 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	0.55	4/7812 (0.1%)	1.16	72/10592 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	994	GLY	C-OXT	9.40	1.42	1.23
1	A	957	PHE	CA-C	-5.64	1.44	1.52
1	A	959	LEU	CA-C	5.15	1.59	1.52
1	A	798	VAL	CA-CB	5.03	1.61	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASN	N-CA-C	-16.02	94.46	112.57
1	A	113	GLU	N-CA-C	13.36	130.95	109.85
1	A	52	LEU	N-CA-C	-12.93	98.14	114.56
1	A	504	SER	N-CA-C	10.88	125.07	111.69
1	A	959	LEU	N-CA-C	10.83	125.08	110.35
1	A	373	ASP	N-CA-C	-10.62	92.32	108.99
1	A	874	MET	N-CA-C	-10.50	100.77	114.31
1	A	960	LYS	N-CA-C	9.48	131.00	110.80
1	A	5	HIS	N-CA-C	-8.87	100.43	112.94
1	A	957	PHE	N-CA-C	8.32	123.55	113.23
1	A	556	ARG	N-CA-C	-8.12	103.27	113.02
1	A	878	GLU	N-CA-C	-7.95	93.87	110.80
1	A	194	VAL	CA-C-N	7.94	129.76	119.84
1	A	194	VAL	C-N-CA	7.94	129.76	119.84
1	A	159	VAL	CA-C-N	7.91	127.63	119.64
1	A	159	VAL	C-N-CA	7.91	127.63	119.64
1	A	110	ARG	N-CA-C	7.75	121.46	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	958	LYS	CA-C-N	7.73	132.43	120.75
1	A	958	LYS	C-N-CA	7.73	132.43	120.75
1	A	955	MET	N-CA-C	-7.67	102.91	111.28
1	A	106	VAL	CB-CA-C	-7.49	102.29	111.88
1	A	602	PRO	CA-C-N	7.32	127.25	119.85
1	A	602	PRO	C-N-CA	7.32	127.25	119.85
1	A	506	ALA	N-CA-C	7.25	119.33	110.41
1	A	454	VAL	N-CA-C	7.21	121.12	111.17
1	A	48	SER	N-CA-C	-7.06	96.12	108.20
1	A	628	ASN	N-CA-C	6.69	120.18	110.28
1	A	916	LEU	N-CA-C	-6.68	104.87	113.16
1	A	643	GLY	N-CA-C	-6.66	103.62	112.82
1	A	973	ILE	N-CA-C	-6.51	107.15	113.53
1	A	743	ILE	N-CA-C	-6.49	104.16	110.72
1	A	115	ALA	N-CA-C	-6.45	104.10	112.23
1	A	924	ARG	N-CA-C	-6.42	105.60	113.50
1	A	601	ASP	CA-C-N	6.42	126.99	120.38
1	A	601	ASP	C-N-CA	6.42	126.99	120.38
1	A	350	SER	N-CA-C	6.38	119.90	109.06
1	A	508	VAL	N-CA-C	6.34	117.75	109.58
1	A	607	VAL	N-CA-C	6.30	116.47	110.42
1	A	235	ILE	N-CA-C	-6.25	104.42	110.42
1	A	654	THR	N-CA-C	-6.10	100.96	110.42
1	A	732	GLU	N-CA-C	-5.98	106.15	113.50
1	A	606	GLU	N-CA-C	5.93	120.51	113.16
1	A	602	PRO	N-CA-C	5.92	117.92	110.70
1	A	13	LEU	N-CA-C	-5.84	104.83	111.14
1	A	114	ASN	N-CA-C	5.72	117.38	109.15
1	A	44	GLU	CA-C-N	-5.69	114.87	122.72
1	A	44	GLU	C-N-CA	-5.69	114.87	122.72
1	A	943	LEU	N-CA-C	-5.69	106.50	113.50
1	A	499	SER	CA-C-N	5.68	125.96	119.83
1	A	499	SER	C-N-CA	5.68	125.96	119.83
1	A	715	GLU	N-CA-C	-5.63	105.29	111.82
1	A	392	GLU	N-CA-C	5.62	118.05	109.62
1	A	938	CYS	N-CA-C	-5.56	105.12	111.07
1	A	132	ALA	N-CA-C	5.53	118.02	111.33
1	A	301	ALA	N-CA-C	-5.50	107.11	113.88
1	A	59	ASP	N-CA-C	-5.48	99.12	110.80
1	A	106	VAL	N-CA-C	5.48	116.11	110.36
1	A	285	GLY	N-CA-C	5.46	126.12	113.18
1	A	967	TRP	N-CA-C	-5.34	105.37	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	GLU	N-CA-C	-5.32	103.93	110.31
1	A	903	VAL	N-CA-C	-5.27	105.47	110.42
1	A	605	LYS	N-CA-C	5.25	117.69	111.33
1	A	113	GLU	CA-C-N	5.22	129.80	121.66
1	A	113	GLU	C-N-CA	5.22	129.80	121.66
1	A	4	ALA	CA-C-N	5.18	130.34	122.37
1	A	4	ALA	C-N-CA	5.18	130.34	122.37
1	A	44	GLU	N-CA-C	-5.17	102.02	110.20
1	A	601	ASP	N-CA-C	-5.17	98.45	108.59
1	A	780	ALA	N-CA-C	-5.10	107.05	113.28
1	A	196	ASP	N-CA-C	5.05	119.75	109.60
1	A	794	TRP	N-CA-C	-5.04	105.70	111.14
1	A	880	HIS	N-CA-C	5.04	119.80	113.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7766	649	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	649	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 42.

All (649) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:ASN:HD22	1:A:111:ASN:C	1.69	1.00
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: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:326:MET:HE1	1:A:339:VAL:HG22	1.53	0.90
1:A:957:PHE:C	1:A:958:LYS:HG2	1.98	0.89
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: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: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
1:A:449:VAL:HG21	1:A:472:ASN:CG	2.04	0.83
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:THR:HG21	1:A:340:GLU:CD	2.09	0.76
1:A:111:ASN:O	1:A:112:ALA:C	2.25	0.76
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:887:ASP:CG	1:A:890:ILE:HD11	2.12	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:239:MET:HE3	1:A:708:ALA:HB1	1.69	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: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:111:ASN:C	1:A:111:ASN:ND2	2.38	0.73
1:A:75:LEU:HD21	1:A:296:PHE:HB3	1.70	0.72
1:A:476:ARG:NH1	1:A:476:ARG:HB2	2.03	0.72
1:A:957:PHE:O	1:A:958:LYS:HG2	1.88	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:51:GLU:HA	1:A:54:ILE:CD1	2.25	0.66
1:A:449:VAL:HG21	1:A:472:ASN:ND2	2.09	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:383:SER:C	1:A:384:ILE:HD13	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:298:ILE:C	1:A:298:ILE:HD12	2.22	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:544:LYS:HD3	1:A:544:LYS:C	2.22	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:606:GLU:H	1:A:606:GLU:CD	2.07	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:369:ILE:HG13	1:A:528:VAL:HG11	1.81	0.62
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:803:PRO:HG2	1:A:909:MET:HE1	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:969:MET:HE2	1:A:973:ILE:HD11	1.81	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:VAL:HG11	1:A:943:LEU:HD13	1.82	0.60
1:A:800:ASP:C	1:A:803:PRO:HD2	2.26	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:111:ASN:C	1:A:113:GLU:N	2.59	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:421:ASN:HD22	1:A:421:ASN:C	2.09	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:971:LEU:C	1:A:973:ILE:H	2.09	0.59
1:A:353:THR:HA	1:A:357:THR:OG1	2.03	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
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:679:VAL:HB	1:A:683:HIS:HB2	1.84	0.58
1:A:275:ASN:C	1:A:277:GLY:H	2.12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ALA:C	1:A:392:GLU:H	2.11	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:777:LEU:C	1:A:779:ALA:H	2.12	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:962:LEU:C	1:A:964:LEU:H	2.13	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:684:LYS:NZ	1:A:707:ASP:OD1	2.39	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HD2	1:A:138:GLN:CD	2.31	0.56
1:A:356:LEU:HB3	1:A:639:ILE:HD11	1.87	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:342:LEU:CD1	1:A:716:ILE:HD13	2.36	0.55
1:A:838:MET:HE3	1:A:838:MET:O	2.05	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: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: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: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:358:THR:O	1:A:359:ASN:HB3	2.06	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:456:ASN:O	1:A:457:THR:C	2.51	0.54
1:A:880:HIS:C	1:A:882:HIS:H	2.16	0.54
1:A:198:ARG:NH1	1:A:660:ASP:OD1	2.41	0.53
1:A:895:GLU:N	1:A:896:PRO:HD2	2.23	0.53
1:A:948:LEU:C	1:A:949:TYR:HD1	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:897:MET:C	1:A:899:MET:H	2.17	0.53
1:A:963:ASP:O	1:A:964:LEU:C	2.52	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:329:LYS:O	1:A:330:ASN:HB2	2.08	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: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:421:ASN:ND2	1:A:421:ASN:C	2.67	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:944:HIS:C	1:A:946:LEU:H	2.17	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
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:429:GLU:CD	1:A:429:GLU:H	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:962:LEU:C	1:A:964:LEU:N	2.67	0.51
1:A:255:GLU:HG3	1:A:256:PHE:N	2.26	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:355:THR:HG23	1:A:720:MET:HE3	1.93	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:768:ASN:N	1:A:768:ASN:ND2	2.57	0.50
1:A:760:PHE:CD1	1:A:760:PHE:C	2.90	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: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:929:VAL:HG12	1:A:929:VAL:O	2.12	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:950:VAL:C	1:A:952:PRO:HD2	2.38	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LYS:HB3	1:A:574:GLU:OE2	2.12	0.48
1:A:326:MET:HE1	1:A:339:VAL:CG2	2.33	0.48
1:A:581:SER:HA	1:A:584:PHE:CZ	2.48	0.48
1:A:798:VAL:O	1:A:799:THR:C	2.56	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: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:428:ASN:OD1	1:A:428:ASN:C	2.56	0.48
1:A:500:PRO:HD2	1:A:510:ASN:HD22	1.77	0.48
1:A:924:ARG:C	1:A:926:PRO:HD3	2.39	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: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:890:ILE:C	1:A:892:GLU:H	2.21	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLN:OE1	1:A:872:HIS:HD2	1.98	0.47
1:A:110:ARG:C	1:A:112:ALA:H	2.20	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:491:ARG:HH11	1:A:588:GLU:CD	2.23	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: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:897:MET:C	1:A:899:MET:N	2.71	0.47
1:A:969:MET:O	1:A:973:ILE:HG13	2.15	0.47
1:A:154:ALA:O	1:A:155:VAL:C	2.58	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:236:ARG:HD3	1:A:236:ARG:C	2.40	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:366:MET:HE3	1:A:384:ILE:HD11	1.96	0.46
1:A:558:THR:O	1:A:559:LEU:HD23	2.16	0.46
1:A:879:ASP:CG	1:A:885:GLY:HA3	2.40	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:880:HIS:C	1:A:882:HIS:N	2.73	0.46
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.15	0.46
1:A:56:GLN:HE22	1:A:105:GLY:C	2.23	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:487:PHE:C	1:A:487:PHE:CD2	2.94	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:204:LYS:C	1:A:206:ASN:H	2.24	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:366:MET:HE1	1:A:448:LEU:HD11	1.97	0.45
1:A:557:ASP:O	1:A:558:THR:C	2.59	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:715:GLU:C	1:A:716:ILE:HG13	2.41	0.45
1:A:178:SER:HB3	1:A:183:GLU:C	2.41	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:957:PHE:C	1:A:958:LYS:CG	2.69	0.45
1:A:556:ARG:H	1:A:556:ARG:CD	2.18	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:846:ALA:C	1:A:848:THR:H	2.23	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:367:PHE:C	1:A:367:PHE:CD2	2.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:298:ILE:C	1:A:298:ILE:CD1	2.90	0.45
1:A:622:ILE:CD1	1:A:691:LEU:HD21	2.46	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:518:PRO:O	1:A:519:GLU:C	2.60	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:108:GLN:CD	1:A:336:LEU:HD11	2.40	0.44
1:A:290:ARG:C	1:A:292:ALA:H	2.26	0.44
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.45	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:71:ILE:C	1:A:73:PHE:H	2.25	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:756:ASN:CG	1:A:810:ASN:HB2	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:201:ASN:C	1:A:203:ASP:H	2.26	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
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:249:LEU:O	1:A:250:GLN:C	2.61	0.43
1:A:255:GLU:O	1:A:259:GLN:HG2	2.19	0.43
1:A:426:ASP:OD2	1:A:426:ASP:C	2.60	0.43
1:A:584:PHE:N	1:A:584:PHE:CD2	2.84	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:971:LEU:C	1:A:973:ILE:N	2.75	0.43
1:A:75:LEU:HD12	1:A:75:LEU:N	2.33	0.43
1:A:857:MET:HE1	1:A:867:TYR:HA	2.01	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:259:GLN:C	1:A:261:SER:N	2.75	0.43
1:A:333:VAL:HG11	1:A:339:VAL:CG2	2.48	0.43
1:A:616:ASP:C	1:A:618:GLY:H	2.26	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:855:TRP:HD1	1:A:856:PHE:CE1	2.37	0.43
1:A:828:LEU:HD12	5:A:999:TG1:H291	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:855:TRP:C	1:A:859:ALA:HB2	2.44	0.42
1:A:868:HIS:O	1:A:868:HIS:CG	2.72	0.42
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:402:ILE:HD13	1:A:402:ILE:N	2.35	0.42
1:A:890:ILE:C	1:A:892:GLU:N	2.78	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:629:LYS:NZ	1:A:657:GLU:OE2	2.51	0.42
1:A:849:VAL:O	1:A:852:ALA:HB3	2.20	0.42
1:A:974:SER:O	1:A:977:VAL:HG12	2.19	0.42
1:A:114:ASN:C	1:A:729:THR:HG21	2.45	0.42
1:A:242:THR:OG1	1:A:712:LYS:HE3	2.20	0.42
1:A:366:MET:HE2	1:A:448:LEU:HD11	2.02	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:864:GLY:C	1:A:866:THR:H	2.28	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:629:LYS:O	1:A:630:GLY:C	2.62	0.41
1:A:775:ILE:HA	1:A:778:THR:CG2	2.50	0.41
1:A:47:LYS:CD	1:A:52:LEU:CD1	2.95	0.41
1:A:275:ASN:C	1:A:277:GLY:N	2.77	0.41
1:A:200:VAL:O	1:A:203:ASP:HB2	2.20	0.41
1:A:555:GLY:C	1:A:557:ASP:H	2.28	0.41
1:A:611:ILE:HG13	1:A:639:ILE:CG2	2.50	0.41
1:A:777:LEU:C	1:A:779:ALA:N	2.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:944:HIS:C	1:A:946:LEU:N	2.79	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: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:201:ASN:C	1:A:203:ASP:N	2.79	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:326:MET:HE3	1:A:333:VAL:HG21	2.03	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

5.3.1 Protein backbone

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%)	3	19

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	PRO
1	A	289	ILE
1	A	263	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	787 (94%)	53 (6%)	16	48

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	53	VAL
1	A	55	GLU
1	A	58	GLU
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	228	VAL
1	A	328	LYS
1	A	356	LEU
1	A	388	THR
1	A	396	LEU
1	A	402	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	LEU
1	A	421	ASN
1	A	436	LYS
1	A	441	THR
1	A	457	THR
1	A	460	ARG
1	A	467	ARG
1	A	476	ARG
1	A	491	ARG
1	A	508	VAL
1	A	511	LYS
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	601	ASP
1	A	613	LEU
1	A	665	GLU
1	A	691	LEU
1	A	705	VAL
1	A	768	ASN
1	A	783	LEU
1	A	788	ILE
1	A	794	TRP
1	A	799	THR
1	A	814	LEU
1	A	928	TRP
1	A	967	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	796	ASN
1	A	872	HIS
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 oligosaccharides 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
5	TG1	A	999	-	44,48,48	2.20	13 (29%)	47,72,72	2.05	13 (27%)
3	ALF	A	2002	1,6,2	4,4,4	1.21	0	-		

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	TG1	O4-C21	5.96	1.33	1.21
5	A	999	TG1	O1-C13	4.39	1.46	1.34
5	A	999	TG1	C9-C8	4.18	1.57	1.52
5	A	999	TG1	C11-C7	4.17	1.60	1.55
5	A	999	TG1	O3-C3	3.97	1.52	1.44
5	A	999	TG1	O6-C7	3.91	1.49	1.43
5	A	999	TG1	C34-C11	3.69	1.58	1.53
5	A	999	TG1	O7-C27	3.30	1.43	1.34
5	A	999	TG1	C9-C10	3.25	1.59	1.54
5	A	999	TG1	C31-C10	3.08	1.58	1.52
5	A	999	TG1	C21-C22	2.97	1.59	1.50
5	A	999	TG1	O7-C8	2.48	1.50	1.46
5	A	999	TG1	O11-C11	2.47	1.47	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	TG1	C10-O9-C32	7.68	139.35	121.36
5	A	999	TG1	O12-C12-C11	-4.05	124.18	128.28
5	A	999	TG1	C6-O5-C12	-3.59	105.82	110.80
5	A	999	TG1	C7-C6-C5	3.45	124.48	115.41
5	A	999	TG1	C24-C22-C21	3.39	133.51	120.79
5	A	999	TG1	O5-C12-O12	2.96	125.44	121.60
5	A	999	TG1	C23-C22-C21	-2.61	109.41	116.12
5	A	999	TG1	C3-O3-C21	2.47	122.11	116.96
5	A	999	TG1	C8-O7-C27	2.37	122.35	118.03
5	A	999	TG1	O1-C2-C3	-2.27	105.89	110.18
5	A	999	TG1	O11-C11-C12	-2.19	98.88	106.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	TG1	O7-C27-O8	2.16	128.76	123.70
5	A	999	TG1	C26-C4-C3	-2.15	117.66	121.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

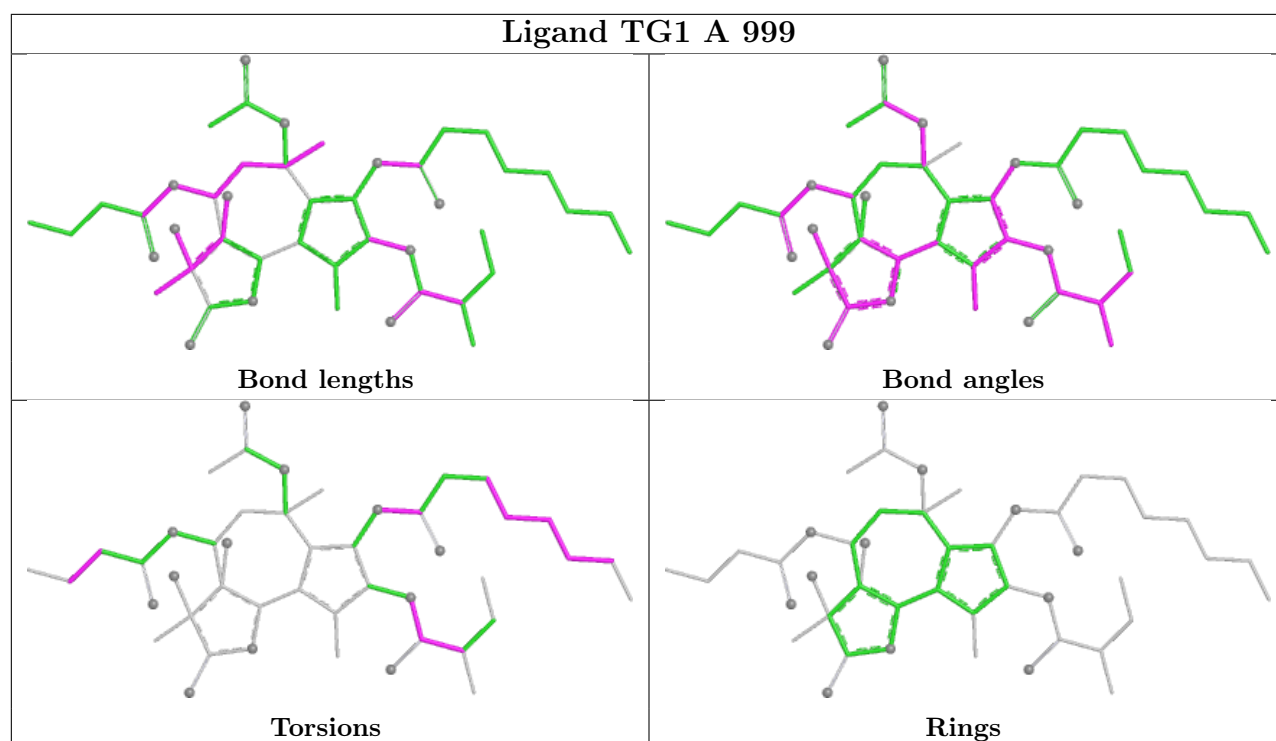
Mol	Chain	Res	Type	Atoms
5	A	999	TG1	O3-C21-C22-C23
5	A	999	TG1	O4-C21-C22-C23
5	A	999	TG1	O4-C21-C22-C24
5	A	999	TG1	O3-C21-C22-C24
5	A	999	TG1	C22-C21-O3-C3
5	A	999	TG1	C14-C13-O1-C2
5	A	999	TG1	O2-C13-O1-C2
5	A	999	TG1	O4-C21-O3-C3
5	A	999	TG1	C15-C16-C17-C18
5	A	999	TG1	C16-C17-C18-C19
5	A	999	TG1	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
5	A	999	TG1	11	0
3	A	2002	ALF	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	-0.02	27 (2%)	56 33	27, 72, 163, 197	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	GLU	3.4
1	A	891	PHE	3.4
1	A	260	LEU	3.4
1	A	108	GLN	3.4
1	A	870	LEU	2.9
1	A	336	LEU	2.7
1	A	300	VAL	2.7
1	A	890	ILE	2.6
1	A	873	PHE	2.5
1	A	1	MET	2.5
1	A	962	LEU	2.4
1	A	268	CYS	2.4
1	A	504	SER	2.4
1	A	868	HIS	2.3
1	A	959	LEU	2.3
1	A	964	LEU	2.3
1	A	994	GLY	2.3
1	A	278	HIS	2.2
1	A	256	PHE	2.2
1	A	871	THR	2.1
1	A	277	GLY	2.1
1	A	53	VAL	2.1
1	A	501	ALA	2.0
1	A	786	ALA	2.0
1	A	961	ALA	2.0
1	A	61	LEU	2.0
1	A	289	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

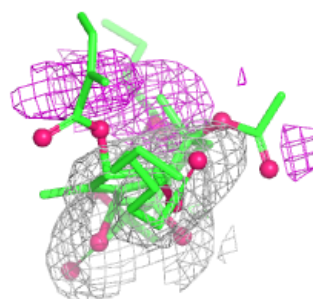
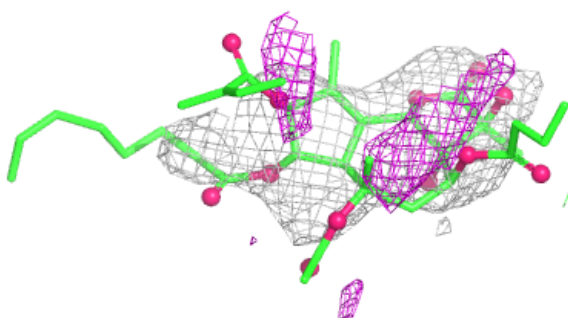
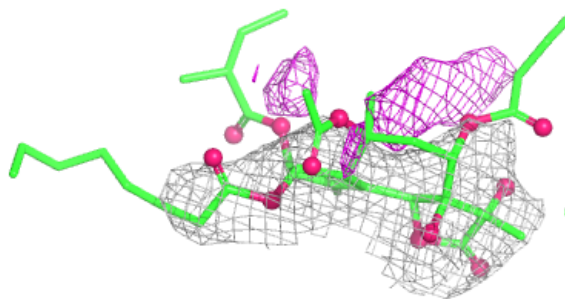
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TG1	A	999	46/46	0.81	0.23	107,139,152,155	0
4	K	A	2003	1/1	0.97	0.07	67,67,67,67	0
3	ALF	A	2002	5/5	0.98	0.06	41,56,58,63	0
2	MG	A	2001	1/1	0.99	0.10	33,33,33,33	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.

Electron density around TG1 A 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.