



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:59 PM EDT

PDB ID : 3B9R / pdb_00003b9r
Title : SERCA Ca²⁺-ATPase E2 aluminium fluoride complex without thapsigargin
Authors : Olesen, C.; Picard, M.; Winther, A.M.L.; Morth, J.P.; Moller, J.V.; Nissen, P.
Deposited on : 2007-11-06
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

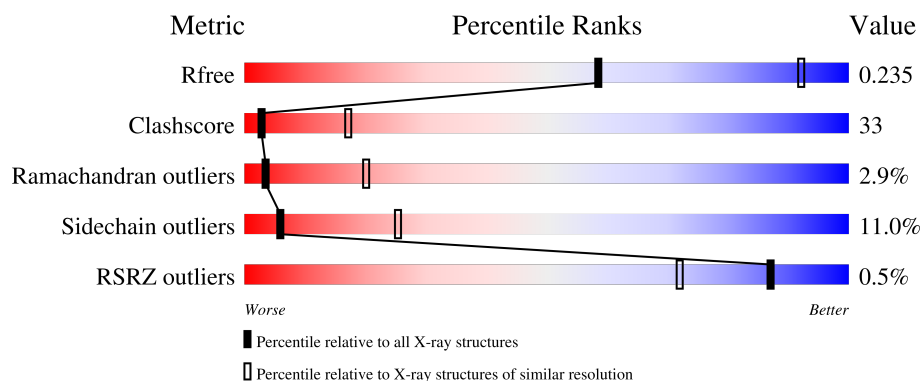
1 Overall quality at a glance

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	 46% 44% 9% .
1	B	994	 46% 44% 9% .

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

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

2 Entry composition [i](#)

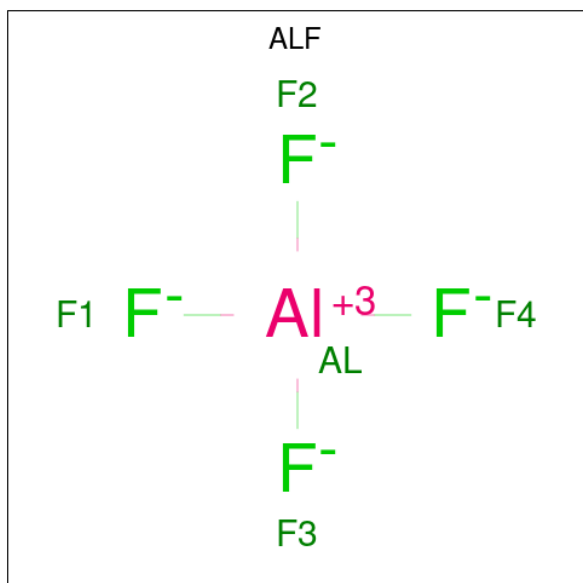
There are 6 unique types of molecules in this entry. The entry contains 15426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



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

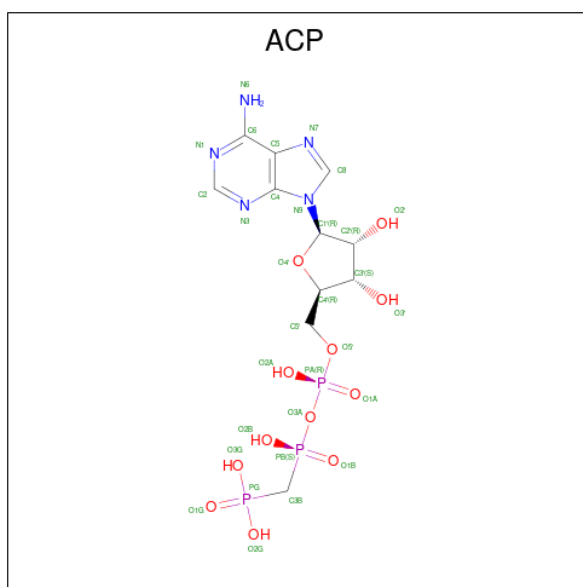
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

- Molecule 6 is water.

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

Continued on next page...

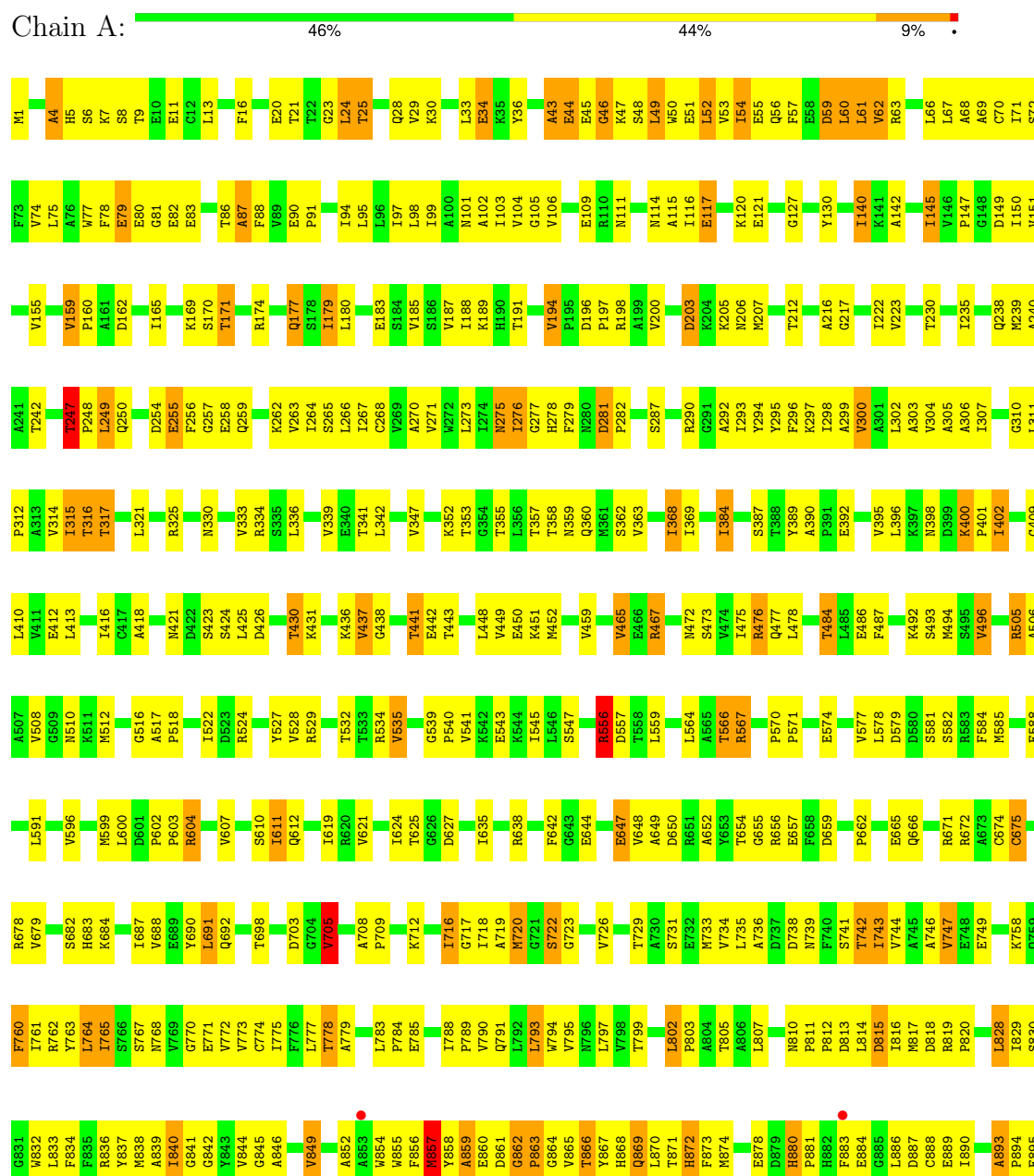
Continued from previous page...

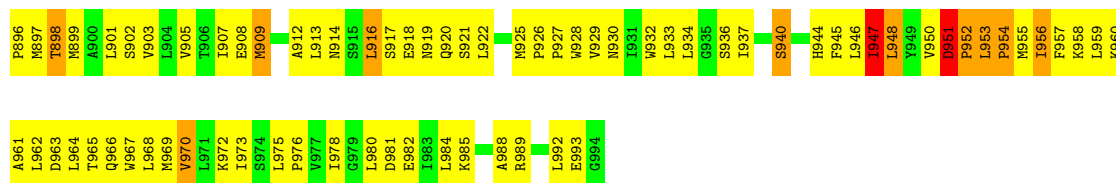
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	O	0	0
			4	4		

3 Residue-property plots

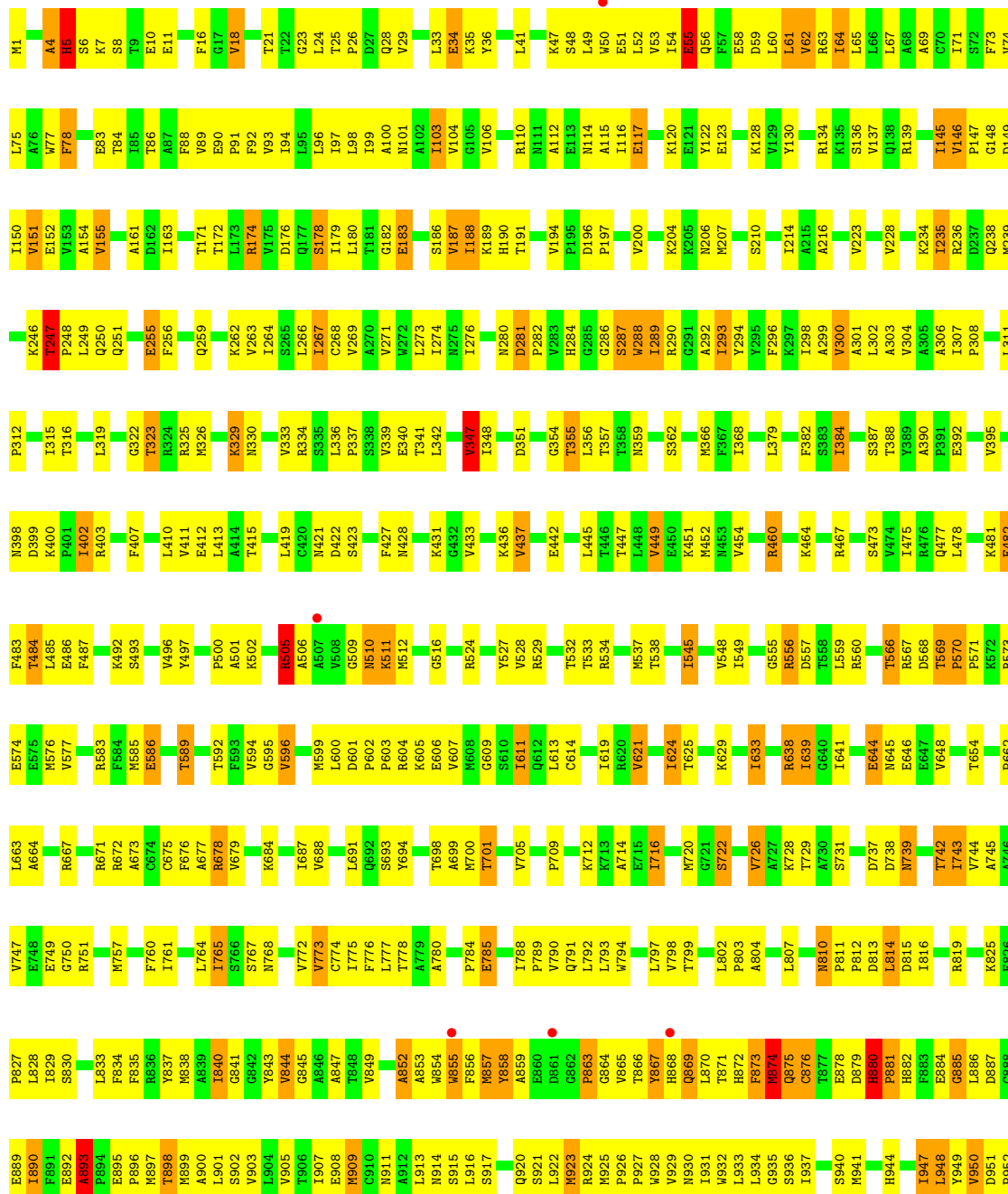
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



L953	P954	M955	I956	F957	K958	L959	K960	A961	D962	L963	L964	T965	Q966	W967	L968	H969	V970	L971	S974	L975	P976	V977	I978	E982	I983	L984	K985	F986	I987	A988	R989	N990	Y991	L992	E993	G994
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

●

●

●

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 94.43Å 136.18Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.99-3.00) 99.3 (19.99-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.185 , 0.235 0.189 , 0.235	Depositor DCC
R_{free} test set	1039 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 104.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15426	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

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

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, K, 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	0.79	3/7812 (0.0%)	1.22	57/10592 (0.5%)
1	B	0.71	0/7812	1.13	48/10592 (0.5%)
All	All	0.75	3/15624 (0.0%)	1.17	105/21184 (0.5%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	675	CYS	CA-CB	6.07	1.62	1.53
1	A	705	VAL	CA-CB	5.35	1.62	1.54
1	A	674	CYS	CA-C	5.07	1.58	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	GLN	N-CA-C	-12.24	99.33	114.75
1	B	194	VAL	CA-C-N	9.77	129.89	119.05
1	B	194	VAL	C-N-CA	9.77	129.89	119.05
1	A	819	ARG	CA-C-N	9.62	130.29	120.38
1	A	819	ARG	C-N-CA	9.62	130.29	120.38
1	A	951	ASP	CA-C-N	9.59	131.83	119.84
1	A	951	ASP	C-N-CA	9.59	131.83	119.84
1	A	893	ALA	CA-C-N	9.20	129.41	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	ALA	C-N-CA	9.20	129.41	119.28
1	A	400	LYS	CA-C-N	8.87	128.95	119.90
1	A	400	LYS	C-N-CA	8.87	128.95	119.90
1	B	146	VAL	CA-C-N	-8.69	111.04	119.90
1	B	146	VAL	C-N-CA	-8.69	111.04	119.90
1	A	247	THR	CA-C-N	8.56	128.56	119.05
1	A	247	THR	C-N-CA	8.56	128.56	119.05
1	A	947	ILE	N-CA-C	-8.55	104.69	112.90
1	B	570	PRO	O-C-N	8.34	125.07	121.15
1	B	5	HIS	N-CA-C	-8.06	103.47	113.38
1	A	4	ALA	N-CA-C	7.99	121.43	108.32
1	A	556	ARG	N-CA-C	-7.87	103.68	113.28
1	B	601	ASP	CA-C-N	7.76	128.37	120.38
1	B	601	ASP	C-N-CA	7.76	128.37	120.38
1	B	505	ARG	N-CA-C	-7.70	97.77	109.79
1	A	862	GLY	CA-C-N	7.63	129.38	119.84
1	A	862	GLY	C-N-CA	7.63	129.38	119.84
1	A	820	PRO	N-CA-C	7.49	119.84	110.70
1	B	569	THR	CA-C-N	7.45	125.03	119.66
1	B	569	THR	C-N-CA	7.45	125.03	119.66
1	B	4	ALA	N-CA-C	7.39	121.40	108.75
1	A	459	VAL	CB-CA-C	-7.34	103.73	110.63
1	A	43	ALA	N-CA-C	7.34	119.90	110.65
1	B	855	TRP	N-CA-C	-7.29	103.96	112.92
1	A	317	THR	N-CA-C	-7.28	105.58	114.75
1	B	641	ILE	N-CA-C	-7.28	102.09	112.35
1	A	5	HIS	N-CA-C	-7.24	104.05	113.17
1	B	909	MET	N-CA-C	-7.08	104.77	113.41
1	A	77	TRP	N-CA-C	-6.86	105.85	114.56
1	B	874	MET	N-CA-C	-6.69	105.03	113.72
1	A	159	VAL	CA-C-N	6.67	128.18	119.84
1	A	159	VAL	C-N-CA	6.67	128.18	119.84
1	A	655	GLY	N-CA-C	-6.51	104.95	112.50
1	B	814	LEU	N-CA-C	6.42	118.81	111.11
1	B	235	ILE	N-CA-C	-6.40	104.02	111.00
1	A	505	ARG	N-CA-C	6.33	119.85	111.75
1	B	548	VAL	N-CA-C	-6.26	105.63	111.45
1	A	579	ASP	N-CA-C	-6.21	106.02	113.97
1	A	916	LEU	N-CA-C	-6.21	105.57	113.02
1	B	728	LYS	N-CA-C	-6.01	104.85	111.82
1	A	712	LYS	N-CA-C	5.92	117.81	111.36
1	A	535	VAL	CA-C-N	-5.91	113.88	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	VAL	C-N-CA	-5.91	113.88	119.85
1	A	897	MET	N-CA-C	-5.82	106.31	113.41
1	A	25	THR	CA-C-N	5.77	126.17	119.47
1	A	25	THR	C-N-CA	5.77	126.17	119.47
1	A	854	TRP	N-CA-C	-5.76	105.63	114.16
1	A	121	GLU	N-CA-C	-5.71	106.31	113.28
1	A	194	VAL	CA-C-N	5.68	125.21	119.19
1	A	194	VAL	C-N-CA	5.68	125.21	119.19
1	B	935	GLY	N-CA-C	-5.68	108.10	114.40
1	A	852	ALA	N-CA-C	-5.64	105.51	112.90
1	B	556	ARG	N-CA-C	-5.62	106.27	113.01
1	A	50	TRP	N-CA-C	-5.62	104.53	111.33
1	A	909	MET	N-CA-C	-5.58	107.11	114.31
1	B	247	THR	CA-C-N	5.54	125.21	119.56
1	B	247	THR	C-N-CA	5.54	125.21	119.56
1	B	545	ILE	CB-CA-C	-5.52	102.24	111.29
1	B	505	ARG	CA-C-N	5.49	131.57	121.70
1	B	505	ARG	C-N-CA	5.49	131.57	121.70
1	A	4	ALA	CA-C-N	5.46	131.55	122.54
1	A	4	ALA	C-N-CA	5.46	131.55	122.54
1	A	390	ALA	CA-C-N	5.41	126.60	119.84
1	A	390	ALA	C-N-CA	5.41	126.60	119.84
1	B	967	TRP	N-CA-C	-5.38	106.72	113.72
1	B	570	PRO	CA-C-O	-5.36	116.50	120.73
1	A	857	MET	N-CA-C	5.35	118.60	111.75
1	A	720	MET	N-CA-C	-5.35	101.56	110.17
1	B	122	TYR	N-CA-C	-5.34	106.45	113.17
1	B	570	PRO	CA-C-N	5.33	125.33	119.89
1	B	570	PRO	C-N-CA	5.33	125.33	119.89
1	A	127	GLY	CA-C-O	-5.32	116.94	121.57
1	A	203	ASP	N-CA-C	-5.32	106.92	113.41
1	B	810	ASN	CA-C-N	5.31	125.85	120.38
1	B	810	ASN	C-N-CA	5.31	125.85	120.38
1	B	155	VAL	CB-CA-C	-5.29	103.35	111.71
1	A	430	THR	N-CA-C	5.28	116.72	110.97
1	B	852	ALA	N-CA-C	-5.26	106.26	113.30
1	B	931	ILE	N-CA-C	-5.25	106.42	112.98
1	B	621	VAL	N-CA-C	5.24	115.59	107.78
1	A	362	SER	N-CA-C	5.24	116.95	108.41
1	A	866	THR	N-CA-C	5.24	117.76	109.96
1	B	893	ALA	CA-C-N	5.22	125.91	120.12
1	B	893	ALA	C-N-CA	5.22	125.91	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	ILE	CB-CA-C	-5.16	105.28	112.04
1	A	217	GLY	N-CA-C	5.14	118.28	111.70
1	B	963	ASP	N-CA-C	5.14	119.29	112.30
1	B	570	PRO	CB-CA-C	-5.11	106.37	111.17
1	A	818	ASP	N-CA-C	-5.09	107.10	113.72
1	B	639	ILE	N-CA-C	-5.09	108.33	113.47
1	B	16	PHE	N-CA-C	-5.08	107.08	113.28
1	B	183	GLU	N-CA-C	5.08	116.81	108.52
1	A	478	LEU	N-CA-C	5.04	116.86	111.36
1	B	347	VAL	CB-CA-C	-5.03	103.07	110.82
1	A	771	GLU	N-CA-C	-5.03	106.32	112.90
1	A	541	VAL	N-CA-C	-5.01	105.96	110.82
1	A	70	CYS	N-CA-C	-5.01	106.86	113.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	55	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7762	509	0
1	B	7671	0	7762	506	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	14	2	0
5	B	31	0	14	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	15426	0	15552	1016	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1016) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TRP:O	1:B:53:VAL:HG12	1.43	1.16
1:B:264:ILE:HD11	1:B:306:ALA:HB3	1.30	1.12
1:A:953:LEU:HB2	1:A:954:PRO:HD2	1.23	1.12
1:A:720:MET:HE1	1:A:735:LEU:HD12	1.35	1.05
1:A:951:ASP:HB3	1:A:952:PRO:HD2	1.38	1.04
1:A:951:ASP:HB3	1:A:952:PRO:CD	1.89	1.02
1:B:985:LYS:HB3	1:B:989:ARG:HH12	1.20	1.02
1:A:25:THR:H	1:A:28:GLN:HE21	1.05	1.02
1:B:678:ARG:HG3	1:B:678:ARG:HH11	1.24	1.01
1:B:855:TRP:HE1	1:B:899:MET:HG3	1.30	0.93
1:A:60:LEU:HD12	1:A:61:LEU:N	1.82	0.93
1:A:953:LEU:HB2	1:A:954:PRO:CD	1.98	0.93
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.51	0.92
1:B:171:THR:HG21	1:B:486:GLU:OE1	1.70	0.92
1:B:1:MET:HB2	1:B:36:TYR:CE1	2.06	0.91
1:B:65:LEU:HD21	1:B:307:ILE:HG13	1.52	0.90
1:B:481:LYS:HG3	1:B:496:VAL:CG1	2.02	0.90
1:A:951:ASP:CB	1:A:952:PRO:HD2	2.03	0.89
1:A:105:GLY:O	1:A:109:GLU:HG2	1.73	0.89
1:B:151:VAL:HG11	1:B:163:ILE:HD13	1.52	0.89
1:A:278:HIS:HA	1:A:282:PRO:HD2	1.55	0.88
1:B:556:ARG:HD2	1:B:644:GLU:O	1.75	0.87
1:B:869:GLN:HG3	1:B:872:HIS:ND1	1.90	0.86
1:A:49:LEU:HD13	1:A:51:GLU:HB2	1.59	0.85
1:A:436:LYS:HB2	1:A:443:THR:HG21	1.58	0.85
1:B:785:GLU:HG3	1:B:897:MET:HE2	1.58	0.84
1:B:962:LEU:O	1:B:966:GLN:HB2	1.76	0.84
1:A:436:LYS:HE2	1:A:438:GLY:O	1.78	0.83
1:A:449:VAL:HG23	1:A:472:ASN:ND2	1.93	0.83
1:A:656:ARG:HG3	1:A:656:ARG:HH11	1.42	0.82
1:A:527:TYR:CG	1:A:534:ARG:HD3	2.14	0.82
1:B:187:VAL:HG22	1:B:189:LYS:HE2	1.60	0.82
1:A:865:VAL:HB	1:A:868:HIS:CD2	2.15	0.82
1:B:500:PRO:HD3	1:B:509:GLY:HA3	1.62	0.82
1:A:880:HIS:CD2	1:A:881:PRO:HD3	2.15	0.82
1:A:788:ILE:HG13	1:A:791:GLN:HG3	1.61	0.81
1:B:873:PHE:CE1	1:B:876:CYS:HA	2.15	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLN:HE21	1:A:871:THR:HG23	1.45	0.81
1:A:964:LEU:HD12	1:A:965:THR:HG23	1.61	0.80
1:B:964:LEU:HA	1:B:968:LEU:CD1	2.12	0.80
1:A:917:SER:OG	1:A:920:GLN:HB2	1.81	0.80
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.81	0.79
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.82	0.79
1:B:151:VAL:HG11	1:B:163:ILE:CD1	2.11	0.78
1:B:880:HIS:N	1:B:881:PRO:HD3	1.99	0.78
1:B:878:GLU:HB3	1:B:880:HIS:CD2	2.18	0.78
1:B:460:ARG:HH11	1:B:460:ARG:HB2	1.46	0.78
1:B:876:CYS:SG	1:B:882:HIS:HE1	2.05	0.78
1:A:950:VAL:HG21	1:A:953:LEU:HD12	1.65	0.78
1:B:739:ASN:HB3	1:B:742:THR:HG22	1.66	0.78
1:A:60:LEU:C	1:A:62:VAL:H	1.89	0.78
1:A:436:LYS:CB	1:A:443:THR:HG21	2.13	0.78
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.19	0.78
1:A:316:THR:O	1:A:316:THR:HG22	1.83	0.77
1:A:99:ILE:O	1:A:103:ILE:HG12	1.84	0.77
1:A:961:ALA:HB1	1:A:966:GLN:HB2	1.66	0.77
1:B:264:ILE:HD11	1:B:306:ALA:CB	2.11	0.77
1:A:953:LEU:C	1:A:955:MET:H	1.92	0.77
1:B:855:TRP:NE1	1:B:899:MET:HG3	2.00	0.77
1:A:649:ALA:O	1:A:650:ASP:HB3	1.85	0.77
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.13	0.77
1:A:4:ALA:HB3	1:A:7:LYS:HG2	1.67	0.76
1:B:288:TRP:C	1:B:290:ARG:H	1.92	0.76
1:B:366:MET:HG2	1:B:384:ILE:HD11	1.66	0.76
1:A:922:LEU:HB3	1:A:927:PRO:HG3	1.67	0.76
1:A:293:ILE:O	1:A:297:LYS:HB2	1.86	0.76
1:B:964:LEU:HD12	1:B:964:LEU:O	1.85	0.76
1:A:155:VAL:HG12	1:A:216:ALA:HA	1.68	0.76
1:A:336:LEU:O	1:A:339:VAL:HG22	1.86	0.76
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.21	0.75
1:B:411:VAL:O	1:B:415:THR:HG23	1.86	0.75
1:B:922:LEU:HB3	1:B:927:PRO:HG3	1.66	0.75
1:A:239:MET:HE1	1:A:708:ALA:HB1	1.69	0.75
1:B:51:GLU:O	1:B:54:ILE:HB	1.87	0.75
1:B:481:LYS:HG3	1:B:496:VAL:HG11	1.67	0.75
1:B:837:TYR:HA	1:B:840:ILE:HB	1.69	0.75
1:B:678:ARG:HH11	1:B:678:ARG:CG	1.99	0.74
1:B:930:ASN:O	1:B:934:LEU:HG	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ALA:O	1:B:103:ILE:HG22	1.87	0.74
1:B:264:ILE:CD1	1:B:306:ALA:HB3	2.13	0.74
1:B:256:PHE:HZ	1:B:765:ILE:HD12	1.51	0.74
1:A:880:HIS:CG	1:A:881:PRO:HD3	2.23	0.74
1:B:765:ILE:HA	1:B:768:ASN:HB2	1.70	0.73
1:A:845:GLY:O	1:A:849:VAL:HG13	1.87	0.73
1:B:281:ASP:HB3	1:B:284:HIS:CD2	2.23	0.73
1:A:79:GLU:O	1:A:79:GLU:HG2	1.88	0.73
1:B:60:LEU:HA	1:B:63:ARG:HB3	1.70	0.73
1:B:101:ASN:O	1:B:104:VAL:HG22	1.88	0.73
1:B:985:LYS:HB3	1:B:989:ARG:NH1	2.00	0.72
1:A:60:LEU:HD13	1:A:307:ILE:HD12	1.70	0.72
1:B:922:LEU:HD12	1:B:922:LEU:H	1.53	0.72
1:A:647:GLU:O	1:A:647:GLU:HG3	1.89	0.72
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.71	0.72
1:A:894:PRO:HB3	1:A:959:LEU:H	1.53	0.72
1:B:347:VAL:HG21	1:B:691:LEU:HD22	1.72	0.71
1:A:985:LYS:O	1:A:989:ARG:HG2	1.91	0.71
1:B:50:TRP:O	1:B:53:VAL:CG1	2.31	0.71
1:A:449:VAL:HG23	1:A:472:ASN:HD21	1.51	0.71
1:A:870:LEU:HB3	1:A:873:PHE:CZ	2.25	0.71
1:B:948:LEU:HD11	1:B:961:ALA:HB3	1.73	0.71
1:B:964:LEU:HA	1:B:968:LEU:HD12	1.73	0.71
1:A:947:ILE:O	1:A:954:PRO:HD3	1.91	0.71
1:A:947:ILE:HD13	1:A:953:LEU:HD13	1.73	0.71
1:A:948:LEU:O	1:A:954:PRO:HG3	1.91	0.71
1:B:844:VAL:HB	1:B:907:ILE:HG21	1.72	0.71
1:B:764:LEU:HD21	1:B:804:ALA:HB2	1.73	0.70
1:B:930:ASN:HB3	1:B:933:LEU:H	1.56	0.70
1:A:865:VAL:CA	1:A:868:HIS:HD2	2.04	0.70
1:B:859:ALA:HB3	1:B:864:GLY:CA	2.20	0.70
1:A:281:ASP:CG	1:A:282:PRO:HD3	2.16	0.70
1:B:238:GLN:HG2	1:B:709:PRO:HB3	1.72	0.70
1:B:298:ILE:HD12	1:B:299:ALA:N	2.06	0.70
1:A:919:ASN:O	1:A:989:ARG:HD3	1.91	0.70
1:B:47:LYS:HG3	1:B:47:LYS:O	1.92	0.70
1:B:1:MET:HB2	1:B:36:TYR:HE1	1.52	0.70
1:B:249:LEU:HD11	1:B:340:GLU:HG2	1.74	0.70
1:A:903:VAL:HG23	1:A:970:VAL:HG22	1.73	0.69
1:B:876:CYS:SG	1:B:882:HIS:CE1	2.85	0.69
1:A:988:ALA:O	1:A:992:LEU:HB3	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:CG2	1:B:189:LYS:HE2	2.22	0.69
1:A:926:PRO:O	1:A:929:VAL:HG23	1.91	0.69
1:B:859:ALA:HB3	1:B:864:GLY:HA2	1.75	0.69
1:B:866:THR:HG22	1:B:867:TYR:CD1	2.28	0.69
1:A:765:ILE:HA	1:A:768:ASN:HD22	1.57	0.69
1:A:869:GLN:HG3	1:A:871:THR:OG1	1.93	0.69
1:A:813:ASP:O	1:A:816:ILE:HB	1.92	0.69
1:A:235:ILE:O	1:A:239:MET:HG2	1.93	0.68
1:A:473:SER:O	1:A:477:GLN:HG2	1.92	0.68
1:B:895:GLU:HA	1:B:898:THR:HG22	1.75	0.68
1:B:235:ILE:O	1:B:239:MET:HG3	1.93	0.68
1:A:961:ALA:HB1	1:A:966:GLN:CB	2.24	0.68
1:B:280:ASN:C	1:B:282:PRO:HD2	2.18	0.68
1:A:247:THR:HG23	1:A:250:GLN:HB3	1.76	0.68
1:B:483:PHE:HZ	1:B:576:MET:HE1	1.59	0.67
1:A:981:ASP:O	1:A:985:LYS:HB2	1.93	0.67
1:A:828:LEU:HD12	1:A:829:ILE:HG12	1.75	0.67
1:A:662:PRO:HG2	1:A:665:GLU:HB2	1.77	0.67
1:B:814:LEU:HD12	1:B:815:ASP:N	2.08	0.67
1:A:72:SER:O	1:A:91:PRO:HG3	1.94	0.67
1:A:189:LYS:HE3	1:A:207:MET:O	1.94	0.67
1:A:775:ILE:HA	1:A:778:THR:HG22	1.77	0.67
1:B:481:LYS:HG3	1:B:496:VAL:HG13	1.77	0.67
1:A:278:HIS:HA	1:A:282:PRO:CD	2.24	0.67
1:A:832:TRP:CH2	1:A:988:ALA:HB2	2.30	0.66
1:A:865:VAL:C	1:A:868:HIS:HD2	2.02	0.66
1:B:899:MET:CE	1:B:966:GLN:HB3	2.25	0.66
1:B:648:VAL:HG12	1:B:648:VAL:O	1.95	0.66
1:A:424:SER:HB3	1:A:437:VAL:HG22	1.77	0.66
1:A:833:LEU:HD12	1:A:836:ARG:HD3	1.78	0.66
1:B:560:ARG:HH12	5:B:998:ACP:H2'	1.61	0.66
1:A:893:ALA:O	1:A:896:PRO:HD2	1.96	0.66
1:B:573:ARG:HA	1:B:576:MET:HE2	1.77	0.66
1:B:917:SER:OG	1:B:920:GLN:HB2	1.96	0.66
1:B:950:VAL:O	1:B:954:PRO:HD2	1.96	0.66
1:A:869:GLN:HE21	1:A:871:THR:CG2	2.10	0.65
1:B:743:ILE:O	1:B:747:VAL:HG23	1.95	0.65
1:A:95:LEU:O	1:A:99:ILE:HG12	1.96	0.65
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.76	0.65
1:A:870:LEU:HB3	1:A:873:PHE:CE1	2.31	0.65
1:A:953:LEU:CB	1:A:954:PRO:CD	2.74	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HG22	1:B:293:ILE:O	1.96	0.65
1:B:500:PRO:CD	1:B:509:GLY:HA3	2.26	0.65
1:A:292:ALA:O	1:A:296:PHE:HB2	1.96	0.65
1:A:767:SER:HB3	1:A:908:GLU:CD	2.22	0.65
1:A:683:HIS:O	1:A:687:ILE:HG13	1.97	0.65
1:B:256:PHE:CZ	1:B:765:ILE:HD12	2.32	0.65
1:A:889:GLU:O	1:A:889:GLU:HG2	1.95	0.65
1:B:624:ILE:HD11	1:B:687:ILE:HG21	1.77	0.65
1:A:656:ARG:HG3	1:A:656:ARG:NH1	2.06	0.65
1:A:832:TRP:CZ3	1:A:836:ARG:HD2	2.32	0.65
1:B:256:PHE:HZ	1:B:765:ILE:CD1	2.09	0.65
1:A:294:TYR:O	1:A:298:ILE:HG13	1.97	0.64
1:A:316:THR:O	1:A:316:THR:CG2	2.44	0.64
1:B:524:ARG:HD3	1:B:585:MET:HE3	1.79	0.64
1:A:953:LEU:O	1:A:955:MET:N	2.29	0.64
1:B:751:ARG:HB3	1:B:816:ILE:HD11	1.80	0.64
1:B:856:PHE:HE1	1:B:896:PRO:HG2	1.62	0.64
1:A:249:LEU:HD12	1:A:250:GLN:N	2.12	0.64
1:A:717:GLY:O	1:A:731:SER:HB2	1.97	0.64
1:A:815:ASP:CG	1:A:815:ASP:O	2.39	0.64
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.16	0.64
1:A:963:ASP:OD1	1:A:964:LEU:N	2.30	0.64
1:B:106:VAL:O	1:B:110:ARG:HB2	1.97	0.64
1:B:916:LEU:HD13	1:B:933:LEU:CD2	2.28	0.64
1:A:25:THR:H	1:A:28:GLN:NE2	1.88	0.64
1:A:899:MET:SD	1:A:970:VAL:HG23	2.38	0.64
1:A:859:ALA:HB3	1:A:864:GLY:CA	2.28	0.64
1:B:342:LEU:HD13	1:B:716:ILE:HD13	1.80	0.63
1:B:828:LEU:O	1:B:829:ILE:HD13	1.97	0.63
1:B:844:VAL:HB	1:B:907:ILE:HD13	1.80	0.63
1:A:62:VAL:HG12	1:A:63:ARG:N	2.14	0.63
1:A:298:ILE:C	1:A:298:ILE:HD12	2.24	0.63
1:A:816:ILE:HG23	1:A:817:MET:HG2	1.80	0.63
1:A:247:THR:HG23	1:A:250:GLN:CB	2.28	0.63
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.78	0.63
1:B:52:LEU:O	1:B:55:GLU:HB2	1.99	0.63
1:A:716:ILE:HD12	1:A:716:ILE:N	2.13	0.63
1:B:266:LEU:O	1:B:269:VAL:HG22	1.99	0.63
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.81	0.63
1:B:916:LEU:HD13	1:B:933:LEU:HD22	1.79	0.63
1:B:246:LYS:HD2	1:B:250:GLN:HE22	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG21	1:A:486:GLU:OE1	1.97	0.63
1:B:428:ASN:ND2	1:B:431:LYS:HD2	2.13	0.62
1:A:53:VAL:HG13	1:A:106:VAL:HG21	1.79	0.62
1:B:174:ARG:HD3	1:B:188:ILE:HD13	1.81	0.62
1:B:390:ALA:C	1:B:392:GLU:H	2.07	0.62
1:B:964:LEU:O	1:B:965:THR:HB	1.99	0.62
1:A:270:ALA:HA	1:A:273:LEU:HD23	1.81	0.62
1:B:145:ILE:HD11	1:B:223:VAL:HG21	1.82	0.62
1:B:775:ILE:HA	1:B:778:THR:HG22	1.82	0.62
1:A:774:CYS:O	1:A:778:THR:HB	2.00	0.62
1:A:975:LEU:HB2	1:A:976:PRO:HD3	1.81	0.62
1:B:857:MET:SD	1:B:867:TYR:HA	2.39	0.62
1:B:941:MET:HA	1:B:944:HIS:HB3	1.81	0.62
1:A:94:ILE:O	1:A:98:LEU:HB2	2.00	0.62
1:A:264:ILE:HD11	1:A:306:ALA:HB3	1.80	0.62
1:B:174:ARG:HG3	1:B:216:ALA:HB3	1.82	0.62
1:B:624:ILE:HD13	1:B:687:ILE:HD13	1.80	0.62
1:A:743:ILE:O	1:A:747:VAL:HG12	2.00	0.62
1:A:51:GLU:HB3	1:A:54:ILE:HG13	1.80	0.62
1:A:90:GLU:O	1:A:94:ILE:HG12	1.99	0.62
1:A:484:THR:HB	1:A:496:VAL:HG23	1.81	0.62
1:B:247:THR:HB	1:B:248:PRO:HD2	1.82	0.62
1:B:529:ARG:NH2	1:B:592:THR:HG21	2.15	0.62
1:B:239:MET:O	1:B:712:LYS:HE3	2.00	0.61
1:A:846:ALA:O	1:A:849:VAL:HG22	2.00	0.61
1:B:77:TRP:HD1	1:B:78:PHE:CD1	2.18	0.61
1:A:951:ASP:CB	1:A:952:PRO:CD	2.64	0.61
1:A:733:MET:HE3	1:A:735:LEU:HD21	1.82	0.61
1:B:447:THR:HG22	1:B:451:LYS:HE3	1.82	0.61
1:B:844:VAL:CB	1:B:907:ILE:HG21	2.30	0.61
1:A:927:PRO:HD2	1:A:928:TRP:CZ3	2.35	0.61
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.80	0.61
1:B:671:ARG:HH21	1:B:694:TYR:HB3	1.65	0.61
1:A:556:ARG:HH11	1:A:644:GLU:HB3	1.66	0.61
1:B:905:VAL:O	1:B:909:MET:HG2	2.00	0.61
1:A:992:LEU:HG	1:A:993:GLU:N	2.15	0.61
1:A:413:LEU:HD11	1:A:564:LEU:HD12	1.83	0.61
1:B:288:TRP:C	1:B:290:ARG:N	2.59	0.61
1:B:483:PHE:HZ	1:B:576:MET:CE	2.14	0.61
1:B:784:PRO:HD3	1:B:870:LEU:HD22	1.82	0.61
1:A:333:VAL:HG21	1:A:339:VAL:CG1	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ILE:HD13	1:A:837:TYR:CE1	2.36	0.60
1:B:60:LEU:CA	1:B:63:ARG:HB3	2.30	0.60
1:B:84:THR:HG22	1:B:86:THR:H	1.65	0.60
1:A:198:ARG:HH21	1:A:659:ASP:HB3	1.64	0.60
1:B:607:VAL:O	1:B:611:ILE:HG12	2.01	0.60
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.82	0.60
1:A:784:PRO:HD3	1:A:873:PHE:CZ	2.36	0.60
1:B:484:THR:HB	1:B:496:VAL:HG22	1.84	0.60
1:A:52:LEU:C	1:A:52:LEU:HD23	2.26	0.60
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.01	0.60
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.00	0.60
1:B:511:LYS:HZ2	1:B:568:ASP:HA	1.67	0.60
1:B:567:ARG:NH1	1:B:571:PRO:HD3	2.16	0.60
1:B:629:LYS:O	1:B:633:ILE:HG13	2.01	0.60
1:A:60:LEU:C	1:A:62:VAL:N	2.58	0.60
1:B:803:PRO:O	1:B:807:LEU:HG	2.01	0.60
1:A:359:ASN:C	1:A:360:GLN:HG2	2.27	0.60
1:A:412:GLU:OE2	1:A:566:THR:CG2	2.49	0.60
1:A:865:VAL:O	1:A:868:HIS:HB2	2.02	0.60
1:A:963:ASP:O	1:A:964:LEU:HG	2.02	0.60
1:B:920:GLN:HB3	1:B:925:MET:HB2	1.83	0.60
1:B:722:SER:OG	1:B:738:ASP:OD1	2.20	0.60
1:B:964:LEU:HA	1:B:968:LEU:HD11	1.84	0.60
1:B:5:HIS:CD2	1:B:6:SER:N	2.69	0.59
1:B:974:SER:C	1:B:976:PRO:HD2	2.27	0.59
1:A:932:TRP:HA	1:A:932:TRP:CE3	2.37	0.59
1:B:869:GLN:HE21	1:B:872:HIS:CE1	2.21	0.59
1:A:484:THR:HB	1:A:496:VAL:CG2	2.32	0.59
1:A:720:MET:HE1	1:A:735:LEU:CD1	2.23	0.59
1:B:62:VAL:HG13	1:B:98:LEU:HD22	1.83	0.59
1:A:649:ALA:O	1:A:650:ASP:CB	2.50	0.59
1:B:304:VAL:HG13	1:B:792:LEU:HD12	1.84	0.59
1:B:625:THR:HA	2:B:995:ALF:F1	1.93	0.59
1:B:843:TYR:OH	1:B:976:PRO:HB2	2.02	0.59
1:B:844:VAL:CG1	1:B:907:ILE:HG21	2.32	0.59
1:A:13:LEU:HD21	1:A:20:GLU:HB2	1.85	0.59
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.38	0.59
1:A:256:PHE:HA	1:A:259:GLN:HG2	1.85	0.59
1:A:450:GLU:OE2	1:A:467:ARG:NH2	2.36	0.59
1:A:778:THR:OG1	1:A:785:GLU:HA	2.02	0.59
1:A:951:ASP:O	1:A:953:LEU:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:C	1:A:396:LEU:HD23	2.27	0.59
1:A:829:ILE:HD12	1:A:837:TYR:HE2	1.67	0.59
1:B:909:MET:SD	1:B:937:ILE:HG23	2.43	0.59
1:A:912:ALA:O	1:A:933:LEU:HD21	2.03	0.58
1:B:286:GLY:O	1:B:287:SER:C	2.46	0.58
1:B:567:ARG:CZ	1:B:571:PRO:HD3	2.33	0.58
1:B:992:LEU:O	1:B:992:LEU:HG	2.03	0.58
1:A:239:MET:HE1	1:A:708:ALA:CB	2.32	0.58
1:B:128:LYS:HB3	1:B:137:VAL:CG2	2.33	0.58
1:B:413:LEU:HD12	1:B:595:GLY:HA3	1.84	0.58
1:B:445:LEU:O	1:B:449:VAL:HG13	2.02	0.58
1:A:505:ARG:O	1:A:506:ALA:HB3	2.02	0.58
1:A:960:LYS:HD2	1:A:960:LYS:O	2.03	0.58
1:B:25:THR:OG1	1:B:28:GLN:HG3	2.02	0.58
1:B:322:GLY:HA2	1:B:325:ARG:HB2	1.84	0.58
1:A:880:HIS:CE1	1:A:881:PRO:HG3	2.38	0.58
1:A:947:ILE:CD1	1:A:953:LEU:HD13	2.33	0.58
1:B:161:ALA:HA	1:B:210:SER:HB2	1.85	0.58
1:B:921:SER:HB2	1:B:982:GLU:OE1	2.03	0.58
1:A:109:GLU:C	1:A:111:ASN:H	2.10	0.58
1:B:501:ALA:O	1:B:502:LYS:HG2	2.04	0.58
1:B:874:MET:HG2	1:B:874:MET:O	2.02	0.58
1:B:916:LEU:HD11	1:B:930:ASN:ND2	2.19	0.58
1:A:47:LYS:HE2	1:A:242:THR:HG23	1.86	0.58
1:A:60:LEU:O	1:A:62:VAL:N	2.37	0.58
1:A:267:ILE:O	1:A:271:VAL:HG13	2.04	0.58
1:A:355:THR:O	1:A:604:ARG:HD2	2.03	0.58
1:B:161:ALA:CA	1:B:210:SER:HB2	2.34	0.58
1:B:334:ARG:HD3	1:B:731:SER:O	2.04	0.58
1:B:791:GLN:HB3	1:B:901:LEU:HD12	1.86	0.58
1:A:145:ILE:CD1	1:A:223:VAL:HG21	2.34	0.57
1:B:600:LEU:O	1:B:602:PRO:HD3	2.03	0.57
1:A:115:ALA:HA	1:A:729:THR:HG21	1.85	0.57
1:A:384:ILE:HG23	1:A:395:VAL:HG22	1.85	0.57
1:A:930:ASN:HB3	1:A:933:LEU:H	1.68	0.57
1:B:333:VAL:HG11	1:B:339:VAL:HG22	1.86	0.57
1:B:810:ASN:HB3	1:B:811:PRO:HD2	1.85	0.57
1:B:340:GLU:HA	1:B:750:GLY:HA2	1.85	0.57
1:B:856:PHE:HD2	1:B:870:LEU:HD11	1.69	0.57
1:B:120:LYS:HA	1:B:123:GLU:HG3	1.84	0.57
1:A:791:GLN:O	1:A:795:VAL:HG23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:VAL:O	1:A:909:MET:HG2	2.04	0.57
1:A:52:LEU:HD22	1:A:106:VAL:HG22	1.85	0.57
1:A:648:VAL:O	1:A:649:ALA:C	2.46	0.57
1:A:832:TRP:CH2	1:A:836:ARG:HD2	2.38	0.57
1:A:988:ALA:HB1	1:A:992:LEU:HD22	1.86	0.57
1:B:319:LEU:HB3	1:B:336:LEU:HB3	1.87	0.57
1:A:79:GLU:HG3	1:A:87:ALA:HB2	1.86	0.57
1:A:539:GLY:N	1:A:540:PRO:HD2	2.20	0.57
1:B:965:THR:H	1:B:968:LEU:HD12	1.69	0.57
1:A:872:HIS:CE1	1:A:874:MET:HB3	2.39	0.57
1:A:51:GLU:O	1:A:52:LEU:C	2.48	0.57
1:B:911:ASN:HA	1:B:914:ASN:HB2	1.87	0.57
1:A:8:SER:OG	1:A:11:GLU:HG3	2.04	0.57
1:A:101:ASN:O	1:A:104:VAL:HG22	2.05	0.57
1:B:4:ALA:HB1	1:B:6:SER:OG	2.05	0.57
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.86	0.56
1:A:863:PRO:HB2	1:A:890:ILE:HG21	1.86	0.56
1:B:830:SER:H	1:B:833:LEU:HB3	1.70	0.56
1:A:255:GLU:HA	1:A:258:GLU:HB3	1.88	0.56
1:A:760:PHE:CD1	1:A:760:PHE:C	2.83	0.56
1:A:865:VAL:C	1:A:868:HIS:CD2	2.83	0.56
1:B:5:HIS:HD2	1:B:6:SER:N	2.03	0.56
1:B:301:ALA:HA	1:B:789:PRO:HG3	1.88	0.56
1:B:926:PRO:O	1:B:929:VAL:HG23	2.04	0.56
1:A:436:LYS:HB2	1:A:443:THR:CG2	2.34	0.56
1:B:987:ILE:O	1:B:987:ILE:HG22	2.03	0.56
1:A:722:SER:OG	1:A:738:ASP:OD1	2.24	0.56
1:A:901:LEU:CD2	1:A:944:HIS:HE1	2.18	0.56
1:B:354:GLY:N	1:B:359:ASN:HB2	2.20	0.56
1:B:609:GLY:O	1:B:613:LEU:HD13	2.06	0.56
1:A:936:SER:O	1:A:940:SER:HB2	2.06	0.56
1:A:953:LEU:C	1:A:955:MET:N	2.59	0.56
1:B:248:PRO:HD2	1:B:341:THR:HG22	1.85	0.56
1:B:965:THR:HG22	1:B:965:THR:O	2.06	0.56
1:A:775:ILE:HA	1:A:778:THR:CG2	2.36	0.56
1:B:624:ILE:HD13	1:B:687:ILE:CD1	2.36	0.56
1:A:803:PRO:O	1:A:807:LEU:HG	2.06	0.56
1:A:828:LEU:CD1	1:A:829:ILE:HG12	2.36	0.56
1:B:834:PHE:O	1:B:838:MET:HG2	2.05	0.56
1:B:8:SER:OG	1:B:11:GLU:HG3	2.04	0.56
1:A:44:GLU:HB2	1:A:116:ILE:HD12	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:O	1:A:300:VAL:HG13	2.06	0.56
1:A:767:SER:HB3	1:A:908:GLU:OE1	2.06	0.56
1:A:863:PRO:CB	1:A:890:ILE:HG21	2.35	0.55
1:A:79:GLU:HG3	1:A:87:ALA:CB	2.36	0.55
1:A:183:GLU:OE2	1:A:627:ASP:HB2	2.06	0.55
1:B:251:GLN:O	1:B:255:GLU:HG3	2.05	0.55
1:A:4:ALA:HB1	1:A:6:SER:H	1.72	0.55
1:A:777:LEU:C	1:A:779:ALA:H	2.14	0.55
1:A:946:LEU:O	1:A:950:VAL:CG2	2.55	0.55
1:B:24:LEU:CD1	1:B:149:ASP:HB3	2.37	0.55
1:A:739:ASN:O	1:A:742:THR:HG23	2.07	0.55
1:A:927:PRO:HD2	1:A:928:TRP:CE3	2.41	0.55
1:A:248:PRO:HG2	1:A:341:THR:HG22	1.89	0.55
1:A:865:VAL:O	1:A:865:VAL:HG23	2.06	0.55
1:B:24:LEU:HD12	1:B:149:ASP:HB3	1.88	0.55
1:A:744:VAL:O	1:A:747:VAL:HG13	2.07	0.55
1:B:292:ALA:O	1:B:296:PHE:HB2	2.07	0.55
1:A:901:LEU:HD21	1:A:944:HIS:CE1	2.41	0.55
1:B:329:LYS:O	1:B:330:ASN:HB2	2.06	0.55
1:A:4:ALA:HB1	1:A:6:SER:OG	2.07	0.54
1:A:303:ALA:O	1:A:307:ILE:HG12	2.07	0.54
1:B:34:GLU:OE1	1:B:34:GLU:HA	2.06	0.54
1:B:83:GLU:CD	1:B:83:GLU:H	2.14	0.54
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.23	0.54
1:B:262:LYS:O	1:B:266:LEU:HB2	2.07	0.54
1:B:739:ASN:O	1:B:742:THR:HG22	2.07	0.54
1:B:930:ASN:HB2	1:B:933:LEU:HB3	1.90	0.54
1:B:146:VAL:O	1:B:147:PRO:C	2.49	0.54
1:B:855:TRP:HE1	1:B:899:MET:CG	2.13	0.54
1:B:947:ILE:O	1:B:947:ILE:HG13	2.08	0.54
1:B:354:GLY:O	1:B:604:ARG:NH1	2.40	0.54
1:B:613:LEU:HD23	1:B:744:VAL:HG11	1.88	0.54
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.89	0.54
1:B:100:ALA:O	1:B:104:VAL:HG13	2.08	0.54
1:B:325:ARG:HD2	1:B:749:GLU:OE1	2.07	0.54
1:A:295:TYR:O	1:A:299:ALA:HB2	2.07	0.54
1:B:676:PHE:CD1	1:B:676:PHE:N	2.76	0.54
1:A:259:GLN:O	1:A:263:VAL:HG23	2.07	0.54
1:B:151:VAL:CG1	1:B:163:ILE:HD13	2.32	0.54
1:B:256:PHE:HA	1:B:259:GLN:HG2	1.90	0.54
1:B:411:VAL:HG22	1:B:454:VAL:HB	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:VAL:O	1:A:611:ILE:HG12	2.08	0.54
1:B:342:LEU:O	1:B:747:VAL:HG13	2.07	0.54
1:B:951:ASP:HB2	1:B:952:PRO:HD3	1.90	0.54
1:B:301:ALA:HA	1:B:304:VAL:HG12	1.90	0.53
1:B:18:VAL:HG11	1:B:148:GLY:O	2.08	0.53
1:B:852:ALA:HB2	1:B:900:ALA:HB2	1.91	0.53
1:B:930:ASN:CB	1:B:933:LEU:HB3	2.38	0.53
1:A:90:GLU:OE2	1:A:789:PRO:HB2	2.09	0.53
1:A:524:ARG:HH21	1:A:588:GLU:CB	2.21	0.53
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.08	0.53
1:A:315:ILE:C	1:A:317:THR:H	2.17	0.53
1:B:281:ASP:HB3	1:B:284:HIS:NE2	2.22	0.53
1:A:859:ALA:HB3	1:A:864:GLY:HA3	1.90	0.53
1:B:47:LYS:O	1:B:47:LYS:CG	2.56	0.53
1:B:325:ARG:NH1	1:B:749:GLU:OE2	2.41	0.53
1:A:352:LYS:HD2	1:A:635:ILE:HG13	1.90	0.53
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.44	0.53
1:B:263:VAL:O	1:B:267:ILE:HB	2.09	0.53
1:B:288:TRP:O	1:B:289:ILE:HB	2.09	0.53
1:A:703:ASP:HB2	1:A:723:GLY:HA3	1.90	0.53
1:B:50:TRP:NE1	1:B:51:GLU:HG3	2.24	0.53
1:B:174:ARG:HB3	1:B:186:SER:HB3	1.91	0.53
1:B:415:THR:HA	1:B:475:ILE:HG21	1.91	0.53
1:A:413:LEU:HD11	1:A:564:LEU:CD1	2.38	0.52
1:B:336:LEU:N	1:B:337:PRO:HD2	2.24	0.52
1:A:25:THR:N	1:A:28:GLN:HE21	1.89	0.52
1:B:410:LEU:HB3	1:B:452:MET:CE	2.40	0.52
1:B:739:ASN:HB3	1:B:742:THR:CG2	2.38	0.52
1:B:866:THR:HG22	1:B:867:TYR:HD1	1.73	0.52
1:A:33:LEU:O	1:A:33:LEU:HD23	2.09	0.52
1:A:395:VAL:HG12	1:A:402:ILE:CD1	2.39	0.52
1:B:74:VAL:HG13	1:B:75:LEU:HD12	1.91	0.52
1:B:294:TYR:O	1:B:298:ILE:HG13	2.10	0.52
1:B:296:PHE:O	1:B:300:VAL:HG13	2.09	0.52
1:A:290:ARG:HD2	1:A:874:MET:HE2	1.90	0.52
1:B:59:ASP:C	1:B:61:LEU:H	2.17	0.52
1:A:16:PHE:CD1	1:A:222:ILE:HD11	2.45	0.52
1:A:169:LYS:HD3	1:A:169:LYS:N	2.24	0.52
1:A:898:THR:HG21	1:A:961:ALA:HB2	1.91	0.52
1:B:825:LYS:O	1:B:827:PRO:HD3	2.10	0.52
1:A:739:ASN:C	1:A:739:ASN:HD22	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:PRO:HG2	1:A:890:ILE:HD12	1.92	0.52
1:A:901:LEU:CD2	1:A:944:HIS:CE1	2.93	0.52
1:B:235:ILE:O	1:B:239:MET:CG	2.58	0.52
1:A:194:VAL:HG23	1:A:206:ASN:ND2	2.24	0.52
1:B:873:PHE:HD1	1:B:875:GLN:CD	2.18	0.52
1:A:330:ASN:HB3	1:A:736:ALA:HB3	1.92	0.52
5:A:998:ACP:O2B	5:A:998:ACP:H5'2	2.09	0.52
1:A:114:ASN:OD1	1:A:117:GLU:HB2	2.10	0.51
1:A:778:THR:HG23	1:A:778:THR:O	2.10	0.51
1:B:382:PHE:CE1	1:B:410:LEU:HD21	2.45	0.51
1:B:500:PRO:HD3	1:B:509:GLY:CA	2.38	0.51
1:B:847:ALA:O	1:B:903:VAL:HG11	2.10	0.51
1:B:865:VAL:HB	1:B:868:HIS:CG	2.45	0.51
1:A:758:LYS:O	1:A:762:ARG:HG3	2.10	0.51
1:B:460:ARG:HB2	1:B:460:ARG:NH1	2.22	0.51
1:A:387:SER:HB2	1:A:602:PRO:HG2	1.92	0.51
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.91	0.51
1:B:96:LEU:HD23	1:B:96:LEU:O	2.10	0.51
1:A:23:GLY:HA3	1:A:130:TYR:O	2.10	0.51
1:A:51:GLU:O	1:A:53:VAL:N	2.44	0.51
1:A:666:GLN:NE2	1:A:690:TYR:OH	2.44	0.51
1:A:720:MET:HA	1:A:720:MET:HE2	1.92	0.51
1:B:268:CYS:HB3	1:B:302:LEU:CD2	2.41	0.51
1:B:855:TRP:CZ2	1:B:966:GLN:HG3	2.45	0.51
1:B:873:PHE:CZ	1:B:881:PRO:HG2	2.46	0.51
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.40	0.51
1:A:264:ILE:HD11	1:A:306:ALA:CB	2.40	0.51
1:A:678:ARG:O	1:A:678:ARG:HG2	2.11	0.51
1:A:957:PHE:O	1:A:958:LYS:HD3	2.10	0.51
1:B:115:ALA:HA	1:B:729:THR:HG21	1.93	0.51
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.92	0.51
1:B:323:THR:OG1	1:B:336:LEU:HD22	2.10	0.51
1:B:893:ALA:O	1:B:896:PRO:HD2	2.11	0.51
1:B:815:ASP:OD1	1:B:819:ARG:NH2	2.44	0.51
1:A:718:ILE:HG23	1:A:733:MET:HE2	1.92	0.51
1:A:969:MET:O	1:A:973:ILE:HG13	2.10	0.51
1:B:97:ILE:O	1:B:101:ASN:HB2	2.10	0.51
1:B:757:MET:HG2	1:B:760:PHE:CZ	2.45	0.51
1:B:880:HIS:N	1:B:881:PRO:CD	2.69	0.51
1:B:881:PRO:HD2	1:B:882:HIS:H	1.76	0.51
1:A:857:MET:SD	1:A:867:TYR:HA	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:LEU:O	1:A:954:PRO:CG	2.59	0.51
1:B:247:THR:HB	1:B:248:PRO:CD	2.40	0.51
1:A:79:GLU:O	1:A:79:GLU:CG	2.56	0.51
1:A:688:VAL:O	1:A:692:GLN:HG3	2.11	0.50
1:A:859:ALA:HB3	1:A:864:GLY:HA2	1.93	0.50
1:B:5:HIS:CD2	1:B:6:SER:HB3	2.46	0.50
1:B:281:ASP:N	1:B:282:PRO:CD	2.74	0.50
1:B:878:GLU:CB	1:B:880:HIS:CD2	2.92	0.50
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.92	0.50
1:B:89:VAL:HG21	1:B:956:ILE:HG21	1.92	0.50
1:B:509:GLY:O	1:B:510:ASN:C	2.54	0.50
1:B:844:VAL:HG11	1:B:907:ILE:HG21	1.93	0.50
1:A:30:LYS:O	1:A:34:GLU:HB2	2.11	0.50
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.94	0.50
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.92	0.50
1:A:865:VAL:CB	1:A:868:HIS:CD2	2.91	0.50
1:A:946:LEU:O	1:A:950:VAL:HG21	2.11	0.50
1:B:354:GLY:CA	1:B:359:ASN:HB2	2.42	0.50
1:A:472:ASN:O	1:A:476:ARG:HG2	2.10	0.50
1:B:89:VAL:HG21	1:B:956:ILE:CG2	2.41	0.50
1:A:768:ASN:O	1:A:772:VAL:HG23	2.12	0.50
1:A:963:ASP:C	1:A:965:THR:H	2.19	0.50
1:B:892:GLU:O	1:B:893:ALA:C	2.54	0.50
1:B:897:MET:SD	1:B:958:LYS:HE2	2.51	0.50
1:A:262:LYS:O	1:A:266:LEU:HB2	2.11	0.50
1:B:292:ALA:C	1:B:294:TYR:H	2.18	0.50
1:B:326:MET:HE3	1:B:326:MET:HA	1.94	0.50
1:B:154:ALA:O	1:B:214:ILE:HB	2.11	0.50
1:B:950:VAL:HB	1:B:953:LEU:HD12	1.92	0.50
1:A:60:LEU:HD12	1:A:61:LEU:H	1.72	0.50
1:A:188:ILE:HD13	1:A:487:PHE:CE2	2.46	0.50
1:A:449:VAL:CG2	1:A:472:ASN:HD21	2.22	0.50
1:A:760:PHE:C	1:A:760:PHE:HD1	2.20	0.50
1:B:48:SER:O	1:B:49:LEU:C	2.55	0.50
1:B:853:ALA:C	1:B:854:TRP:CD1	2.89	0.50
1:A:300:VAL:O	1:A:300:VAL:HG23	2.10	0.50
1:B:322:GLY:O	1:B:326:MET:HG2	2.12	0.50
1:B:921:SER:HB2	1:B:982:GLU:CD	2.36	0.50
1:B:25:THR:HB	1:B:26:PRO:CD	2.42	0.49
1:B:171:THR:HG21	1:B:486:GLU:CD	2.36	0.49
1:B:859:ALA:HB3	1:B:864:GLY:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:ILE:O	1:B:982:GLU:HB2	2.12	0.49
1:A:198:ARG:NH2	1:A:659:ASP:HB3	2.28	0.49
1:B:757:MET:O	1:B:761:ILE:HG13	2.12	0.49
1:B:899:MET:HE1	1:B:966:GLN:HB3	1.94	0.49
1:A:114:ASN:OD1	1:A:117:GLU:CB	2.61	0.49
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.93	0.49
1:A:947:ILE:HD12	1:A:957:PHE:CE1	2.47	0.49
1:B:899:MET:HE3	1:B:966:GLN:HB3	1.95	0.49
1:B:915:SER:C	1:B:917:SER:H	2.19	0.49
1:A:325:ARG:NH1	1:A:749:GLU:OE2	2.45	0.49
1:A:793:LEU:HD23	1:A:793:LEU:N	2.27	0.49
1:B:505:ARG:HG3	1:B:506:ALA:HA	1.95	0.49
1:A:508:VAL:C	1:A:510:ASN:H	2.19	0.49
1:B:23:GLY:HA3	1:B:130:TYR:O	2.12	0.49
1:A:878:GLU:HG3	1:A:878:GLU:O	2.12	0.49
1:B:421:ASN:HD22	1:B:422:ASP:H	1.61	0.49
1:A:4:ALA:CB	1:A:7:LYS:HG2	2.39	0.49
1:A:67:LEU:O	1:A:69:ALA:N	2.45	0.49
1:B:487:PHE:CE1	1:B:492:LYS:HA	2.47	0.49
1:B:948:LEU:HD22	1:B:949:TYR:CE1	2.47	0.49
1:A:200:VAL:O	1:A:203:ASP:HB2	2.12	0.49
1:B:65:LEU:HB2	1:B:98:LEU:HD21	1.94	0.49
1:B:172:THR:HG21	1:B:174:ARG:HH21	1.78	0.49
1:A:716:ILE:HD12	1:A:716:ILE:H	1.78	0.49
1:A:880:HIS:CG	1:A:881:PRO:CD	2.94	0.49
1:B:51:GLU:HG2	1:B:54:ILE:HD12	1.94	0.48
1:B:493:SER:HB3	1:B:516:GLY:HA3	1.95	0.48
1:A:625:THR:HA	2:A:995:ALF:F3	2.03	0.48
1:B:288:TRP:H	1:B:288:TRP:CD1	2.30	0.48
1:A:357:THR:HA	1:A:603:PRO:HA	1.94	0.48
1:A:908:GLU:O	1:A:909:MET:HE2	2.13	0.48
1:B:773:VAL:CG1	1:B:845:GLY:HA3	2.43	0.48
1:B:873:PHE:HB2	1:B:875:GLN:HG3	1.96	0.48
1:A:57:PHE:HA	1:A:62:VAL:HG21	1.95	0.48
1:B:624:ILE:CD1	1:B:687:ILE:HG21	2.43	0.48
1:B:932:TRP:O	1:B:936:SER:HB3	2.12	0.48
1:A:398:ASN:C	1:A:400:LYS:H	2.22	0.48
1:A:424:SER:HB3	1:A:437:VAL:CG2	2.42	0.48
1:A:518:PRO:O	1:A:522:ILE:HG13	2.14	0.48
1:A:762:ARG:HD3	1:A:833:LEU:HD21	1.95	0.48
1:A:898:THR:CG2	1:A:961:ALA:HB2	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:GLY:C	1:B:557:ASP:H	2.21	0.48
1:B:23:GLY:HA2	1:B:150:ILE:HG12	1.95	0.48
1:B:65:LEU:HD21	1:B:307:ILE:CG1	2.35	0.48
1:B:863:PRO:HB2	1:B:890:ILE:HD11	1.96	0.48
1:B:884:GLU:O	1:B:886:LEU:N	2.47	0.48
1:A:83:GLU:HG2	1:A:83:GLU:O	2.14	0.48
1:A:559:LEU:CD2	1:A:600:LEU:HD13	2.44	0.48
1:A:856:PHE:HB3	1:A:865:VAL:HG22	1.94	0.48
1:A:858:TYR:O	1:A:860:GLU:N	2.46	0.48
1:B:362:SER:O	1:B:599:MET:HA	2.14	0.48
1:A:505:ARG:O	1:A:506:ALA:CB	2.62	0.48
1:A:884:GLU:HB3	1:A:887:ASP:OD2	2.13	0.48
1:A:894:PRO:CB	1:A:959:LEU:H	2.24	0.48
1:A:952:PRO:O	1:A:955:MET:HE2	2.13	0.48
1:B:351:ASP:OD2	1:B:355:THR:CG2	2.61	0.48
1:B:529:ARG:HH22	1:B:568:ASP:CG	2.22	0.48
1:B:654:THR:HA	1:B:677:ALA:O	2.14	0.48
1:A:25:THR:O	1:A:29:VAL:HG23	2.14	0.48
1:A:840:ILE:HG22	1:A:841:GLY:N	2.28	0.48
1:B:421:ASN:HD22	1:B:422:ASP:N	2.10	0.48
1:B:671:ARG:HH21	1:B:694:TYR:CB	2.26	0.48
1:B:720:MET:HE3	1:B:738:ASP:OD2	2.14	0.48
1:B:767:SER:HB3	1:B:908:GLU:CD	2.39	0.48
1:B:921:SER:HB3	1:B:989:ARG:NH2	2.29	0.48
1:B:948:LEU:HD11	1:B:961:ALA:CB	2.42	0.48
1:A:487:PHE:HA	1:A:493:SER:O	2.14	0.48
1:A:839:ALA:HB3	1:A:984:LEU:HD11	1.96	0.48
1:A:962:LEU:O	1:A:965:THR:OG1	2.29	0.48
1:A:964:LEU:HA	1:A:968:LEU:HD21	1.95	0.48
1:A:45:GLU:O	1:A:46:GLY:C	2.57	0.47
1:B:303:ALA:O	1:B:307:ILE:HG12	2.14	0.47
1:B:606:GLU:HG3	1:B:739:ASN:ND2	2.29	0.47
1:A:930:ASN:HB2	1:A:933:LEU:HB3	1.96	0.47
1:B:51:GLU:HA	1:B:54:ILE:HG13	1.96	0.47
1:B:529:ARG:NH2	1:B:568:ASP:OD2	2.47	0.47
1:A:275:ASN:C	1:A:277:GLY:H	2.22	0.47
1:A:298:ILE:C	1:A:298:ILE:CD1	2.87	0.47
1:A:508:VAL:HG23	1:A:508:VAL:O	2.14	0.47
1:A:524:ARG:HH21	1:A:588:GLU:HB2	1.79	0.47
1:B:93:VAL:HG12	1:B:793:LEU:HD13	1.97	0.47
1:B:315:ILE:HG22	1:B:316:THR:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:VAL:HG13	1:B:845:GLY:HA3	1.95	0.47
1:A:719:ALA:HB3	1:A:734:VAL:HG22	1.97	0.47
1:A:895:GLU:N	1:A:896:PRO:CD	2.77	0.47
1:B:190:HIS:O	1:B:206:ASN:HA	2.14	0.47
1:B:452:MET:HE2	1:B:454:VAL:CG1	2.44	0.47
1:B:775:ILE:O	1:B:775:ILE:HG22	2.15	0.47
1:B:268:CYS:O	1:B:271:VAL:HG22	2.15	0.47
1:B:844:VAL:CB	1:B:907:ILE:HD13	2.45	0.47
1:A:52:LEU:HD23	1:A:53:VAL:N	2.29	0.47
1:A:61:LEU:HD21	1:A:312:PRO:CG	2.45	0.47
1:A:74:VAL:HG22	1:A:78:PHE:HE2	1.78	0.47
1:A:865:VAL:CB	1:A:868:HIS:HD2	2.26	0.47
1:A:948:LEU:C	1:A:954:PRO:HG3	2.39	0.47
1:B:53:VAL:HG13	1:B:54:ILE:N	2.30	0.47
1:B:86:THR:O	1:B:89:VAL:HG12	2.14	0.47
1:B:304:VAL:HG11	1:B:789:PRO:HB3	1.97	0.47
1:B:402:ILE:HG12	1:B:403:ARG:N	2.29	0.47
1:B:555:GLY:C	1:B:557:ASP:N	2.69	0.47
1:B:678:ARG:HG3	1:B:678:ARG:NH1	2.05	0.47
1:B:828:LEU:HD12	1:B:829:ILE:HG12	1.96	0.47
1:B:882:HIS:CD2	1:B:885:GLY:HA3	2.49	0.47
1:A:421:ASN:HD22	1:A:423:SER:H	1.61	0.47
1:B:58:GLU:O	1:B:60:LEU:HG	2.15	0.47
1:B:248:PRO:HD2	1:B:341:THR:CG2	2.44	0.47
1:B:667:ARG:NH2	1:B:693:SER:O	2.48	0.47
1:B:971:LEU:HD23	1:B:971:LEU:O	2.15	0.47
1:A:612:GLN:HA	1:A:612:GLN:OE1	2.14	0.47
1:A:829:ILE:CG2	1:A:834:PHE:HB2	2.44	0.47
1:A:865:VAL:HG23	1:A:868:HIS:HB2	1.97	0.47
1:A:903:VAL:O	1:A:907:ILE:HG13	2.14	0.47
1:B:25:THR:HB	1:B:26:PRO:HD2	1.97	0.47
1:B:428:ASN:OD1	1:B:428:ASN:C	2.58	0.47
1:A:83:GLU:HB2	1:A:86:THR:HG22	1.97	0.47
1:A:496:VAL:O	1:A:512:MET:HA	2.15	0.47
1:B:5:HIS:CD2	1:B:5:HIS:C	2.93	0.47
1:B:5:HIS:ND1	1:B:204:LYS:HG2	2.30	0.47
1:B:678:ARG:CG	1:B:678:ARG:NH1	2.68	0.47
1:A:342:LEU:HD13	1:A:716:ILE:HG21	1.96	0.46
1:B:69:ALA:HB2	1:B:94:ILE:HG21	1.96	0.46
1:B:151:VAL:HG13	1:B:152:GLU:N	2.30	0.46
1:B:483:PHE:HE2	1:B:485:LEU:HD21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:LEU:HD23	1:B:901:LEU:O	2.14	0.46
1:B:948:LEU:HD21	1:B:961:ALA:H	1.80	0.46
1:A:353:THR:HA	1:A:357:THR:OG1	2.16	0.46
1:A:53:VAL:C	1:A:55:GLU:N	2.73	0.46
1:A:145:ILE:HD11	1:A:223:VAL:HG21	1.97	0.46
1:A:392:GLU:O	1:A:451:LYS:HE2	2.15	0.46
1:A:921:SER:HB2	1:A:989:ARG:NE	2.31	0.46
1:B:300:VAL:O	1:B:304:VAL:HG12	2.16	0.46
1:B:671:ARG:HA	1:B:671:ARG:HD3	1.80	0.46
1:B:774:CYS:C	1:B:776:PHE:H	2.23	0.46
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.61	0.46
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.98	0.46
1:B:128:LYS:HB3	1:B:137:VAL:HG22	1.98	0.46
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.45	0.46
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.97	0.46
1:B:88:PHE:O	1:B:91:PRO:HD2	2.15	0.46
1:B:672:ARG:HG3	1:B:673:ALA:N	2.30	0.46
1:A:71:ILE:O	1:A:75:LEU:HG	2.16	0.46
1:A:275:ASN:O	1:A:277:GLY:N	2.48	0.46
1:A:921:SER:HA	1:A:985:LYS:HD2	1.98	0.46
1:B:171:THR:HG21	1:B:486:GLU:CG	2.46	0.46
1:B:356:LEU:O	1:B:604:ARG:HG3	2.16	0.46
1:B:557:ASP:HA	1:B:638:ARG:NH2	2.31	0.46
1:B:965:THR:N	1:B:968:LEU:HD12	2.31	0.46
1:A:67:LEU:C	1:A:69:ALA:H	2.23	0.46
1:A:306:ALA:O	1:A:768:ASN:HB3	2.16	0.46
1:B:699:ALA:CB	1:B:716:ILE:HG23	2.45	0.46
1:B:760:PHE:HB3	1:B:807:LEU:HB2	1.96	0.46
1:B:921:SER:HB3	1:B:989:ARG:CZ	2.46	0.46
1:A:90:GLU:HG3	1:A:790:VAL:HG23	1.96	0.46
1:A:290:ARG:HD2	1:A:874:MET:CE	2.45	0.46
1:A:334:ARG:HD3	1:A:731:SER:O	2.15	0.46
1:A:762:ARG:CD	1:A:833:LEU:HD21	2.46	0.46
1:A:834:PHE:O	1:A:838:MET:HB2	2.15	0.46
1:B:477:GLN:O	1:B:501:ALA:HB3	2.15	0.46
1:B:936:SER:O	1:B:940:SER:HB2	2.16	0.46
1:A:60:LEU:CD2	1:A:257:GLY:HA2	2.45	0.46
1:B:89:VAL:HG13	1:B:90:GLU:N	2.31	0.46
1:B:684:LYS:O	1:B:688:VAL:HG23	2.16	0.46
1:A:36:TYR:CD2	1:A:147:PRO:HG2	2.51	0.46
1:A:57:PHE:HD1	1:A:62:VAL:HG13	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:O	1:A:262:LYS:HD3	2.16	0.46
1:A:387:SER:HB2	1:A:602:PRO:CG	2.45	0.46
1:B:25:THR:O	1:B:29:VAL:HG23	2.16	0.46
1:B:354:GLY:HA2	1:B:359:ASN:HB2	1.98	0.46
1:B:500:PRO:CG	1:B:509:GLY:HA3	2.46	0.46
1:A:140:ILE:HD11	1:A:145:ILE:HG22	1.98	0.45
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.16	0.45
1:B:920:GLN:O	1:B:921:SER:C	2.58	0.45
1:A:59:ASP:N	1:A:59:ASP:OD1	2.46	0.45
1:A:174:ARG:HG3	1:A:174:ARG:HH11	1.81	0.45
1:A:600:LEU:O	1:A:602:PRO:HD3	2.16	0.45
1:A:773:VAL:HG21	1:A:842:GLY:HA2	1.99	0.45
1:A:947:ILE:HD13	1:A:947:ILE:HA	1.72	0.45
1:B:64:ILE:HG22	1:B:65:LEU:HD23	1.98	0.45
1:B:421:ASN:HD21	1:B:442:GLU:HB3	1.82	0.45
1:B:481:LYS:CG	1:B:496:VAL:HG13	2.46	0.45
1:B:933:LEU:O	1:B:933:LEU:HG	2.16	0.45
1:A:53:VAL:C	1:A:55:GLU:H	2.24	0.45
1:A:279:PHE:CD1	1:A:279:PHE:C	2.94	0.45
1:B:948:LEU:HD23	1:B:948:LEU:C	2.41	0.45
1:B:785:GLU:O	1:B:897:MET:HG2	2.16	0.45
1:A:61:LEU:HD21	1:A:312:PRO:HG2	1.98	0.45
1:A:142:ALA:O	1:A:145:ILE:HG23	2.15	0.45
1:B:97:ILE:CD1	1:B:797:LEU:HD22	2.46	0.45
1:B:944:HIS:O	1:B:944:HIS:CD2	2.70	0.45
1:A:79:GLU:OE1	1:A:79:GLU:N	2.50	0.45
1:A:840:ILE:HD11	1:A:980:LEU:HB2	1.99	0.45
1:B:207:MET:HE3	1:B:207:MET:HB3	1.69	0.45
1:B:473:SER:O	1:B:477:GLN:HG2	2.16	0.45
1:B:933:LEU:O	1:B:937:ILE:HG12	2.17	0.45
1:A:49:LEU:C	1:A:51:GLU:N	2.73	0.45
1:B:700:MET:HE3	1:B:701:THR:O	2.17	0.45
1:B:873:PHE:HD1	1:B:875:GLN:NE2	2.15	0.45
1:B:879:ASP:C	1:B:881:PRO:HD3	2.42	0.45
1:A:512:MET:HE2	1:A:512:MET:HB3	1.74	0.45
1:A:869:GLN:NE2	1:A:871:THR:HG23	2.25	0.45
1:A:913:LEU:O	1:A:922:LEU:HD21	2.17	0.45
1:A:799:THR:HG22	1:A:909:MET:HE3	1.98	0.45
1:B:4:ALA:HB1	1:B:6:SER:H	1.82	0.45
1:B:114:ASN:OD1	1:B:117:GLU:HB2	2.16	0.45
1:B:302:LEU:HD12	1:B:772:VAL:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:HB	1:B:621:VAL:HG22	1.99	0.45
1:B:351:ASP:OD2	1:B:355:THR:HG23	2.16	0.45
1:B:625:THR:O	1:B:679:VAL:HG22	2.16	0.45
1:A:165:ILE:HG13	1:A:206:ASN:O	2.16	0.45
1:A:396:LEU:HD23	1:A:396:LEU:N	2.32	0.45
1:A:543:GLU:O	1:A:547:SER:HB3	2.17	0.45
1:B:629:LYS:HA	1:B:677:ALA:CB	2.47	0.45
1:B:889:GLU:O	1:B:889:GLU:HG3	2.17	0.45
1:B:901:LEU:HD23	1:B:901:LEU:C	2.42	0.45
1:A:115:ALA:CA	1:A:729:THR:HG21	2.46	0.44
1:A:155:VAL:HG23	1:A:155:VAL:O	2.17	0.44
1:A:978:ILE:O	1:A:982:GLU:HG2	2.17	0.44
1:A:988:ALA:HA	1:A:992:LEU:CB	2.33	0.44
1:B:281:ASP:N	1:B:282:PRO:HD2	2.31	0.44
1:B:583:ARG:O	1:B:586:GLU:HG2	2.17	0.44
1:A:275:ASN:C	1:A:277:GLY:N	2.76	0.44
1:A:60:LEU:HD12	1:A:60:LEU:C	2.42	0.44
1:A:179:ILE:CG2	1:A:212:THR:HG22	2.48	0.44
1:A:421:ASN:HA	1:A:442:GLU:OE2	2.18	0.44
1:B:110:ARG:NH2	1:B:112:ALA:HB2	2.33	0.44
1:B:794:TRP:O	1:B:798:VAL:HB	2.17	0.44
1:B:951:ASP:O	1:B:953:LEU:N	2.51	0.44
1:A:311:LEU:HG	1:A:315:ILE:HD12	1.98	0.44
1:A:342:LEU:HD23	1:A:746:ALA:HB3	1.98	0.44
1:A:642:PHE:CZ	1:A:648:VAL:HG13	2.52	0.44
1:A:922:LEU:HA	1:A:925:MET:O	2.18	0.44
1:B:410:LEU:HB3	1:B:452:MET:HE3	2.00	0.44
1:B:922:LEU:HA	1:B:925:MET:HE3	2.00	0.44
1:B:983:ILE:O	1:B:987:ILE:HG13	2.18	0.44
1:A:358:THR:O	1:A:359:ASN:HB3	2.18	0.44
1:A:359:ASN:O	1:A:360:GLN:HG2	2.17	0.44
1:B:264:ILE:HA	1:B:267:ILE:HG22	2.00	0.44
1:B:500:PRO:HG3	1:B:509:GLY:HA3	1.98	0.44
1:A:79:GLU:O	1:A:81:GLY:N	2.48	0.44
1:A:174:ARG:HG3	1:A:174:ARG:NH1	2.32	0.44
1:A:793:LEU:HD23	1:A:793:LEU:H	1.83	0.44
1:B:55:GLU:OE1	1:B:58:GLU:HB3	2.18	0.44
1:B:423:SER:HB2	1:B:437:VAL:O	2.18	0.44
1:B:776:PHE:O	1:B:780:ALA:HB3	2.17	0.44
1:B:953:LEU:C	1:B:955:MET:N	2.74	0.44
1:A:418:ALA:HB3	1:A:475:ILE:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:LEU:HB3	1:A:965:THR:OG1	2.18	0.44
1:B:863:PRO:CB	1:B:890:ILE:HD11	2.48	0.44
1:A:23:GLY:HA2	1:A:150:ILE:HG12	2.00	0.44
1:B:50:TRP:CD1	1:B:51:GLU:HG3	2.52	0.44
1:B:182:GLY:HA3	2:B:995:ALF:F3	2.08	0.44
1:B:236:ARG:C	1:B:236:ARG:HD3	2.43	0.44
1:B:407:PHE:N	1:B:407:PHE:CD2	2.85	0.44
1:B:964:LEU:O	1:B:965:THR:CB	2.64	0.44
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.79	0.44
1:A:567:ARG:HG3	1:A:591:LEU:HD23	2.00	0.44
1:A:672:ARG:NH1	1:A:672:ARG:HG2	2.33	0.44
1:B:35:LYS:HD3	1:B:36:TYR:CZ	2.53	0.44
1:B:645:ASN:O	1:B:646:GLU:C	2.61	0.44
1:B:799:THR:HG21	1:B:905:VAL:HG22	2.00	0.44
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.62	0.43
1:A:189:LYS:HD2	1:A:205:LYS:O	2.18	0.43
1:A:492:LYS:HB3	1:A:517:ALA:HB2	2.00	0.43
1:B:276:ILE:HG22	1:B:276:ILE:O	2.18	0.43
1:B:527:TYR:CE2	1:B:534:ARG:NH1	2.86	0.43
1:A:179:ILE:O	1:A:705:VAL:HG22	2.17	0.43
1:A:870:LEU:HB3	1:A:873:PHE:HZ	1.79	0.43
1:B:298:ILE:O	1:B:302:LEU:HB2	2.18	0.43
1:A:302:LEU:HD22	1:A:772:VAL:HG13	1.99	0.43
1:A:333:VAL:HG21	1:A:339:VAL:HG12	1.99	0.43
1:A:430:THR:HG22	1:A:431:LYS:N	2.29	0.43
1:A:557:ASP:O	1:A:557:ASP:OD1	2.37	0.43
1:B:41:LEU:HG	1:B:123:GLU:OE1	2.19	0.43
1:B:856:PHE:CE1	1:B:896:PRO:HG2	2.48	0.43
1:A:276:ILE:HD12	1:A:278:HIS:CE1	2.53	0.43
1:A:368:ILE:HD12	1:A:409:GLY:HA3	2.00	0.43
1:A:672:ARG:HG2	1:A:672:ARG:HH11	1.82	0.43
1:A:764:LEU:O	1:A:768:ASN:ND2	2.51	0.43
1:A:932:TRP:HA	1:A:932:TRP:HE3	1.81	0.43
1:B:23:GLY:HA2	1:B:150:ILE:CG1	2.48	0.43
1:B:614:CYS:O	1:B:619:ILE:HB	2.18	0.43
1:B:807:LEU:HA	1:B:810:ASN:ND2	2.34	0.43
1:A:179:ILE:HD12	1:A:179:ILE:HG21	1.86	0.43
1:A:679:VAL:HB	1:A:683:HIS:HB2	2.01	0.43
1:A:948:LEU:HD12	1:A:948:LEU:HA	1.88	0.43
1:A:972:LYS:HA	1:A:972:LYS:HD2	1.76	0.43
1:B:814:LEU:HD12	1:B:815:ASP:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:LEU:O	1:B:993:GLU:HB2	2.18	0.43
1:A:7:LYS:HB3	1:A:11:GLU:HB2	2.01	0.43
1:A:13:LEU:CD2	1:A:20:GLU:HB2	2.47	0.43
1:A:57:PHE:CA	1:A:62:VAL:HG11	2.48	0.43
1:A:196:ASP:OD1	1:A:196:ASP:C	2.61	0.43
1:A:610:SER:OG	1:A:741:SER:HA	2.18	0.43
1:B:234:LYS:O	1:B:238:GLN:HB2	2.19	0.43
1:B:482:GLU:HB3	1:B:483:PHE:H	1.72	0.43
1:B:913:LEU:HD23	1:B:933:LEU:HD21	2.00	0.43
1:B:923:MET:CE	1:B:924:ARG:HD2	2.48	0.43
1:A:559:LEU:HD23	1:A:600:LEU:HD13	2.00	0.43
1:B:511:LYS:HZ2	1:B:568:ASP:CA	2.28	0.43
1:B:648:VAL:O	1:B:648:VAL:CG1	2.63	0.43
1:B:761:ILE:O	1:B:761:ILE:CG2	2.67	0.43
1:A:88:PHE:O	1:A:88:PHE:CD1	2.72	0.43
1:A:441:THR:HG22	1:A:599:MET:SD	2.59	0.43
1:B:926:PRO:HB3	1:B:928:TRP:NE1	2.34	0.43
1:B:948:LEU:HD22	1:B:949:TYR:CD1	2.54	0.43
1:A:239:MET:O	1:A:240:ALA:C	2.62	0.43
1:A:773:VAL:HG11	1:A:845:GLY:HA3	1.95	0.43
1:B:895:GLU:H	1:B:896:PRO:HD2	1.83	0.43
1:A:53:VAL:O	1:A:55:GLU:N	2.52	0.43
1:B:246:LYS:HD2	1:B:250:GLN:NE2	2.31	0.43
1:B:496:VAL:O	1:B:512:MET:HA	2.19	0.43
1:B:662:PRO:O	1:B:664:ALA:N	2.52	0.43
1:B:893:ALA:HB3	1:B:896:PRO:HG2	2.01	0.43
1:A:16:PHE:HD1	1:A:222:ILE:HD11	1.84	0.42
1:A:75:LEU:HD22	1:A:293:ILE:HD13	2.00	0.42
1:A:901:LEU:HD21	1:A:944:HIS:HE1	1.82	0.42
1:A:933:LEU:O	1:A:937:ILE:HG13	2.18	0.42
1:A:958:LYS:HD3	1:A:958:LYS:HA	1.87	0.42
1:B:368:ILE:HG23	1:B:410:LEU:HD23	2.00	0.42
1:B:873:PHE:CE2	1:B:881:PRO:HG2	2.54	0.42
1:B:913:LEU:HD23	1:B:933:LEU:CD2	2.49	0.42
1:B:951:ASP:C	1:B:953:LEU:N	2.77	0.42
1:A:268:CYS:O	1:A:271:VAL:HG22	2.18	0.42
1:A:305:ALA:HB3	1:A:772:VAL:HG22	2.01	0.42
1:B:329:LYS:NZ	1:B:745:ALA:HB1	2.33	0.42
1:B:777:LEU:HD12	1:B:849:VAL:HG21	2.01	0.42
1:B:923:MET:HE3	1:B:924:ARG:HD2	2.02	0.42
1:A:642:PHE:CE2	1:A:648:VAL:HG13	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:PRO:O	1:A:793:LEU:HG	2.19	0.42
1:A:886:LEU:O	1:A:886:LEU:HG	2.19	0.42
1:A:963:ASP:C	1:A:965:THR:N	2.77	0.42
1:B:556:ARG:NH1	1:B:644:GLU:HB3	2.34	0.42
1:A:177:GLN:HA	1:A:212:THR:HG22	2.00	0.42
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.55	0.42
1:B:51:GLU:O	1:B:54:ILE:CB	2.65	0.42
1:A:120:LYS:HB3	1:A:120:LYS:HE2	1.79	0.42
1:A:247:THR:HG23	1:A:250:GLN:HB2	1.99	0.42
1:B:90:GLU:C	1:B:92:PHE:N	2.76	0.42
1:B:477:GLN:HA	1:B:477:GLN:OE1	2.20	0.42
1:B:855:TRP:C	1:B:859:ALA:HB2	2.45	0.42
1:A:63:ARG:HD2	1:A:63:ARG:HA	1.71	0.42
1:A:333:VAL:HG11	1:A:339:VAL:HG13	2.02	0.42
1:B:196:ASP:HA	1:B:197:PRO:HD3	1.87	0.42
1:B:875:GLN:O	1:B:876:CYS:C	2.63	0.42
1:A:342:LEU:HD23	1:A:746:ALA:CB	2.49	0.42
1:A:557:ASP:O	1:A:557:ASP:CG	2.63	0.42
1:A:947:ILE:HD13	1:A:953:LEU:CD1	2.46	0.42
1:B:567:ARG:NH1	1:B:569:THR:O	2.52	0.42
1:B:761:ILE:O	1:B:761:ILE:HG22	2.20	0.42
1:B:840:ILE:CG2	1:B:911:ASN:HD21	2.33	0.42
1:B:844:VAL:HG11	1:B:907:ILE:CG2	2.49	0.42
1:A:67:LEU:C	1:A:69:ALA:N	2.75	0.42
1:A:539:GLY:N	1:A:540:PRO:CD	2.83	0.42
1:A:807:LEU:HA	1:A:810:ASN:CG	2.44	0.42
1:B:77:TRP:CD1	1:B:78:PHE:CE1	3.03	0.42
1:B:357:THR:HA	1:B:603:PRO:HA	2.01	0.42
1:B:421:ASN:ND2	1:B:423:SER:H	2.18	0.42
1:B:497:TYR:CD2	1:B:576:MET:HE1	2.55	0.42
1:A:1:MET:HB2	1:A:36:TYR:OH	2.20	0.42
1:A:90:GLU:CD	1:A:789:PRO:HB2	2.44	0.42
1:A:310:GLY:O	1:A:314:VAL:HG23	2.19	0.42
1:B:67:LEU:HD12	1:B:67:LEU:HA	1.84	0.42
1:B:412:GLU:HG2	1:B:594:VAL:HG11	2.01	0.42
1:B:452:MET:HE2	1:B:454:VAL:HG12	2.01	0.42
1:B:840:ILE:HD12	1:B:911:ASN:HD21	1.83	0.42
1:A:421:ASN:HD22	1:A:421:ASN:C	2.28	0.42
1:A:611:ILE:HG23	1:A:621:VAL:HG21	2.02	0.42
1:A:717:GLY:C	1:A:731:SER:HB2	2.44	0.42
1:A:961:ALA:HB1	1:A:966:GLN:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ILE:HA	1:B:308:PRO:HD3	1.77	0.42
1:B:773:VAL:HG11	1:B:841:GLY:O	2.20	0.42
1:B:840:ILE:O	1:B:844:VAL:HG13	2.20	0.42
1:B:965:THR:O	1:B:965:THR:CG2	2.68	0.42
1:A:97:ILE:HD12	1:A:797:LEU:HD22	2.02	0.41
1:A:421:ASN:ND2	1:A:423:SER:H	2.18	0.41
1:A:828:LEU:HG	1:A:829:ILE:H	1.84	0.41
1:B:161:ALA:C	1:B:210:SER:HB2	2.45	0.41
1:B:176:ASP:OD1	1:B:176:ASP:C	2.60	0.41
1:B:304:VAL:HG11	1:B:789:PRO:CB	2.50	0.41
1:B:483:PHE:CZ	1:B:576:MET:HE1	2.47	0.41
1:B:898:THR:O	1:B:898:THR:HG23	2.20	0.41
1:A:8:SER:O	1:A:9:THR:C	2.63	0.41
1:A:249:LEU:HD12	1:A:250:GLN:H	1.84	0.41
1:A:276:ILE:HD12	1:A:276:ILE:HA	1.89	0.41
1:A:652:ALA:HA	1:A:675:CYS:O	2.19	0.41
1:A:955:MET:HE2	1:A:955:MET:HB3	1.85	0.41
1:B:501:ALA:O	1:B:502:LYS:CG	2.66	0.41
1:B:778:THR:O	1:B:778:THR:HG23	2.20	0.41
1:A:103:ILE:O	1:A:103:ILE:HG22	2.20	0.41
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.72	0.41
1:A:524:ARG:HH21	1:A:588:GLU:HB3	1.84	0.41
1:A:527:TYR:CB	1:A:534:ARG:HD3	2.51	0.41
1:B:336:LEU:N	1:B:337:PRO:CD	2.82	0.41
1:B:390:ALA:C	1:B:392:GLU:N	2.77	0.41
1:A:162:ASP:OD1	1:A:230:THR:HB	2.20	0.41
1:A:916:LEU:HD13	1:A:933:LEU:CD2	2.50	0.41
1:B:178:SER:HB3	1:B:183:GLU:C	2.45	0.41
1:B:726:VAL:O	1:B:726:VAL:HG23	2.19	0.41
1:B:793:LEU:HD23	1:B:793:LEU:HA	1.82	0.41
1:A:441:THR:O	1:A:599:MET:HE1	2.20	0.41
1:A:872:HIS:O	1:A:873:PHE:CD1	2.74	0.41
1:B:4:ALA:HB3	1:B:7:LYS:HG2	2.02	0.41
1:B:114:ASN:C	1:B:729:THR:HG21	2.45	0.41
1:B:549:ILE:HD11	1:B:596:VAL:HG21	2.03	0.41
1:B:586:GLU:O	1:B:589:THR:HG22	2.21	0.41
1:A:276:ILE:O	1:A:279:PHE:CD2	2.74	0.41
1:A:814:LEU:HG	1:A:815:ASP:N	2.35	0.41
1:B:78:PHE:CD1	1:B:78:PHE:N	2.88	0.41
1:B:921:SER:C	1:B:923:MET:N	2.78	0.41
1:B:965:THR:H	1:B:968:LEU:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:NE2	1:A:102:ALA:HA	2.35	0.41
1:A:74:VAL:HG13	1:A:75:LEU:N	2.34	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	0.41
1:A:545:ILE:HG21	1:A:545:ILE:HD13	1.81	0.41
1:A:861:ASP:CG	1:A:862:GLY:N	2.74	0.41
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.90	0.41
1:B:483:PHE:CZ	1:B:576:MET:CE	3.00	0.41
1:B:957:PHE:O	1:B:958:LYS:HD3	2.19	0.41
1:A:44:GLU:OE1	1:A:114:ASN:HB3	2.21	0.41
1:A:793:LEU:O	1:A:794:TRP:C	2.62	0.41
1:A:857:MET:HA	1:A:866:THR:HA	2.02	0.41
1:A:902:SER:HB2	1:A:970:VAL:HG21	2.03	0.41
1:A:917:SER:CB	1:A:920:GLN:HB2	2.50	0.41
1:B:73:PHE:C	1:B:75:LEU:N	2.77	0.41
1:B:422:ASP:HB2	1:B:442:GLU:OE1	2.21	0.41
1:B:788:ILE:HG12	1:B:791:GLN:NE2	2.36	0.41
1:B:878:GLU:CB	1:B:880:HIS:NE2	2.83	0.41
1:B:902:SER:O	1:B:970:VAL:HG13	2.20	0.41
1:A:67:LEU:O	1:A:71:ILE:N	2.43	0.41
1:A:298:ILE:HD12	1:A:299:ALA:N	2.35	0.41
1:A:413:LEU:CD1	1:A:564:LEU:CD1	2.99	0.41
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.91	0.41
1:A:581:SER:HA	1:A:584:PHE:CD1	2.56	0.41
1:A:716:ILE:N	1:A:716:ILE:CD1	2.80	0.41
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.82	0.41
1:B:145:ILE:HD11	1:B:223:VAL:CG2	2.49	0.41
1:B:246:LYS:HB3	1:B:250:GLN:HB2	2.03	0.41
1:B:274:ILE:HG21	1:B:780:ALA:HA	2.03	0.41
1:B:336:LEU:HB2	1:B:337:PRO:HD3	2.02	0.41
1:B:528:VAL:HG23	1:B:537:MET:HE2	2.03	0.41
1:B:737:ASP:OD2	1:B:739:ASN:HB2	2.21	0.41
1:B:855:TRP:HB2	1:B:896:PRO:HG3	2.03	0.41
1:B:873:PHE:CZ	1:B:881:PRO:CG	3.04	0.41
1:B:975:LEU:C	1:B:977:VAL:H	2.28	0.41
1:A:945:PHE:CZ	1:A:967:TRP:CZ2	3.09	0.41
1:B:200:VAL:O	1:B:204:LYS:HD2	2.21	0.41
1:B:366:MET:HE2	1:B:384:ILE:CD1	2.50	0.41
1:B:699:ALA:HB2	1:B:716:ILE:HG23	2.02	0.41
1:B:737:ASP:O	1:B:738:ASP:HB2	2.21	0.41
1:A:1:MET:HB2	1:A:36:TYR:CZ	2.56	0.40
1:A:49:LEU:CD1	1:A:52:LEU:N	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:O	1:A:120:LYS:HG3	2.21	0.40
1:A:953:LEU:HA	1:A:956:ILE:HG13	2.02	0.40
1:B:814:LEU:HD12	1:B:815:ASP:CA	2.52	0.40
1:B:857:MET:O	1:B:858:TYR:CD2	2.74	0.40
1:A:410:LEU:HB3	1:A:452:MET:CE	2.51	0.40
1:A:624:ILE:HG22	1:A:684:LYS:HG2	2.03	0.40
1:A:739:ASN:C	1:A:739:ASN:ND2	2.76	0.40
1:A:901:LEU:C	1:A:901:LEU:HD23	2.46	0.40
1:A:934:LEU:HD23	1:A:934:LEU:HA	1.77	0.40
1:B:267:ILE:HG23	1:B:302:LEU:HD21	2.02	0.40
1:B:419:LEU:O	1:B:481:LYS:HE2	2.21	0.40
1:B:566:THR:HG23	1:B:594:VAL:HG21	2.03	0.40
1:A:739:ASN:HB3	1:A:742:THR:HG22	2.03	0.40
1:A:921:SER:HA	1:A:985:LYS:CD	2.52	0.40
1:A:925:MET:HA	1:A:926:PRO:HD3	1.97	0.40
1:B:319:LEU:HA	1:B:319:LEU:HD23	1.83	0.40
1:B:398:ASN:O	1:B:399:ASP:HB2	2.20	0.40
1:B:427:PHE:CZ	1:B:464:LYS:HD3	2.56	0.40
1:A:24:LEU:HB2	1:A:149:ASP:HB3	2.03	0.40
1:A:51:GLU:OE1	1:A:54:ILE:HG13	2.22	0.40
1:A:57:PHE:HA	1:A:62:VAL:HG11	2.02	0.40
1:A:516:GLY:HA2	5:A:998:ACP:N3	2.36	0.40
1:A:524:ARG:HD3	1:A:585:MET:HE3	2.04	0.40
1:A:894:PRO:O	1:A:958:LYS:HB3	2.22	0.40
1:B:5:HIS:HD2	1:B:6:SER:CA	2.35	0.40
1:B:410:LEU:O	1:B:452:MET:HE1	2.21	0.40
1:B:545:ILE:HD13	1:B:545:ILE:HG21	1.84	0.40
1:B:624:ILE:HG22	1:B:679:VAL:HG21	2.03	0.40
1:B:951:ASP:C	1:B:953:LEU:H	2.30	0.40
1:A:43:ALA:O	1:A:44:GLU:C	2.62	0.40
1:A:179:ILE:HG22	1:A:212:THR:HG22	2.04	0.40
1:A:917:SER:OG	1:A:918:GLU:N	2.50	0.40
1:A:992:LEU:CG	1:A:993:GLU:N	2.85	0.40
1:B:340:GLU:HA	1:B:750:GLY:CA	2.51	0.40
1:B:835:PHE:HE2	1:B:984:LEU:HD21	1.86	0.40
1:B:934:LEU:C	1:B:936:SER:H	2.28	0.40

There are no symmetry-related clashes.

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%)	858 (86%)	106 (11%)	28 (3%)	4	21
1	B	992/994 (100%)	853 (86%)	110 (11%)	29 (3%)	3	20
All	All	1984/1988 (100%)	1711 (86%)	216 (11%)	57 (3%)	3	20

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	571	PRO
1	A	859	ALA
1	A	863	PRO
1	A	883	PHE
1	A	952	PRO
1	A	953	LEU
1	A	954	PRO
1	B	288	TRP
1	B	289	ILE
1	B	881	PRO
1	A	46	GLY
1	A	54	ILE
1	A	62	VAL
1	A	68	ALA
1	A	869	GLN
1	B	55	GLU
1	B	287	SER
1	B	785	GLU
1	B	813	ASP
1	B	863	PRO
1	B	867	TYR
1	B	876	CYS
1	B	885	GLY
1	A	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	275	ASN
1	A	276	ILE
1	A	770	GLY
1	A	888	CYS
1	B	644	GLU
1	B	663	LEU
1	B	714	ALA
1	B	887	ASP
1	B	948	LEU
1	B	957	PHE
1	A	80	GLU
1	A	287	SER
1	A	465	VAL
1	B	858	TYR
1	B	893	ALA
1	A	44	GLU
1	A	59	ASP
1	A	281	ASP
1	A	316	THR
1	B	510	ASN
1	B	638	ARG
1	B	739	ASN
1	B	880	HIS
1	A	87	ALA
1	B	281	ASP
1	B	293	ILE
1	B	950	VAL
1	A	951	ASP
1	B	812	PRO
1	B	247	THR
1	A	880	HIS
1	B	947	ILE

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%)	750 (89%)	90 (11%)	6	26
1	B	840/840 (100%)	745 (89%)	95 (11%)	5	24
All	All	1680/1680 (100%)	1495 (89%)	185 (11%)	6	25

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	24	LEU
1	A	34	GLU
1	A	48	SER
1	A	49	LEU
1	A	60	LEU
1	A	66	LEU
1	A	79	GLU
1	A	82	GLU
1	A	117	GLU
1	A	140	ILE
1	A	145	ILE
1	A	151	VAL
1	A	170	SER
1	A	171	THR
1	A	177	GLN
1	A	179	ILE
1	A	180	LEU
1	A	185	VAL
1	A	187	VAL
1	A	191	THR
1	A	238	GLN
1	A	247	THR
1	A	249	LEU
1	A	254	ASP
1	A	255	GLU
1	A	265	SER
1	A	300	VAL
1	A	304	VAL
1	A	315	ILE
1	A	347	VAL
1	A	368	ILE
1	A	384	ILE
1	A	401	PRO
1	A	402	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	426	ASP
1	A	437	VAL
1	A	441	THR
1	A	465	VAL
1	A	467	ARG
1	A	476	ARG
1	A	484	THR
1	A	494	MET
1	A	496	VAL
1	A	532	THR
1	A	535	VAL
1	A	556	ARG
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	577	VAL
1	A	578	LEU
1	A	582	SER
1	A	596	VAL
1	A	604	ARG
1	A	611	ILE
1	A	619	ILE
1	A	647	GLU
1	A	671	ARG
1	A	682	SER
1	A	691	LEU
1	A	705	VAL
1	A	716	ILE
1	A	722	SER
1	A	726	VAL
1	A	742	THR
1	A	743	ILE
1	A	747	VAL
1	A	760	PHE
1	A	761	ILE
1	A	764	LEU
1	A	765	ILE
1	A	778	THR
1	A	793	LEU
1	A	802	LEU
1	A	805	THR
1	A	815	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	828	LEU
1	A	830	SER
1	A	840	ILE
1	A	844	VAL
1	A	849	VAL
1	A	857	MET
1	A	872	HIS
1	A	898	THR
1	A	940	SER
1	A	947	ILE
1	A	948	LEU
1	A	956	ILE
1	A	970	VAL
1	B	5	HIS
1	B	10	GLU
1	B	18	VAL
1	B	21	THR
1	B	33	LEU
1	B	34	GLU
1	B	61	LEU
1	B	62	VAL
1	B	64	ILE
1	B	71	ILE
1	B	78	PHE
1	B	99	ILE
1	B	103	ILE
1	B	116	ILE
1	B	117	GLU
1	B	134	ARG
1	B	136	SER
1	B	139	ARG
1	B	145	ILE
1	B	151	VAL
1	B	155	VAL
1	B	174	ARG
1	B	178	SER
1	B	179	ILE
1	B	180	LEU
1	B	187	VAL
1	B	188	ILE
1	B	191	THR
1	B	228	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	255	GLU
1	B	267	ILE
1	B	273	LEU
1	B	300	VAL
1	B	323	THR
1	B	329	LYS
1	B	347	VAL
1	B	355	THR
1	B	379	LEU
1	B	384	ILE
1	B	387	SER
1	B	388	THR
1	B	395	VAL
1	B	400	LYS
1	B	402	ILE
1	B	433	VAL
1	B	436	LYS
1	B	437	VAL
1	B	449	VAL
1	B	460	ARG
1	B	467	ARG
1	B	478	LEU
1	B	482	GLU
1	B	484	THR
1	B	505	ARG
1	B	511	LYS
1	B	532	THR
1	B	533	THR
1	B	538	THR
1	B	559	LEU
1	B	566	THR
1	B	574	GLU
1	B	577	VAL
1	B	586	GLU
1	B	589	THR
1	B	596	VAL
1	B	605	LYS
1	B	611	ILE
1	B	624	ILE
1	B	633	ILE
1	B	639	ILE
1	B	675	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	678	ARG
1	B	698	THR
1	B	701	THR
1	B	705	VAL
1	B	716	ILE
1	B	722	SER
1	B	726	VAL
1	B	742	THR
1	B	765	ILE
1	B	773	VAL
1	B	790	VAL
1	B	840	ILE
1	B	844	VAL
1	B	857	MET
1	B	869	GLN
1	B	871	THR
1	B	873	PHE
1	B	874	MET
1	B	875	GLN
1	B	880	HIS
1	B	890	ILE
1	B	898	THR
1	B	923	MET
1	B	984	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	56	GLN
1	A	138	GLN
1	A	177	GLN
1	A	213	ASN
1	A	284	HIS
1	A	330	ASN
1	A	406	GLN
1	A	421	ASN
1	A	472	ASN
1	A	510	ASN
1	A	666	GLN
1	A	739	ASN
1	A	759	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	768	ASN
1	A	868	HIS
1	A	869	GLN
1	A	872	HIS
1	A	914	ASN
1	A	930	ASN
1	B	5	HIS
1	B	108	GLN
1	B	201	ASN
1	B	259	GLN
1	B	275	ASN
1	B	421	ASN
1	B	666	GLN
1	B	739	ASN
1	B	759	GLN
1	B	791	GLN
1	B	810	ASN
1	B	872	HIS
1	B	875	GLN
1	B	882	HIS
1	B	911	ASN
1	B	919	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACP	A	998	-	31,33,33	2.16	9 (29%)	47,52,52	2.13	14 (29%)
2	ALF	A	995	6,1	4,4,4	1.33	0	-		
5	ACP	B	998	-	31,33,33	2.43	9 (29%)	47,52,52	2.12	13 (27%)
2	ALF	B	995	6,1	4,4,4	1.24	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	ACP	A	998	-	-	5/19/38/38	0/3/3/3
5	ACP	B	998	-	-	4/19/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	998	ACP	PB-O3A	6.43	1.65	1.58
5	B	998	ACP	PA-O3A	5.78	1.65	1.59
5	B	998	ACP	PG-O1G	5.03	1.60	1.50
5	A	998	ACP	PG-O1G	5.02	1.60	1.50
5	A	998	ACP	C5-C4	4.48	1.47	1.39
5	A	998	ACP	PG-O3G	-4.36	1.45	1.55
5	B	998	ACP	PG-O3G	-4.21	1.45	1.55
5	A	998	ACP	PB-O3A	3.97	1.62	1.58
5	B	998	ACP	C5-C4	3.93	1.46	1.39
5	A	998	ACP	C8-N9	3.14	1.42	1.37
5	A	998	ACP	PA-O3A	3.12	1.62	1.59
5	B	998	ACP	C8-N9	3.06	1.42	1.37
5	B	998	ACP	PG-O2G	2.23	1.59	1.55
5	B	998	ACP	PB-O1B	-2.20	1.46	1.51
5	A	998	ACP	PB-O1B	-2.18	1.46	1.51
5	B	998	ACP	C4-N9	2.15	1.42	1.37
5	A	998	ACP	PG-O2G	2.07	1.59	1.55
5	A	998	ACP	PB-O2B	2.07	1.61	1.56

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	ACP	O4'-C1'-C2'	-6.44	92.84	106.62
5	B	998	ACP	O4'-C4'-C3'	-5.79	93.66	105.15
5	A	998	ACP	O4'-C1'-C2'	-5.73	94.36	106.62
5	B	998	ACP	O3'-C3'-C4'	5.44	126.71	111.08
5	A	998	ACP	O4'-C4'-C3'	-5.18	94.87	105.15
5	A	998	ACP	O3'-C3'-C4'	5.13	125.83	111.08
5	A	998	ACP	O2G-PG-O1G	-4.97	99.52	112.39
5	B	998	ACP	PB-O3A-PA	4.24	146.22	132.37
5	A	998	ACP	O2A-PA-O3A	-3.99	96.50	107.27
5	B	998	ACP	O2G-PG-O1G	-3.58	103.14	112.39
5	A	998	ACP	C2'-C1'-N9	3.27	121.42	113.30
5	B	998	ACP	O2A-PA-O3A	-3.20	98.62	107.27
5	A	998	ACP	O4'-C4'-C5'	-2.91	100.02	109.33
5	B	998	ACP	O3G-PG-O2G	2.90	116.23	107.96
5	A	998	ACP	O3G-PG-C3B	2.87	113.37	106.40
5	A	998	ACP	O3G-PG-O2G	2.86	116.12	107.96
5	B	998	ACP	N3-C4-N9	2.46	131.35	127.17
5	B	998	ACP	O3G-PG-C3B	2.46	112.36	106.40
5	A	998	ACP	C5-C4-N3	-2.44	123.35	126.72
5	B	998	ACP	O4'-C4'-C5'	-2.39	101.68	109.33
5	A	998	ACP	O4'-C1'-N9	-2.29	103.69	108.09
5	B	998	ACP	C5-C4-N3	-2.28	123.58	126.72
5	B	998	ACP	O3G-PG-O1G	-2.15	106.83	112.39
5	A	998	ACP	N3-C4-N9	2.10	130.74	127.17
5	B	998	ACP	C3'-C2'-C1'	2.10	105.43	101.46
5	A	998	ACP	C2'-C3'-C4'	2.09	106.65	102.61
5	A	998	ACP	O3G-PG-O1G	-2.01	107.19	112.39

There are no chirality outliers.

All (9) torsion outliers are listed below:

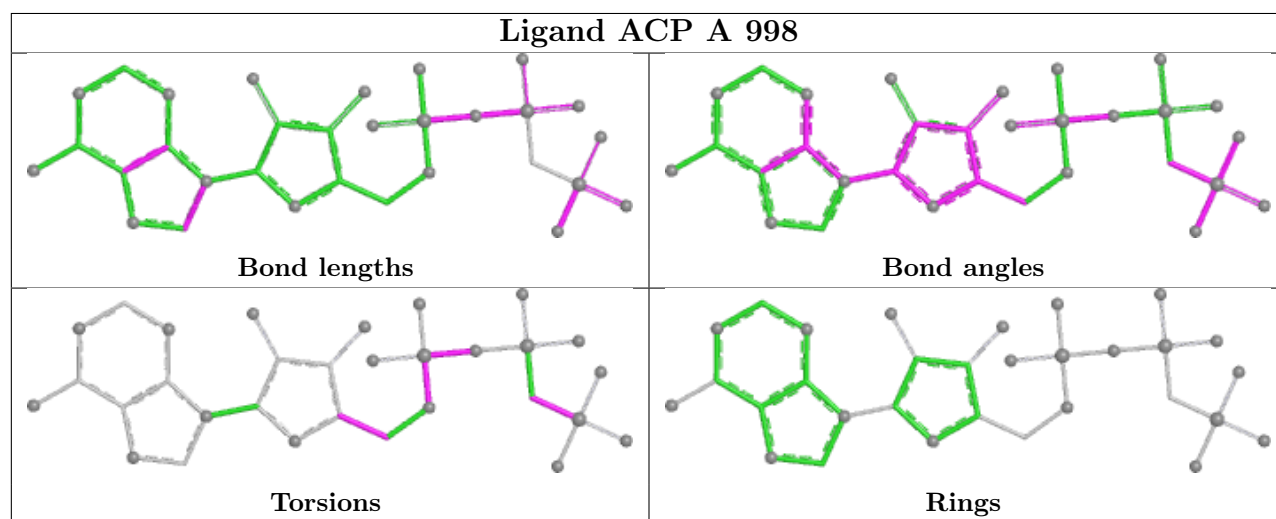
Mol	Chain	Res	Type	Atoms
5	A	998	ACP	C5'-O5'-PA-O1A
5	A	998	ACP	O4'-C4'-C5'-O5'
5	B	998	ACP	PB-C3B-PG-O2G
5	B	998	ACP	C5'-O5'-PA-O1A
5	B	998	ACP	O4'-C4'-C5'-O5'
5	A	998	ACP	C3'-C4'-C5'-O5'
5	A	998	ACP	PB-O3A-PA-O5'
5	B	998	ACP	PB-O3A-PA-O5'
5	A	998	ACP	PB-C3B-PG-O1G

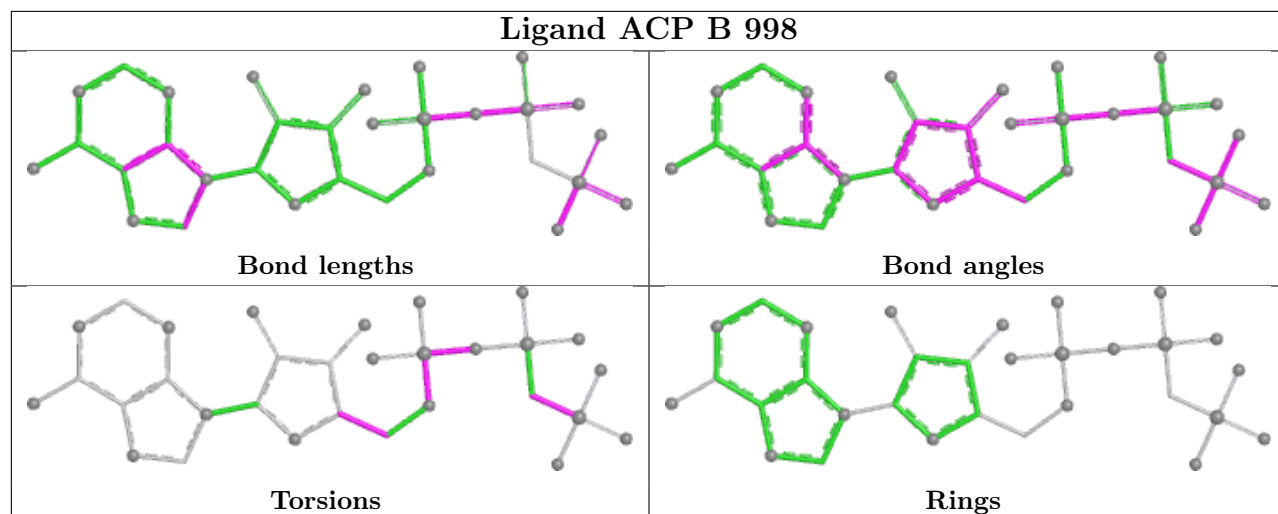
There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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%)	-0.61	2 (0%) 91 83	36, 86, 210, 329	0
1	B	994/994 (100%)	-0.42	8 (0%) 82 64	47, 108, 222, 298	0
All	All	1988/1988 (100%)	-0.51	10 (0%) 87 72	36, 97, 216, 329	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	959	LEU	2.8
1	A	853	ALA	2.7
1	B	861	ASP	2.7
1	B	990	ASN	2.6
1	B	855	TRP	2.4
1	B	868	HIS	2.2
1	A	883	PHE	2.2
1	B	507	ALA	2.1
1	B	992	LEU	2.1
1	B	50	TRP	2.1

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](#)

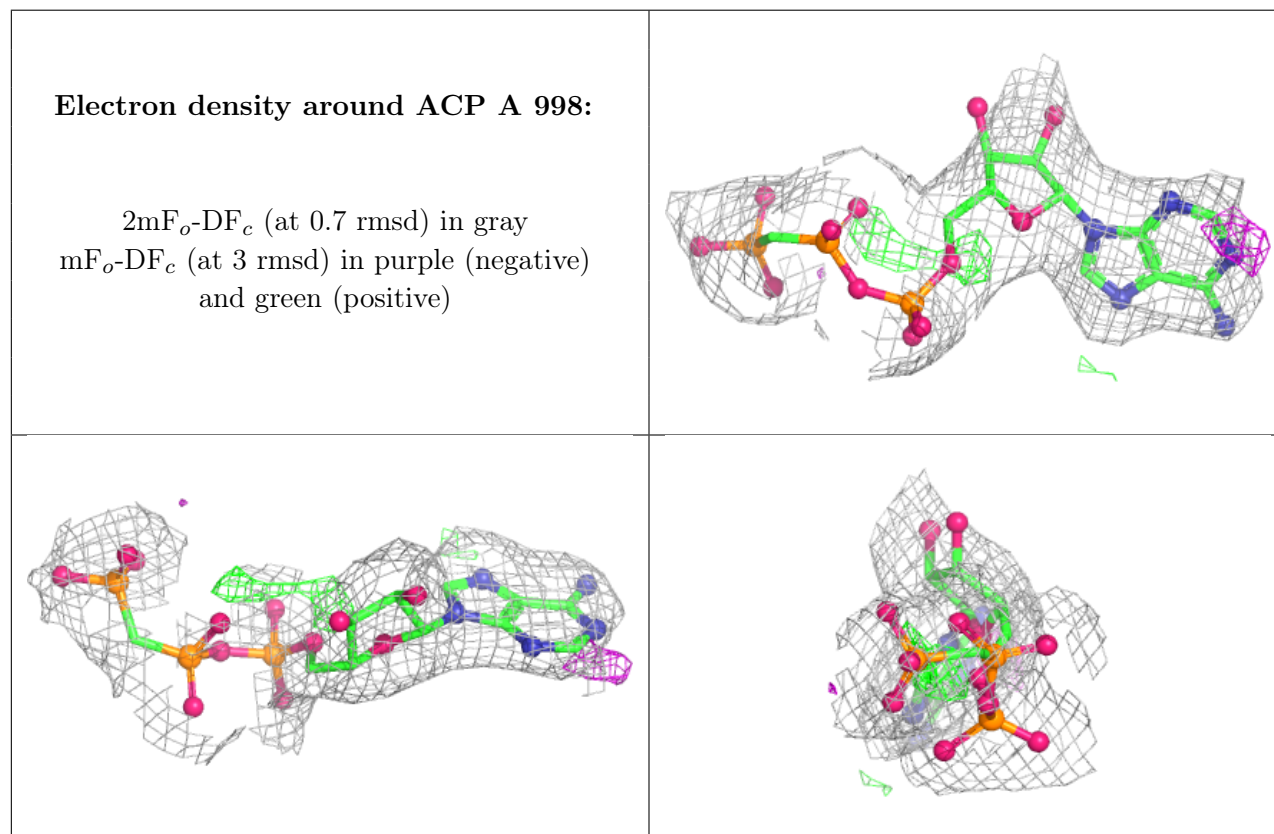
There are no oligosaccharides in this entry.

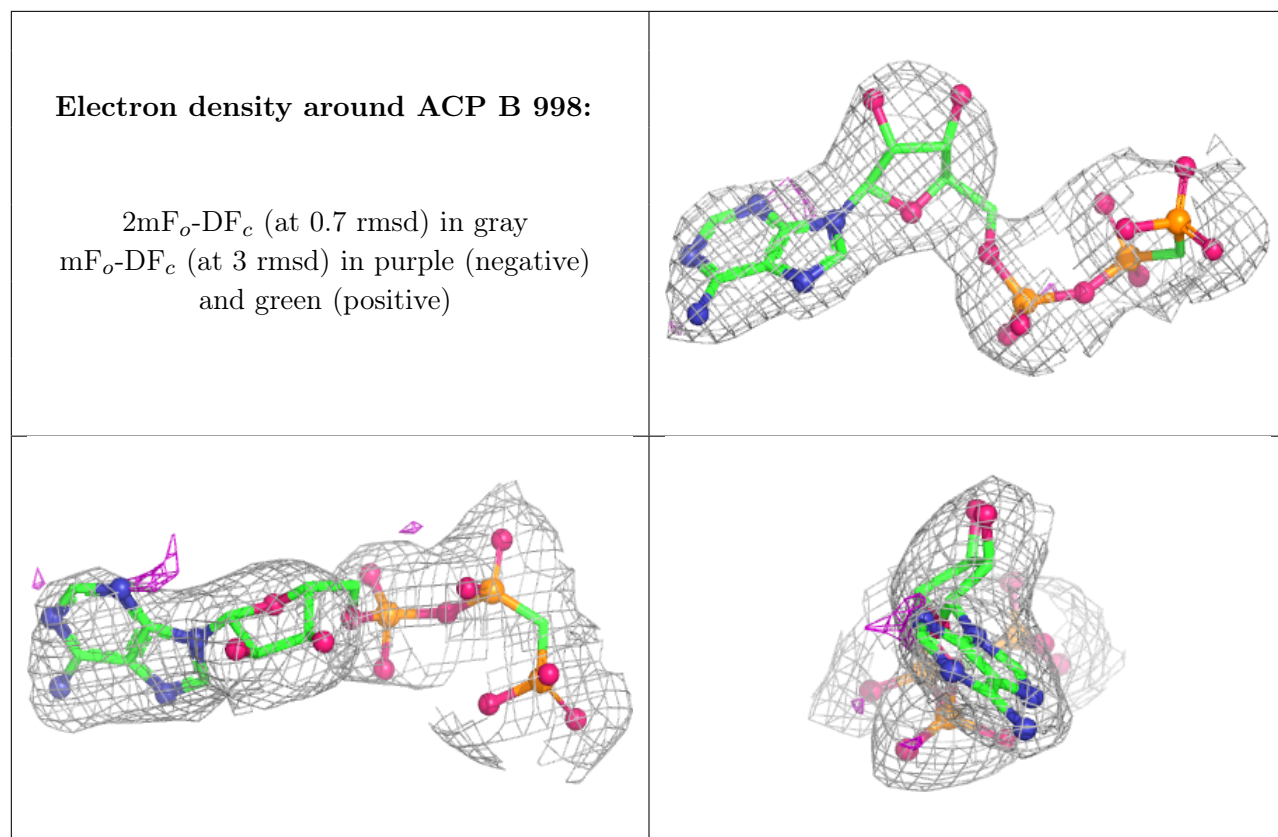
6.4 Ligands ⓘ

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
4	K	A	997	1/1	0.93	0.08	78,78,78,78	0
5	ACP	A	998	31/31	0.93	0.09	63,113,171,279	0
5	ACP	B	998	31/31	0.94	0.08	55,101,210,335	0
4	K	B	997	1/1	0.99	0.05	99,99,99,99	0
2	ALF	B	995	5/5	0.99	0.06	42,50,61,69	0
2	ALF	A	995	5/5	0.99	0.04	18,47,49,50	0
3	MG	A	996	1/1	1.00	0.04	23,23,23,23	0
3	MG	B	996	1/1	1.00	0.03	43,43,43,43	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.