Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 01:47 PM EDT

PDB ID	:	2BDI
Title	:	Human Kallikrein 4 complex with cobalt and p-aminobenzamidine
Authors	:	Debela, M.; Bode, W.; Goettig, P.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2005-10-20
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 (i) 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 (i)) were used in the production of this report:

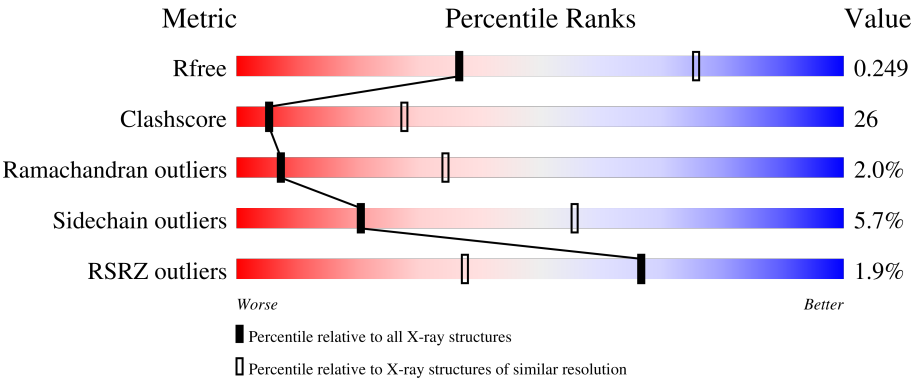
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	223	2% 51% 44%
1	B	223	3% 53% 43%
1	C	223	3% 51% 42% 6%
1	D	223	% 55% 41%
1	E	223	% 52% 44%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	223	52% 43%
1	G	223	50% 42% 8%
1	H	223	54% 41% 5%
1	I	223	52% 43%
1	J	223	50% 45%
1	K	223	53% 43%
1	L	223	52% 44%
1	M	223	54% 42%
1	N	223	52% 42% 5%
1	O	223	57% 40%
1	P	223	54% 41%

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
3	PBZ	A	701	-	X	-	-
3	PBZ	D	704	-	-	X	-
3	PBZ	L	712	-	X	-	-
3	PBZ	O	715	-	X	X	-
3	PBZ	P	716	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27340 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.

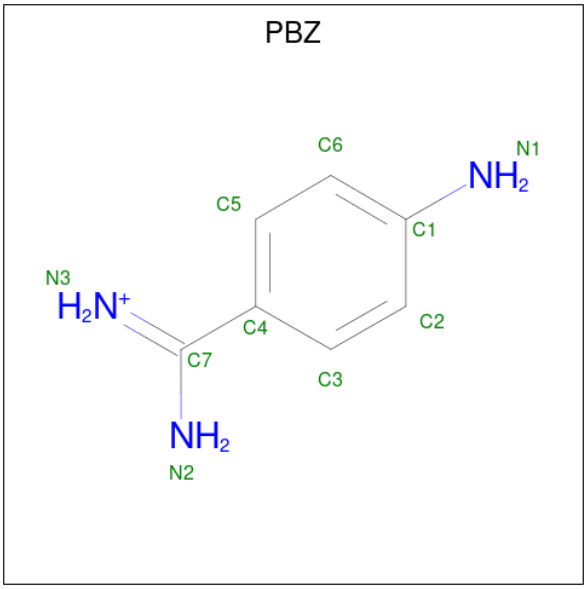
- Molecule 1 is a protein called Kallikrein-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	135	0	0
			1670	1043	281	329	17			
1	B	223	Total	C	N	O	S	80	0	0
			1670	1043	281	329	17			
1	C	223	Total	C	N	O	S	62	0	0
			1670	1043	281	329	17			
1	D	223	Total	C	N	O	S	91	0	0
			1670	1043	281	329	17			
1	E	223	Total	C	N	O	S	90	0	0
			1670	1043	281	329	17			
1	F	223	Total	C	N	O	S	54	0	0
			1670	1043	281	329	17			
1	G	223	Total	C	N	O	S	81	0	0
			1670	1043	281	329	17			
1	H	223	Total	C	N	O	S	120	0	0
			1670	1043	281	329	17			
1	I	223	Total	C	N	O	S	105	0	0
			1670	1043	281	329	17			
1	J	223	Total	C	N	O	S	56	0	0
			1670	1043	281	329	17			
1	K	223	Total	C	N	O	S	78	0	0
			1670	1043	281	329	17			
1	L	223	Total	C	N	O	S	73	0	0
			1670	1043	281	329	17			
1	M	223	Total	C	N	O	S	48	0	0
			1670	1043	281	329	17			
1	N	223	Total	C	N	O	S	63	0	0
			1670	1043	281	329	17			
1	O	223	Total	C	N	O	S	67	0	0
			1670	1043	281	329	17			
1	P	223	Total	C	N	O	S	86	0	0
			1670	1043	281	329	17			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	E	1	Total Co 1 1	0	0
2	I	1	Total Co 1 1	0	0
2	M	1	Total Co 1 1	0	0

- Molecule 3 is P-AMINO BENZAMIDINE (three-letter code: PBZ) (formula: $C_7H_{10}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 7 3	0	0
3	B	1	Total C N 10 7 3	0	0
3	C	1	Total C N 10 7 3	0	0
3	D	1	Total C N 10 7 3	0	0
3	E	1	Total C N 10 7 3	0	0
3	F	1	Total C N 10 7 3	0	0
3	G	1	Total C N 10 7 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C N 10 7 3	0	0
3	I	1	Total C N 10 7 3	0	0
3	J	1	Total C N 10 7 3	0	0
3	K	1	Total C N 10 7 3	0	0
3	L	1	Total C N 10 7 3	0	0
3	M	1	Total C N 10 7 3	0	0
3	N	1	Total C N 10 7 3	0	0
3	O	1	Total C N 10 7 3	0	0
3	P	1	Total C N 10 7 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	27	Total O 27 27	0	0
4	C	30	Total O 30 30	0	0
4	D	37	Total O 37 37	0	0
4	E	26	Total O 26 26	0	0
4	F	36	Total O 36 36	0	0
4	G	25	Total O 25 25	0	0
4	H	21	Total O 21 21	0	0
4	I	20	Total O 20 20	0	0
4	J	22	Total O 22 22	0	0

Continued on next page...

Continued from previous page...

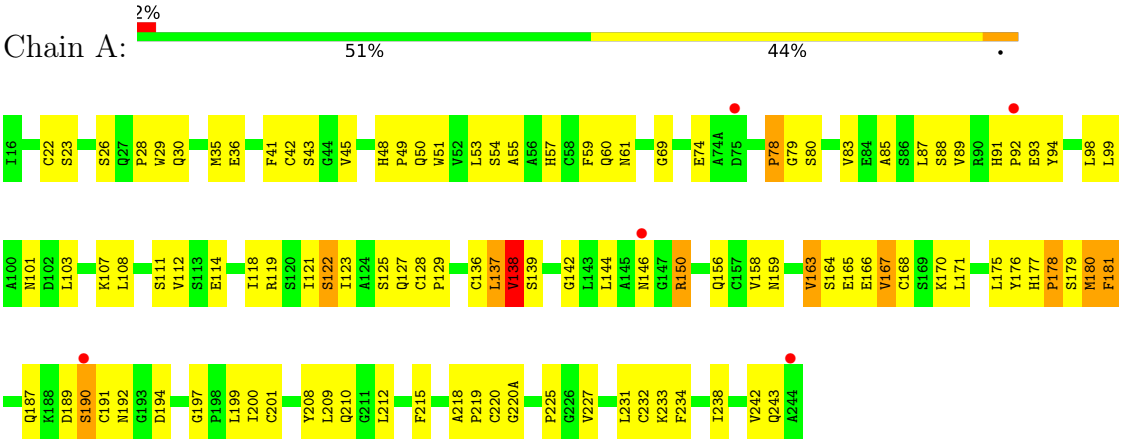
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	21	Total O 21 21	0	0
4	L	39	Total O 39 39	0	0
4	M	37	Total O 37 37	0	0
4	N	29	Total O 29 29	0	0
4	O	28	Total O 28 28	0	0
4	P	32	Total O 32 32	0	0

3 Residue-property plots (i)

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.

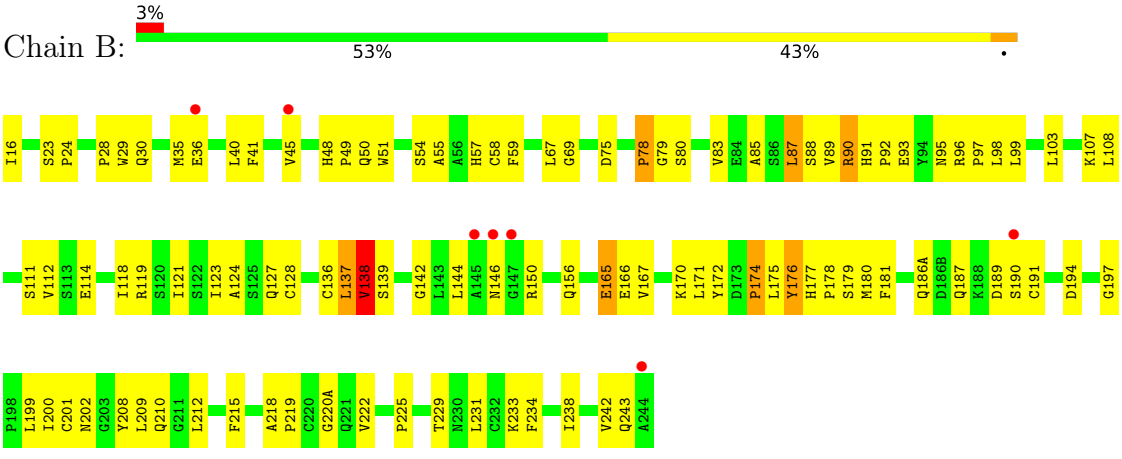
• Molecule 1: Kallikrein-4

Chain A:



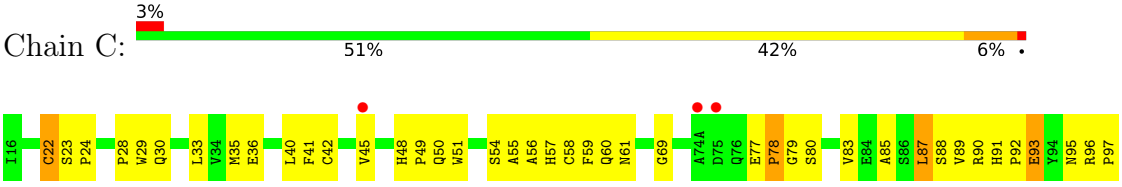
• Molecule 1: Kallikrein-4

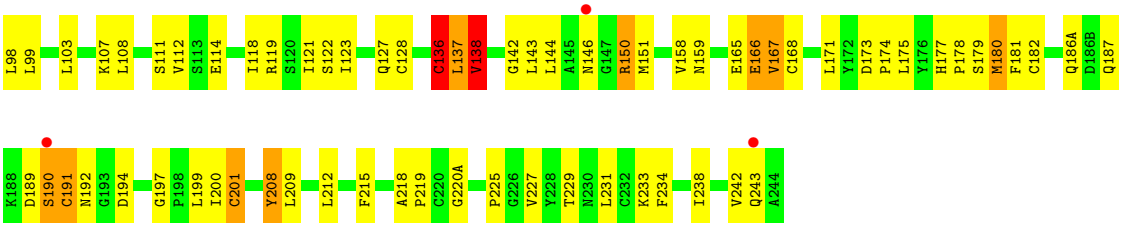
Chain B:



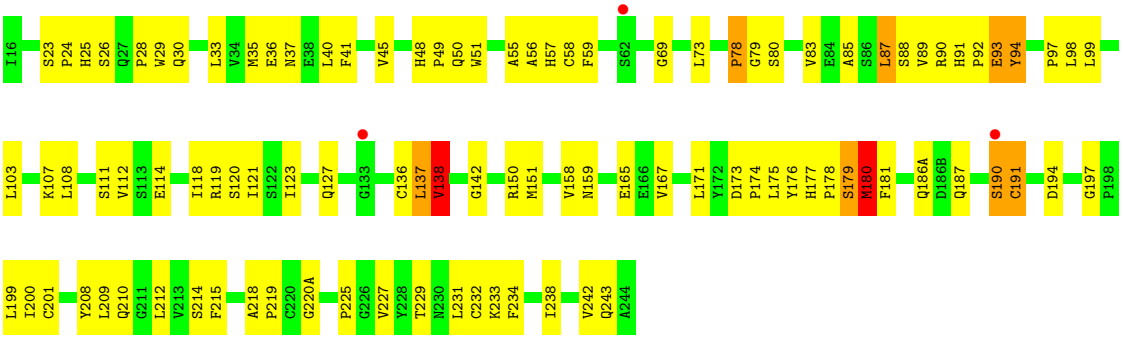
• Molecule 1: Kallikrein-4

Chain C:

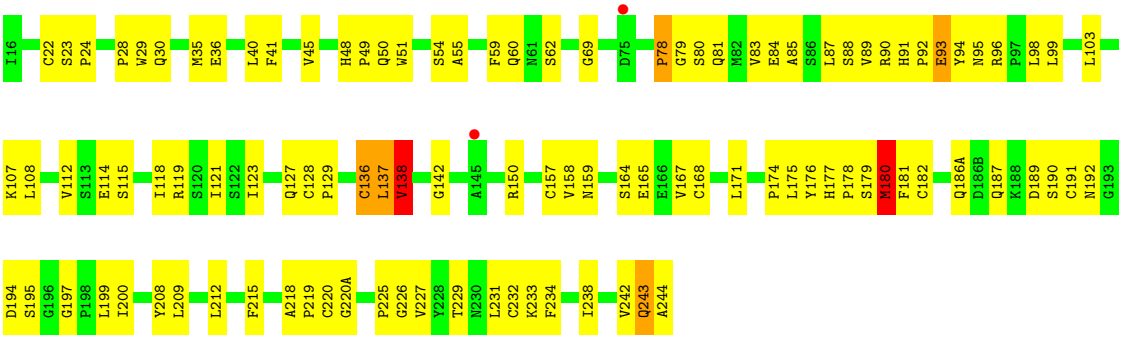




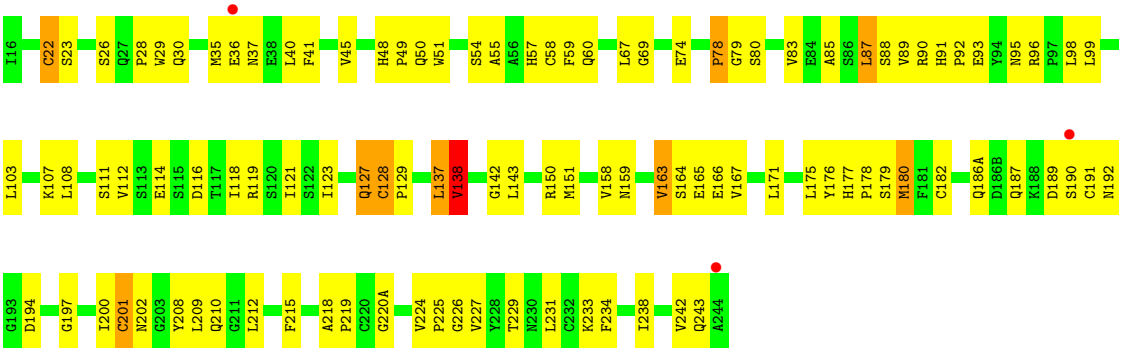
• Molecule 1: Kallikrein-4



• Molecule 1: Kallikrein-4

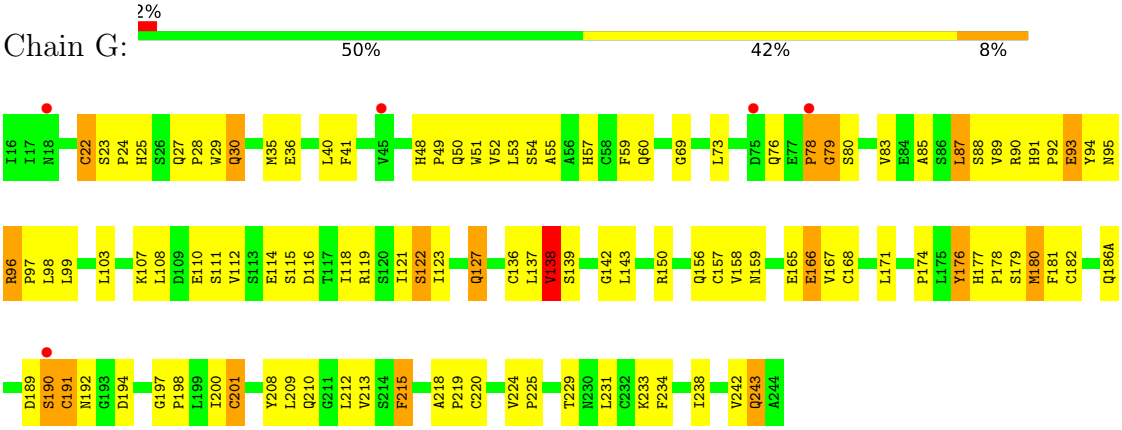


• Molecule 1: Kallikrein-4



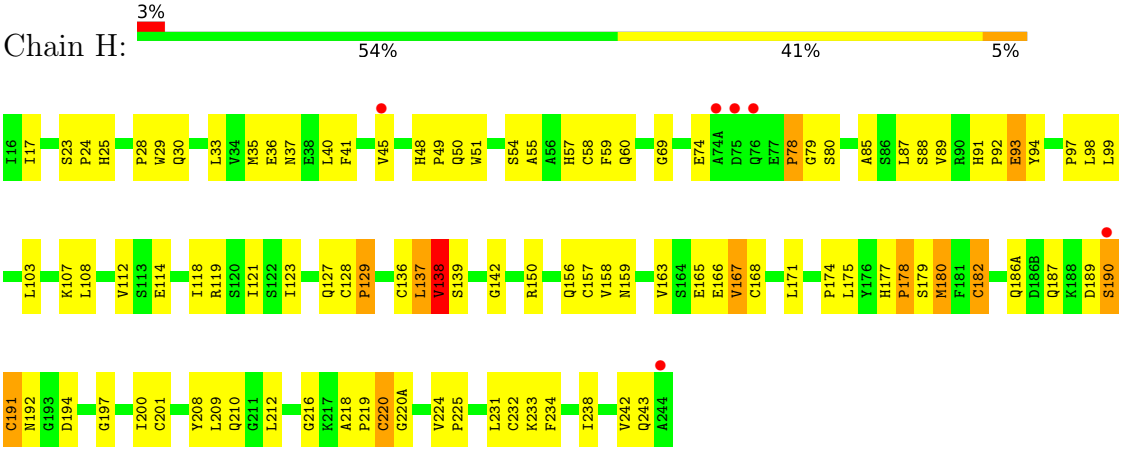
• Molecule 1: Kallikrein-4

Chain G:



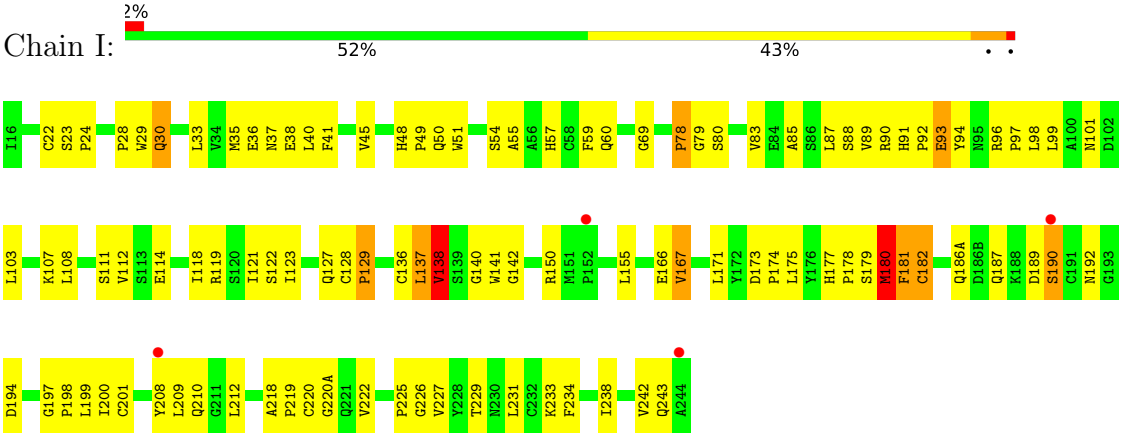
• Molecule 1: Kallikrein-4

Chain H:



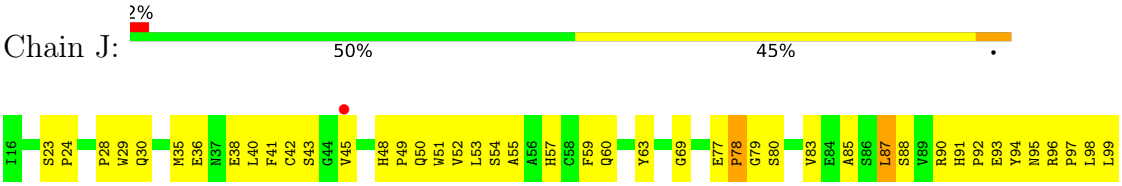
• Molecule 1: Kallikrein-4

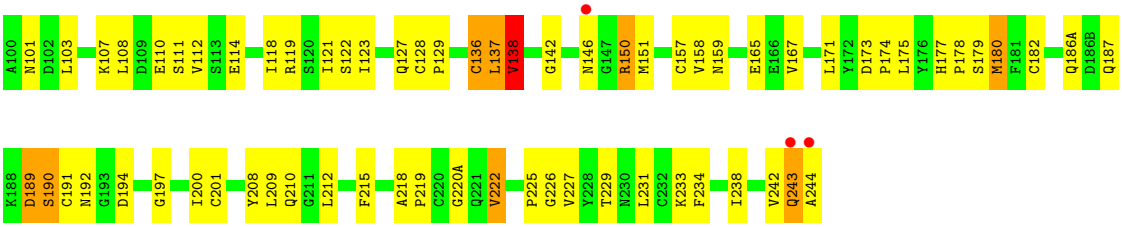
Chain I:



• Molecule 1: Kallikrein-4

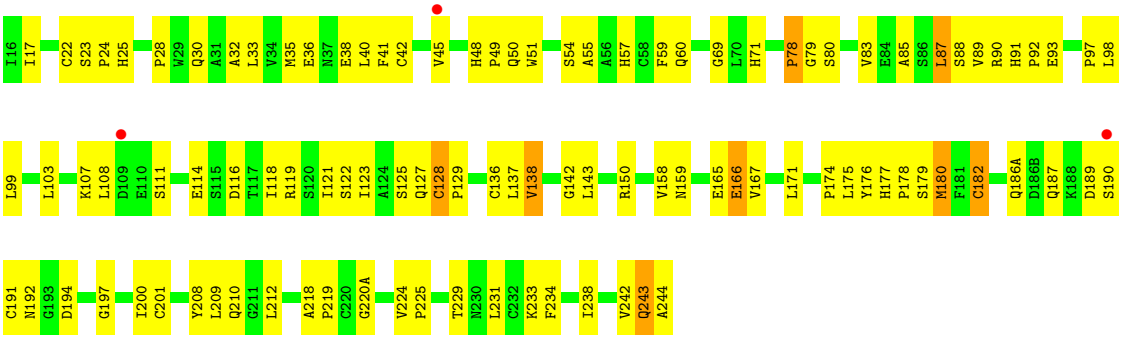
Chain J:





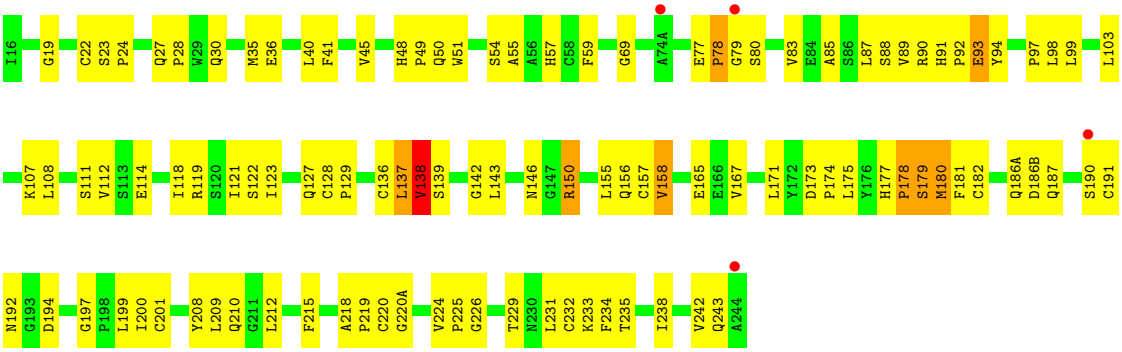
• Molecule 1: Kallikrein-4

Chain K:



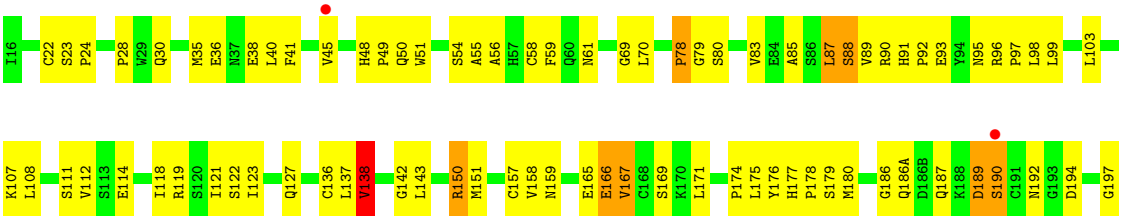
• Molecule 1: Kallikrein-4

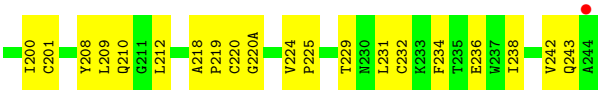
Chain L:



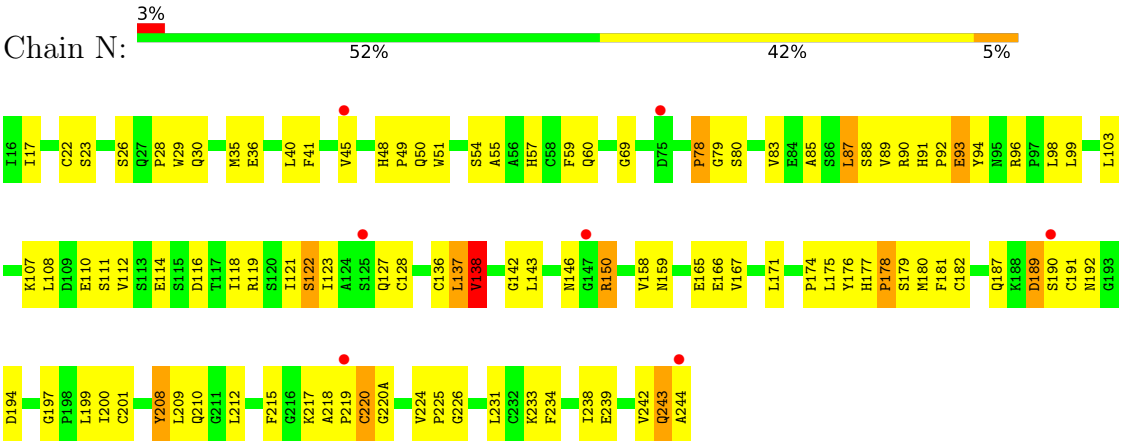
• Molecule 1: Kallikrein-4

Chain M:

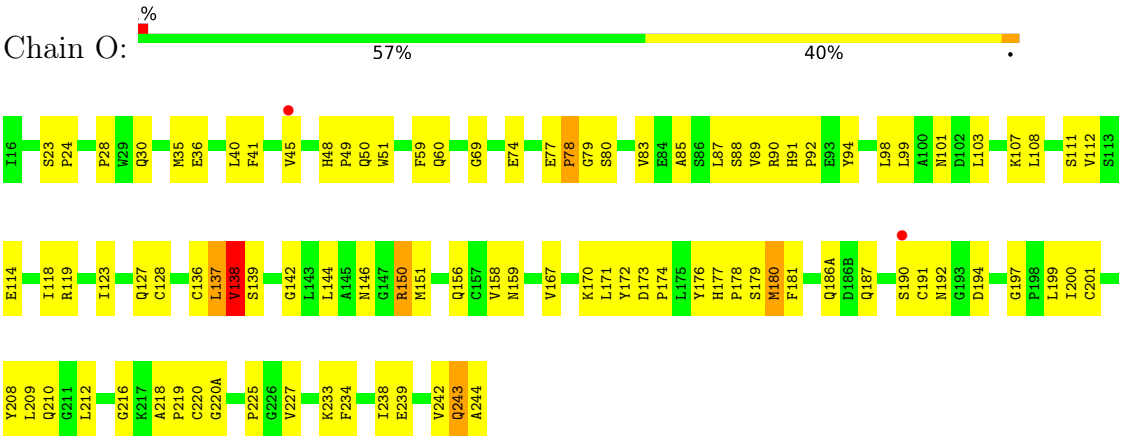




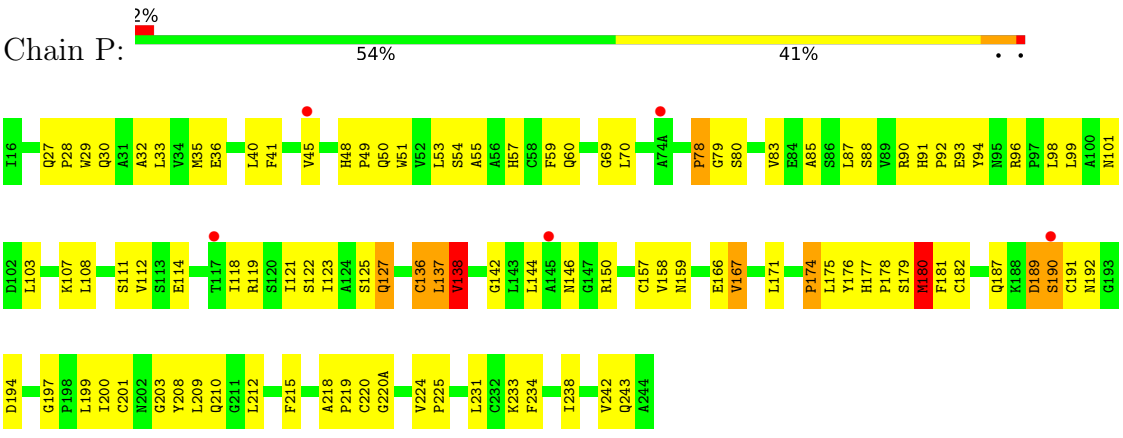
• Molecule 1: Kallikrein-4



• Molecule 1: Kallikrein-4



• Molecule 1: Kallikrein-4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	147.05Å 73.86Å 154.38Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	19.90 – 3.00 19.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.90-3.00) 96.6 (19.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.296 0.245 , 0.249	Depositor DCC
R_{free} test set	3199 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2048e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PBZ, CO

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	1.34	5/1707 (0.3%)	1.06	3/2323 (0.1%)
1	B	1.38	8/1707 (0.5%)	1.03	5/2323 (0.2%)
1	C	1.35	10/1707 (0.6%)	1.05	7/2323 (0.3%)
1	D	1.41	12/1707 (0.7%)	1.04	3/2323 (0.1%)
1	E	1.37	6/1707 (0.4%)	1.05	4/2323 (0.2%)
1	F	1.43	7/1707 (0.4%)	1.04	5/2323 (0.2%)
1	G	1.43	17/1707 (1.0%)	1.09	6/2323 (0.3%)
1	H	1.37	11/1707 (0.6%)	1.08	7/2323 (0.3%)
1	I	1.31	4/1707 (0.2%)	1.04	4/2323 (0.2%)
1	J	1.35	5/1707 (0.3%)	1.02	5/2323 (0.2%)
1	K	1.34	8/1707 (0.5%)	1.03	3/2323 (0.1%)
1	L	1.36	9/1707 (0.5%)	1.05	5/2323 (0.2%)
1	M	1.43	9/1707 (0.5%)	1.02	3/2323 (0.1%)
1	N	1.41	10/1707 (0.6%)	1.04	4/2323 (0.2%)
1	O	1.34	4/1707 (0.2%)	1.02	3/2323 (0.1%)
1	P	1.38	6/1707 (0.4%)	1.06	4/2323 (0.2%)
All	All	1.38	131/27312 (0.5%)	1.05	71/37168 (0.2%)

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	A	0	1
1	B	0	1
1	G	0	1
1	I	0	1
1	K	0	1
1	N	0	1
1	P	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	93	GLU	CD-OE1	9.43	1.36	1.25
1	G	201	CYS	CB-SG	9.03	1.97	1.82
1	J	167	VAL	CB-CG2	-8.77	1.34	1.52
1	C	167	VAL	CB-CG2	-8.74	1.34	1.52
1	B	167	VAL	CB-CG2	-8.60	1.34	1.52
1	M	167	VAL	CB-CG2	-8.51	1.34	1.52
1	D	167	VAL	CB-CG2	-7.88	1.36	1.52
1	L	191	CYS	CB-SG	7.71	1.95	1.82
1	D	180	MET	CG-SD	7.60	2.00	1.81
1	F	89	VAL	CB-CG2	-7.60	1.36	1.52
1	H	167	VAL	CB-CG2	-7.58	1.36	1.52
1	D	191	CYS	CB-SG	7.50	1.95	1.82
1	G	167	VAL	CB-CG2	-7.35	1.37	1.52
1	G	220	CYS	CB-SG	-7.34	1.69	1.82
1	H	191	CYS	CB-SG	7.29	1.94	1.82
1	E	167	VAL	CB-CG2	-7.21	1.37	1.52
1	B	89	VAL	CB-CG2	-7.21	1.37	1.52
1	F	93	GLU	CD-OE1	7.18	1.33	1.25
1	O	167	VAL	CB-CG2	-7.14	1.37	1.52
1	I	89	VAL	CB-CG2	-7.08	1.38	1.52
1	O	89	VAL	CB-CG2	-6.98	1.38	1.52
1	N	167	VAL	CB-CG2	-6.90	1.38	1.52
1	P	167	VAL	CB-CG2	-6.79	1.38	1.52
1	E	138	VAL	CB-CG1	-6.78	1.38	1.52
1	K	167	VAL	CB-CG2	-6.78	1.38	1.52
1	H	138	VAL	CB-CG1	-6.73	1.38	1.52
1	K	224	VAL	CB-CG2	-6.72	1.38	1.52
1	J	138	VAL	CB-CG1	-6.72	1.38	1.52
1	D	93	GLU	CD-OE1	6.71	1.33	1.25
1	N	224	VAL	CB-CG2	-6.70	1.38	1.52
1	L	89	VAL	CB-CG2	-6.67	1.38	1.52
1	A	167	VAL	CB-CG2	-6.67	1.38	1.52
1	H	93	GLU	CD-OE1	6.65	1.32	1.25
1	L	165	GLU	CG-CD	6.65	1.61	1.51
1	L	167	VAL	CB-CG2	-6.63	1.39	1.52
1	E	93	GLU	CD-OE2	6.61	1.32	1.25
1	N	89	VAL	CB-CG2	-6.58	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	VAL	CB-CG2	-6.55	1.39	1.52
1	M	236	GLU	CD-OE2	6.54	1.32	1.25
1	G	180	MET	CG-SD	6.54	1.98	1.81
1	M	169	SER	CB-OG	-6.53	1.33	1.42
1	G	93	GLU	CD-OE1	6.50	1.32	1.25
1	M	22	CYS	CB-SG	-6.41	1.71	1.82
1	A	93	GLU	CD-OE1	6.36	1.32	1.25
1	F	167	VAL	CB-CG2	-6.33	1.39	1.52
1	C	166	GLU	CD-OE2	6.22	1.32	1.25
1	C	138	VAL	CB-CG1	-6.22	1.39	1.52
1	M	93	GLU	CD-OE2	6.20	1.32	1.25
1	G	22	CYS	CA-C	6.18	1.69	1.52
1	N	128	CYS	CA-CB	-6.14	1.40	1.53
1	M	166	GLU	CG-CD	6.14	1.61	1.51
1	I	167	VAL	CB-CG2	-6.10	1.40	1.52
1	C	97	PRO	CA-C	-6.08	1.40	1.52
1	H	97	PRO	CA-C	-6.07	1.40	1.52
1	A	89	VAL	CB-CG2	-6.03	1.40	1.52
1	O	172	TYR	CE2-CZ	-6.02	1.30	1.38
1	L	138	VAL	CB-CG1	-5.97	1.40	1.52
1	D	165	GLU	CD-OE2	5.93	1.32	1.25
1	G	89	VAL	CB-CG2	-5.91	1.40	1.52
1	G	176	TYR	CG-CD2	5.86	1.46	1.39
1	L	179	SER	CB-OG	-5.85	1.34	1.42
1	M	89	VAL	CB-CG2	-5.84	1.40	1.52
1	N	220	CYS	CB-SG	-5.83	1.72	1.81
1	A	168	CYS	CB-SG	5.83	1.92	1.82
1	C	93	GLU	CD-OE1	5.82	1.32	1.25
1	P	136	CYS	C-O	-5.82	1.12	1.23
1	K	93	GLU	CD-OE1	5.82	1.32	1.25
1	N	93	GLU	CD-OE1	5.81	1.32	1.25
1	D	138	VAL	CB-CG1	-5.80	1.40	1.52
1	D	97	PRO	CA-C	-5.80	1.41	1.52
1	H	165	GLU	CG-CD	5.80	1.60	1.51
1	K	182	CYS	CB-SG	-5.78	1.72	1.81
1	K	89	VAL	CB-CG2	-5.75	1.40	1.52
1	E	180	MET	CG-SD	5.74	1.96	1.81
1	C	136	CYS	CA-CB	-5.71	1.41	1.53
1	B	124	ALA	CA-CB	-5.70	1.40	1.52
1	C	89	VAL	CB-CG2	-5.67	1.41	1.52
1	D	165	GLU	CD-OE1	5.66	1.31	1.25
1	P	93	GLU	CD-OE1	5.65	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	GLU	CD-OE1	5.62	1.31	1.25
1	H	128	CYS	CB-SG	5.61	1.91	1.82
1	F	138	VAL	CB-CG1	-5.59	1.41	1.52
1	H	89	VAL	CB-CG2	-5.59	1.41	1.52
1	J	93	GLU	CG-CD	5.56	1.60	1.51
1	P	224	VAL	CB-CG2	-5.51	1.41	1.52
1	G	52	VAL	CA-CB	-5.48	1.43	1.54
1	C	191	CYS	C-O	-5.46	1.12	1.23
1	I	180	MET	CG-SD	5.46	1.95	1.81
1	D	214	SER	CB-OG	-5.43	1.35	1.42
1	F	163	VAL	CA-CB	-5.43	1.43	1.54
1	P	96	ARG	CG-CD	5.42	1.65	1.51
1	M	224	VAL	CB-CG2	-5.42	1.41	1.52
1	A	163	VAL	CA-CB	-5.40	1.43	1.54
1	E	89	VAL	CB-CG2	-5.40	1.41	1.52
1	F	224	VAL	CB-CG2	-5.40	1.41	1.52
1	K	166	GLU	CD-OE2	5.39	1.31	1.25
1	L	97	PRO	CA-C	-5.37	1.42	1.52
1	P	180	MET	CG-SD	5.35	1.95	1.81
1	J	136	CYS	C-O	5.34	1.33	1.23
1	D	179	SER	CB-OG	-5.33	1.35	1.42
1	E	164	SER	CB-OG	-5.33	1.35	1.42
1	H	93	GLU	CD-OE2	5.33	1.31	1.25
1	M	138	VAL	CB-CG1	-5.31	1.41	1.52
1	G	138	VAL	CB-CG1	-5.26	1.41	1.52
1	F	201	CYS	CA-CB	5.26	1.65	1.53
1	O	172	TYR	CG-CD1	-5.25	1.32	1.39
1	G	224	VAL	CB-CG2	-5.25	1.41	1.52
1	N	96	ARG	CG-CD	5.25	1.65	1.51
1	B	58	CYS	CB-SG	-5.21	1.73	1.81
1	G	96	ARG	CG-CD	5.21	1.65	1.51
1	G	215	PHE	CB-CG	-5.20	1.42	1.51
1	H	220	CYS	C-O	-5.20	1.13	1.23
1	B	172	TYR	CE1-CZ	-5.16	1.31	1.38
1	C	208	TYR	CE1-CZ	5.16	1.45	1.38
1	G	166	GLU	CG-CD	5.16	1.59	1.51
1	N	138	VAL	CB-CG1	-5.16	1.42	1.52
1	B	165	GLU	CG-CD	5.13	1.59	1.51
1	G	213	VAL	CB-CG2	-5.13	1.42	1.52
1	D	94	TYR	C-O	-5.11	1.13	1.23
1	N	166	GLU	CG-CD	5.10	1.59	1.51
1	N	208	TYR	CE1-CZ	5.10	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	VAL	CB-CG1	-5.09	1.42	1.52
1	K	97	PRO	CA-C	-5.09	1.42	1.52
1	C	128	CYS	CB-SG	5.08	1.90	1.82
1	K	138	VAL	CB-CG1	-5.08	1.42	1.52
1	J	52	VAL	CA-CB	-5.08	1.44	1.54
1	G	168	CYS	C-O	-5.07	1.13	1.23
1	H	224	VAL	CB-CG2	-5.05	1.42	1.52
1	I	93	GLU	CD-OE1	5.04	1.31	1.25
1	G	224	VAL	CB-CG1	-5.02	1.42	1.52
1	L	224	VAL	CB-CG2	-5.00	1.42	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	157	CYS	CA-CB-SG	-10.44	95.21	114.00
1	G	22	CYS	CA-CB-SG	-9.62	96.67	114.00
1	A	22	CYS	CA-CB-SG	8.11	128.59	114.00
1	N	128	CYS	CA-CB-SG	-7.46	100.58	114.00
1	C	22	CYS	CA-CB-SG	-7.44	100.60	114.00
1	M	22	CYS	CB-CA-C	-7.36	95.68	110.40
1	P	182	CYS	CA-CB-SG	7.31	127.15	114.00
1	E	189	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	E	138	VAL	CG1-CB-CG2	-6.69	100.20	110.90
1	B	138	VAL	CG1-CB-CG2	-6.65	100.27	110.90
1	H	138	VAL	CG1-CB-CG2	-6.62	100.31	110.90
1	G	189	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	H	182	CYS	CB-CA-C	-6.59	97.23	110.40
1	E	168	CYS	CA-CB-SG	6.58	125.85	114.00
1	A	189	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	L	173	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	G	191	CYS	CA-CB-SG	-6.44	102.41	114.00
1	O	138	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	G	201	CYS	CA-CB-SG	6.43	125.58	114.00
1	G	138	VAL	CG1-CB-CG2	-6.39	100.67	110.90
1	F	128	CYS	CA-CB-SG	-6.27	102.72	114.00
1	A	138	VAL	CG1-CB-CG2	-6.25	100.90	110.90
1	H	157	CYS	CA-CB-SG	-6.24	102.77	114.00
1	K	128	CYS	CA-CB-SG	-6.22	102.81	114.00
1	P	189	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	F	138	VAL	CG1-CB-CG2	-6.14	101.08	110.90
1	M	189	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	J	157	CYS	CA-CB-SG	-6.00	103.20	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	CYS	CA-CB-SG	5.99	124.79	114.00
1	G	220	CYS	CA-CB-SG	-5.95	103.29	114.00
1	O	128	CYS	CA-CB-SG	-5.88	103.41	114.00
1	M	138	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	F	22	CYS	N-CA-CB	5.79	121.02	110.60
1	I	182	CYS	CA-CB-SG	5.71	124.27	114.00
1	L	232	CYS	CA-CB-SG	-5.66	103.82	114.00
1	B	90	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	P	138	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	B	189	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	C	136	CYS	CB-CA-C	-5.57	99.26	110.40
1	H	189	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	H	168	CYS	CB-CA-C	5.54	121.47	110.40
1	H	168	CYS	N-CA-CB	-5.54	100.64	110.60
1	J	138	VAL	CG1-CB-CG2	-5.52	102.07	110.90
1	K	182	CYS	CB-CA-C	-5.52	99.37	110.40
1	N	189	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	N	138	VAL	CG1-CB-CG2	-5.47	102.15	110.90
1	L	186(B)	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	H	232	CYS	CA-CB-SG	-5.46	104.17	114.00
1	D	173	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	F	189	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	L	138	VAL	CG1-CB-CG2	-5.38	102.30	110.90
1	D	138	VAL	CG1-CB-CG2	-5.32	102.38	110.90
1	L	220	CYS	CA-CB-SG	-5.32	104.43	114.00
1	C	42	CYS	CA-CB-SG	5.30	123.55	114.00
1	J	173	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	J	189	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	173	ASP	CB-CG-OD1	-5.29	113.53	118.30
1	I	173	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	F	201	CYS	CA-CB-SG	5.25	123.44	114.00
1	C	138	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	O	173	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	222	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	I	138	VAL	CG1-CB-CG2	-5.17	102.64	110.90
1	K	189	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	N	22	CYS	CA-CB-SG	5.13	123.23	114.00
1	B	128	CYS	CA-CB-SG	-5.12	104.78	114.00
1	D	232	CYS	CA-CB-SG	-5.10	104.82	114.00
1	I	222	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	E	136	CYS	CA-CB-SG	-5.04	104.94	114.00
1	J	222	VAL	CG1-CB-CG2	-5.03	102.85	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	201	CYS	CB-CA-C	5.02	120.43	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	PHE	Sidechain
1	B	176	TYR	Sidechain
1	G	181	PHE	Sidechain
1	I	181	PHE	Sidechain
1	K	176	TYR	Sidechain
1	N	176	TYR	Sidechain
1	P	176	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1598	87	0
1	B	1670	0	1598	81	3
1	C	1670	0	1598	90	3
1	D	1670	0	1598	85	0
1	E	1670	0	1600	80	1
1	F	1670	0	1598	86	1
1	G	1670	0	1602	112	1
1	H	1670	0	1598	72	2
1	I	1670	0	1598	83	1
1	J	1670	0	1598	95	0
1	K	1670	0	1598	86	0
1	L	1670	0	1598	80	0
1	M	1670	0	1598	81	0
1	N	1670	0	1600	88	1
1	O	1670	0	1598	76	1
1	P	1670	0	1598	95	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1	0	0	0	0
3	A	10	0	10	2	0
3	B	10	0	10	2	0
3	C	10	0	10	0	0
3	D	10	0	10	7	0
3	E	10	0	10	2	0
3	F	10	0	10	1	0
3	G	10	0	10	2	0
3	H	10	0	8	5	0
3	I	10	0	10	2	0
3	J	10	0	10	2	0
3	K	10	0	10	0	0
3	L	10	0	10	1	0
3	M	10	0	10	2	0
3	N	10	0	10	2	0
3	O	10	0	10	8	0
3	P	10	0	10	6	0
4	A	26	0	0	7	0
4	B	27	0	0	5	0
4	C	30	0	0	3	1
4	D	37	0	0	6	0
4	E	26	0	0	6	0
4	F	36	0	0	8	1
4	G	25	0	0	11	0
4	H	21	0	0	4	0
4	I	20	0	0	7	0
4	J	22	0	0	6	0
4	K	21	0	0	2	1
4	L	39	0	0	8	1
4	M	37	0	0	5	0
4	N	29	0	0	6	0
4	O	28	0	0	1	0
4	P	32	0	0	15	0
All	All	27340	0	25734	1310	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (1310) 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:J:110:GLU:HA	4:J:731:HOH:O	1.31	1.21
1:B:136:CYS:HB3	1:B:200:ILE:O	1.40	1.20
1:I:96:ARG:NH1	4:I:719:HOH:O	1.91	1.02
1:G:116:ASP:HA	4:G:724:HOH:O	1.59	1.02
1:G:243:GLN:HG2	1:K:243:GLN:HB3	1.39	1.01
1:J:77:GLU:OE2	4:J:711:HOH:O	1.79	1.00
1:N:110:GLU:HA	4:N:733:HOH:O	1.61	0.99
1:G:115:SER:CB	1:N:90:ARG:HH22	1.76	0.98
1:G:73:LEU:N	4:G:715:HOH:O	1.94	0.97
1:G:115:SER:HB2	1:N:90:ARG:HH22	1.27	0.97
1:G:243:GLN:HG3	1:K:244:ALA:HB2	1.47	0.95
1:D:83:VAL:HG22	4:D:722:HOH:O	1.66	0.94
1:F:37:ASN:HB3	4:F:728:HOH:O	1.67	0.94
1:A:61:ASN:OD1	4:A:721:HOH:O	1.86	0.92
1:L:98:LEU:O	4:L:750:HOH:O	1.87	0.92
1:C:136:CYS:HB3	1:C:200:ILE:O	1.67	0.92
1:G:110:GLU:OE1	1:N:87:LEU:HG	1.68	0.92
1:P:78:PRO:HG3	4:P:735:HOH:O	1.70	0.91
1:O:77:GLU:OE2	4:O:716:HOH:O	1.88	0.90
1:O:216:GLY:HA3	3:O:715:PBZ:N2	1.86	0.89
1:M:186:GLY:O	4:M:721:HOH:O	1.90	0.89
1:C:77:GLU:OE2	4:C:715:HOH:O	1.89	0.89
1:B:234:PHE:HA	4:B:703:HOH:O	1.73	0.88
1:C:150:ARG:HD3	1:C:151:MET:H	1.37	0.88
1:G:243:GLN:HG2	1:K:244:ALA:H	1.40	0.87
1:L:27:GLN:OE1	4:L:736:HOH:O	1.93	0.86
1:G:208:TYR:CE2	1:K:125:SER:OG	2.28	0.85
1:N:217:LYS:NZ	4:N:725:HOH:O	2.04	0.85
1:E:234:PHE:O	1:E:238:ILE:HG13	1.77	0.84
1:K:177:HIS:HD2	1:K:179:SER:OG	1.61	0.84
1:G:191:CYS:SG	1:G:192:ASN:N	2.50	0.83
1:M:150:ARG:HD3	1:M:151:MET:H	1.43	0.83
1:P:234:PHE:O	1:P:238:ILE:HG13	1.78	0.83
1:F:177:HIS:HD2	1:F:179:SER:OG	1.62	0.82
1:G:186(A):GLN:HG2	1:H:57:HIS:CG	2.14	0.82
1:G:186(A):GLN:HG2	1:H:57:HIS:CD2	2.14	0.82
1:P:78:PRO:CG	4:P:735:HOH:O	2.25	0.82
1:B:201:CYS:HB2	1:B:210:GLN:HE21	1.45	0.82
1:J:150:ARG:HD3	1:J:151:MET:H	1.42	0.82
1:O:150:ARG:HD3	1:O:151:MET:H	1.44	0.82
1:I:187:GLN:HG2	1:I:220(A):GLY:O	1.80	0.81
1:K:136:CYS:HB3	1:K:200:ILE:O	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:177:HIS:HD2	1:L:179:SER:OG	1.64	0.81
1:M:97:PRO:HB2	4:M:731:HOH:O	1.79	0.80
1:H:177:HIS:HD2	1:H:179:SER:OG	1.64	0.80
1:E:177:HIS:HD2	1:E:179:SER:OG	1.63	0.80
1:O:177:HIS:HD2	1:O:179:SER:OG	1.65	0.80
1:C:166:GLU:OE2	1:E:176:TYR:HE1	1.64	0.80
1:D:37:ASN:O	4:D:716:HOH:O	2.00	0.80
1:D:234:PHE:O	1:D:238:ILE:HG13	1.82	0.80
1:A:136:CYS:HB3	1:A:200:ILE:O	1.82	0.80
1:N:177:HIS:HD2	1:N:179:SER:OG	1.66	0.79
1:A:125:SER:OG	4:A:725:HOH:O	1.99	0.79
1:J:97:PRO:HB2	4:J:724:HOH:O	1.82	0.79
1:G:177:HIS:HD2	1:G:179:SER:OG	1.66	0.79
1:O:234:PHE:O	1:O:238:ILE:HG13	1.81	0.79
1:O:216:GLY:HA3	3:O:715:PBZ:HN22	1.43	0.79
1:M:187:GLN:HG2	1:M:220(A):GLY:O	1.83	0.78
1:I:177:HIS:HD2	1:I:179:SER:OG	1.66	0.78
1:D:187:GLN:HG2	1:D:220(A):GLY:O	1.84	0.78
1:D:190:SER:HB2	3:D:704:PBZ:HN22	1.46	0.78
1:P:177:HIS:HD2	1:P:179:SER:OG	1.66	0.78
1:A:234:PHE:O	1:A:238:ILE:HG13	1.84	0.78
1:C:177:HIS:HD2	1:C:179:SER:OG	1.66	0.78
1:J:187:GLN:HG2	1:J:220(A):GLY:O	1.83	0.78
1:G:115:SER:HB2	1:N:90:ARG:NH2	1.98	0.78
1:C:150:ARG:HD3	1:C:151:MET:N	1.97	0.78
1:P:215:PHE:HA	3:P:716:PBZ:C2	2.14	0.78
1:J:177:HIS:HD2	1:J:179:SER:OG	1.64	0.77
1:J:136:CYS:HB3	1:J:200:ILE:O	1.85	0.77
1:P:215:PHE:HA	3:P:716:PBZ:H2	1.67	0.77
1:F:242:VAL:O	4:F:713:HOH:O	2.01	0.76
1:P:78:PRO:CD	4:P:735:HOH:O	2.33	0.76
1:C:93:GLU:HB3	4:C:710:HOH:O	1.84	0.76
1:H:187:GLN:HG2	1:H:220(A):GLY:O	1.85	0.76
1:M:150:ARG:HD3	1:M:151:MET:N	2.00	0.76
1:P:78:PRO:N	4:P:735:HOH:O	2.19	0.76
1:B:57:HIS:NE2	4:B:708:HOH:O	2.19	0.76
1:N:187:GLN:HG2	1:N:220(A):GLY:O	1.85	0.76
1:J:234:PHE:O	1:J:238:ILE:HG13	1.86	0.75
1:K:166:GLU:OE2	1:M:176:TYR:HE1	1.68	0.75
1:J:150:ARG:HD3	1:J:151:MET:N	2.00	0.75
1:L:234:PHE:O	1:L:238:ILE:HG13	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:HG2	1:B:220(A):GLY:O	1.85	0.75
1:B:186(A):GLN:HE22	1:C:215:PHE:CB	1.99	0.75
1:H:234:PHE:O	1:H:238:ILE:HG13	1.86	0.75
1:O:187:GLN:HG2	1:O:220(A):GLY:O	1.86	0.75
1:A:177:HIS:HD2	1:A:179:SER:OG	1.69	0.75
1:C:187:GLN:HG2	1:C:220(A):GLY:O	1.85	0.75
1:B:234:PHE:O	1:B:238:ILE:HG13	1.87	0.75
1:G:234:PHE:O	1:G:238:ILE:HG13	1.87	0.75
1:I:234:PHE:O	1:I:238:ILE:HG13	1.87	0.74
1:N:191:CYS:SG	1:N:192:ASN:N	2.60	0.74
1:F:234:PHE:O	1:F:238:ILE:HG13	1.87	0.74
1:J:28:PRO:HB2	1:J:119:ARG:H	1.49	0.74
1:L:187:GLN:HG2	1:L:220(A):GLY:O	1.88	0.74
1:O:150:ARG:HD3	1:O:151:MET:N	2.01	0.74
1:G:28:PRO:HB2	1:G:119:ARG:H	1.52	0.74
1:L:157:CYS:O	1:L:158:VAL:HB	1.88	0.74
1:K:234:PHE:O	1:K:238:ILE:HG13	1.87	0.74
1:F:74:GLU:OE2	4:F:723:HOH:O	2.06	0.73
1:D:177:HIS:HD2	1:D:179:SER:OG	1.72	0.73
1:E:215:PHE:HB3	1:H:186(A):GLN:HE22	1.54	0.73
1:E:215:PHE:CB	1:H:186(A):GLN:HE22	2.02	0.72
1:G:83:VAL:HG21	1:G:108:LEU:HD22	1.70	0.72
1:J:222:VAL:HB	4:J:732:HOH:O	1.88	0.72
1:N:234:PHE:O	1:N:238:ILE:HG13	1.90	0.72
1:F:187:GLN:HG2	1:F:220(A):GLY:O	1.90	0.72
1:G:115:SER:HA	1:N:90:ARG:NH2	2.05	0.72
1:K:33:LEU:HB2	1:K:42:CYS:O	1.90	0.72
1:A:187:GLN:HG2	1:A:220(A):GLY:O	1.89	0.71
1:E:187:GLN:HG2	1:E:220(A):GLY:O	1.90	0.71
1:M:177:HIS:HD2	1:M:179:SER:OG	1.73	0.71
1:D:120:SER:OG	4:D:715:HOH:O	2.02	0.71
1:F:127:GLN:HA	4:F:725:HOH:O	1.89	0.71
1:P:83:VAL:HG21	1:P:108:LEU:HD22	1.72	0.71
1:I:101:ASN:ND2	4:I:713:HOH:O	2.18	0.71
1:P:187:GLN:HG2	1:P:220(A):GLY:O	1.89	0.71
1:K:187:GLN:HG2	1:K:220(A):GLY:O	1.90	0.71
1:A:28:PRO:HB2	1:A:119:ARG:H	1.54	0.71
1:G:201:CYS:HB3	1:G:210:GLN:HE21	1.56	0.71
1:I:28:PRO:HB2	1:I:119:ARG:H	1.55	0.71
1:L:77:GLU:OE2	4:L:713:HOH:O	2.09	0.71
1:N:201:CYS:HB2	1:N:210:GLN:HE21	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:GLU:CD	1:N:87:LEU:HG	2.11	0.71
1:M:234:PHE:O	1:M:238:ILE:HG13	1.90	0.71
1:B:177:HIS:HD2	1:B:179:SER:OG	1.73	0.70
1:K:28:PRO:HB2	1:K:119:ARG:H	1.56	0.70
1:L:28:PRO:HB2	1:L:119:ARG:H	1.57	0.70
1:M:70:LEU:HB2	4:M:735:HOH:O	1.91	0.70
1:N:103:LEU:H	1:N:103:LEU:HD23	1.55	0.70
1:I:186(A):GLN:HE22	1:J:215:PHE:CB	2.04	0.70
1:A:201:CYS:HB2	1:A:210:GLN:HE21	1.56	0.69
1:O:28:PRO:HB2	1:O:119:ARG:H	1.57	0.69
1:I:186(A):GLN:HE22	1:J:215:PHE:HB3	1.57	0.69
1:M:192:ASN:OD1	3:M:713:PBZ:H2	1.93	0.69
1:N:116:ASP:O	4:N:742:HOH:O	2.11	0.69
1:C:234:PHE:O	1:C:238:ILE:HG13	1.92	0.69
1:G:25:HIS:NE2	4:G:716:HOH:O	2.17	0.68
1:E:28:PRO:HB2	1:E:119:ARG:H	1.57	0.68
1:H:28:PRO:HB2	1:H:119:ARG:H	1.59	0.67
1:D:136:CYS:HB3	1:D:200:ILE:O	1.95	0.67
1:D:28:PRO:HB2	1:D:119:ARG:H	1.58	0.67
1:J:50:GLN:HA	1:J:108:LEU:HD12	1.77	0.67
1:E:81:GLN:OE1	4:E:714:HOH:O	2.11	0.67
1:B:28:PRO:HB2	1:B:119:ARG:H	1.58	0.67
1:E:83:VAL:HG21	1:E:108:LEU:HD22	1.76	0.67
1:K:83:VAL:HG21	1:K:108:LEU:HD22	1.76	0.67
1:B:83:VAL:HG21	1:B:108:LEU:HD22	1.77	0.67
1:D:176:TYR:HE1	1:H:166:GLU:OE2	1.78	0.67
1:D:83:VAL:HG21	1:D:108:LEU:HD22	1.75	0.66
1:F:83:VAL:HG21	1:F:108:LEU:HD22	1.75	0.66
1:P:190:SER:HB2	3:P:716:PBZ:HN32	1.61	0.66
1:P:28:PRO:HB2	1:P:119:ARG:H	1.61	0.66
1:C:28:PRO:HB2	1:C:119:ARG:H	1.60	0.66
1:D:51:TRP:CD1	1:D:242:VAL:HG13	2.30	0.66
1:H:50:GLN:HA	1:H:108:LEU:HD12	1.77	0.66
1:I:83:VAL:HG21	1:I:108:LEU:HD22	1.78	0.66
1:M:28:PRO:HB2	1:M:119:ARG:H	1.61	0.66
1:A:215:PHE:HA	3:A:701:PBZ:C2	2.26	0.65
1:O:83:VAL:HG21	1:O:108:LEU:HD22	1.78	0.65
1:A:166:GLU:OE2	1:G:176:TYR:HE1	1.80	0.65
1:P:78:PRO:CA	4:P:735:HOH:O	2.44	0.65
1:A:51:TRP:CD1	1:A:242:VAL:HG13	2.32	0.65
1:C:50:GLN:HA	1:C:108:LEU:HD12	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:LEU:HD23	1:F:103:LEU:H	1.62	0.65
1:J:83:VAL:HG21	1:J:108:LEU:HD22	1.79	0.65
1:D:103:LEU:HD23	1:D:103:LEU:H	1.62	0.65
1:O:35:MET:O	1:O:36:GLU:C	2.35	0.65
1:A:83:VAL:HG21	1:A:108:LEU:HD22	1.79	0.65
1:F:116:ASP:HB2	4:F:721:HOH:O	1.97	0.65
1:C:83:VAL:HG21	1:C:108:LEU:HD22	1.77	0.64
1:F:28:PRO:HB2	1:F:119:ARG:H	1.60	0.64
1:F:201:CYS:HB2	1:F:210:GLN:HE21	1.62	0.64
1:N:83:VAL:HG21	1:N:108:LEU:HD22	1.77	0.64
1:G:143:LEU:HD13	1:G:192:ASN:HB2	1.79	0.64
1:F:74:GLU:HG3	4:F:723:HOH:O	1.96	0.64
1:G:243:GLN:HB3	1:K:243:GLN:HG2	1.79	0.64
1:I:177:HIS:ND1	1:I:178:PRO:HD2	2.12	0.64
1:C:143:LEU:HD13	1:C:192:ASN:HB2	1.79	0.64
1:M:88:SER:OG	4:M:750:HOH:O	2.06	0.64
1:P:27:GLN:C	4:P:730:HOH:O	2.34	0.64
1:G:50:GLN:HA	1:G:108:LEU:HD12	1.78	0.64
1:D:50:GLN:HA	1:D:108:LEU:HD12	1.80	0.64
1:F:151:MET:HG2	4:F:737:HOH:O	1.98	0.64
1:I:201:CYS:HB2	1:I:210:GLN:HE21	1.63	0.64
1:K:50:GLN:HA	1:K:108:LEU:HD12	1.79	0.63
1:E:85:ALA:HB2	1:E:108:LEU:HA	1.80	0.63
1:J:103:LEU:HD23	1:J:103:LEU:H	1.63	0.63
1:B:50:GLN:HA	1:B:108:LEU:HD12	1.80	0.63
1:E:50:GLN:HA	1:E:108:LEU:HD12	1.80	0.63
1:G:137:LEU:HD11	1:G:157:CYS:HB3	1.79	0.63
1:L:50:GLN:HA	1:L:108:LEU:HD12	1.81	0.63
1:M:83:VAL:HG21	1:M:108:LEU:HD22	1.79	0.63
1:O:50:GLN:HA	1:O:108:LEU:HD12	1.80	0.62
1:B:176:TYR:HE1	1:F:166:GLU:OE2	1.83	0.62
1:O:177:HIS:ND1	1:O:178:PRO:HD2	2.14	0.62
1:N:28:PRO:HB2	1:N:119:ARG:H	1.65	0.62
1:J:190:SER:O	3:J:710:PBZ:N3	2.33	0.62
1:L:83:VAL:HG21	1:L:108:LEU:HD22	1.79	0.62
1:O:216:GLY:CA	3:O:715:PBZ:HN22	2.13	0.62
1:D:215:PHE:HA	3:D:704:PBZ:C6	2.30	0.62
1:P:203:GLY:N	4:P:720:HOH:O	2.03	0.62
1:E:51:TRP:CD1	1:E:242:VAL:HG13	2.35	0.62
1:H:85:ALA:HB2	1:H:108:LEU:HA	1.82	0.62
1:L:103:LEU:H	1:L:103:LEU:HD23	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD13	1:B:41:PHE:N	2.15	0.62
1:G:115:SER:CA	1:N:90:ARG:HH22	2.12	0.62
1:A:50:GLN:HA	1:A:108:LEU:HD12	1.82	0.62
1:H:51:TRP:CD1	1:H:242:VAL:HG13	2.35	0.62
1:B:186(A):GLN:HE22	1:C:215:PHE:HB3	1.64	0.61
1:I:85:ALA:HB2	1:I:108:LEU:HA	1.82	0.61
1:P:50:GLN:HA	1:P:108:LEU:HD12	1.81	0.61
1:N:143:LEU:HD13	1:N:192:ASN:HB2	1.82	0.61
1:P:103:LEU:HD23	1:P:103:LEU:H	1.64	0.61
1:A:57:HIS:CD2	1:D:186(A):GLN:HG2	2.36	0.61
1:A:103:LEU:HD23	1:A:103:LEU:H	1.66	0.61
1:A:41:PHE:CD2	1:A:42:CYS:SG	2.94	0.61
1:A:41:PHE:HD2	1:A:42:CYS:SG	2.24	0.61
1:C:103:LEU:HD23	1:C:103:LEU:H	1.66	0.61
1:H:136:CYS:HB3	1:H:200:ILE:O	1.99	0.61
1:I:51:TRP:CD1	1:I:242:VAL:HG13	2.36	0.61
1:B:16:ILE:O	4:B:718:HOH:O	2.16	0.61
1:B:59:PHE:C	1:B:59:PHE:CD2	2.73	0.61
1:I:50:GLN:HA	1:I:108:LEU:HD12	1.83	0.60
1:L:177:HIS:ND1	1:L:178:PRO:HD2	2.16	0.60
1:M:177:HIS:ND1	1:M:178:PRO:HD2	2.16	0.60
1:P:51:TRP:CD1	1:P:242:VAL:HG13	2.37	0.60
1:A:220:CYS:SG	3:A:701:PBZ:N2	2.74	0.60
1:G:79:GLY:O	4:G:714:HOH:O	2.17	0.60
1:L:59:PHE:C	1:L:59:PHE:CD2	2.75	0.60
1:P:146:ASN:ND2	4:P:741:HOH:O	2.33	0.60
1:F:50:GLN:NE2	4:F:720:HOH:O	2.34	0.60
1:M:50:GLN:HA	1:M:108:LEU:HD12	1.84	0.60
1:B:57:HIS:CD2	4:B:708:HOH:O	2.53	0.60
1:D:50:GLN:HG3	1:D:111:SER:HA	1.82	0.60
1:K:103:LEU:HD23	1:K:103:LEU:H	1.65	0.60
1:L:90:ARG:NH1	4:L:743:HOH:O	2.34	0.60
1:J:51:TRP:CD1	1:J:242:VAL:HG13	2.37	0.60
1:E:103:LEU:H	1:E:103:LEU:HD23	1.66	0.59
1:G:97:PRO:HB2	4:G:713:HOH:O	2.01	0.59
1:K:98:LEU:O	1:K:99:LEU:HB2	2.03	0.59
1:M:40:LEU:HD13	1:M:41:PHE:N	2.17	0.59
1:O:51:TRP:CD1	1:O:242:VAL:HG13	2.37	0.59
1:K:143:LEU:HD13	1:K:192:ASN:HB2	1.83	0.59
1:B:186(A):GLN:HG2	1:C:57:HIS:CD2	2.37	0.59
1:C:142:GLY:N	1:C:194:ASP:OD1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:MET:O	1:G:36:GLU:C	2.41	0.59
1:G:51:TRP:CD1	1:G:242:VAL:HG13	2.38	0.59
1:G:59:PHE:HB2	1:G:90:ARG:HD3	1.85	0.59
1:A:35:MET:O	1:A:36:GLU:C	2.41	0.59
1:J:59:PHE:C	1:J:59:PHE:CD2	2.76	0.59
1:H:35:MET:O	1:H:36:GLU:C	2.40	0.59
1:L:51:TRP:CD1	1:L:242:VAL:HG13	2.37	0.59
1:M:85:ALA:HB2	1:M:108:LEU:HA	1.85	0.59
1:O:192:ASN:OD1	3:O:715:PBZ:H2	2.02	0.59
1:P:59:PHE:C	1:P:59:PHE:CD2	2.76	0.59
1:B:50:GLN:HG3	1:B:111:SER:HA	1.85	0.59
1:F:50:GLN:HA	1:F:108:LEU:HD12	1.84	0.59
1:D:85:ALA:HB2	1:D:108:LEU:HA	1.83	0.59
1:D:151:MET:HG2	4:D:728:HOH:O	2.02	0.59
1:I:59:PHE:C	1:I:59:PHE:CD2	2.76	0.59
1:K:85:ALA:HB2	1:K:108:LEU:HA	1.85	0.59
1:L:143:LEU:HD13	1:L:192:ASN:HB2	1.84	0.59
1:P:177:HIS:ND1	1:P:178:PRO:HD2	2.18	0.59
1:H:25:HIS:NE2	4:H:717:HOH:O	2.21	0.58
1:M:143:LEU:HD13	1:M:192:ASN:HB2	1.83	0.58
1:P:85:ALA:HB2	1:P:108:LEU:HA	1.85	0.58
1:G:59:PHE:C	1:G:59:PHE:CD2	2.76	0.58
1:K:50:GLN:HG3	1:K:111:SER:HA	1.85	0.58
1:N:59:PHE:C	1:N:59:PHE:CD2	2.75	0.58
1:C:35:MET:O	1:C:36:GLU:C	2.40	0.58
1:F:85:ALA:HB2	1:F:108:LEU:HA	1.85	0.58
1:L:180:MET:HB3	4:L:746:HOH:O	2.02	0.58
1:C:50:GLN:HG3	1:C:111:SER:HA	1.85	0.58
1:G:243:GLN:HG3	1:K:244:ALA:CB	2.28	0.58
1:H:191:CYS:HA	3:H:708:PBZ:HN32	1.68	0.58
1:A:85:ALA:HB2	1:A:108:LEU:HA	1.84	0.58
1:D:177:HIS:ND1	1:D:178:PRO:HD2	2.18	0.58
1:I:59:PHE:HB2	1:I:90:ARG:HD3	1.84	0.58
1:A:159:ASN:ND2	1:K:116:ASP:OD2	2.36	0.58
1:K:51:TRP:CD1	1:K:242:VAL:HG13	2.39	0.58
1:O:98:LEU:O	1:O:99:LEU:HB2	2.04	0.58
1:D:98:LEU:HG	1:D:99:LEU:HG	1.86	0.58
1:G:115:SER:CB	1:N:90:ARG:NH2	2.58	0.58
1:K:177:HIS:ND1	1:K:178:PRO:HD2	2.19	0.58
1:P:78:PRO:O	1:P:80:SER:N	2.36	0.58
1:A:177:HIS:ND1	1:A:178:PRO:HD2	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:PHE:C	1:D:59:PHE:CD2	2.77	0.58
1:M:51:TRP:CD1	1:M:242:VAL:HG13	2.39	0.58
1:G:177:HIS:ND1	1:G:178:PRO:HD2	2.19	0.57
1:P:190:SER:C	3:P:716:PBZ:N3	2.57	0.57
1:B:103:LEU:H	1:B:103:LEU:HD23	1.68	0.57
1:N:59:PHE:HB2	1:N:90:ARG:HD3	1.85	0.57
1:P:35:MET:O	1:P:36:GLU:C	2.42	0.57
1:B:51:TRP:CD1	1:B:242:VAL:HG13	2.39	0.57
1:E:177:HIS:ND1	1:E:178:PRO:HD2	2.19	0.57
1:M:59:PHE:C	1:M:59:PHE:CD2	2.77	0.57
1:N:50:GLN:HA	1:N:108:LEU:HD12	1.84	0.57
1:D:59:PHE:HB2	1:D:90:ARG:HD3	1.86	0.57
1:I:40:LEU:HD13	1:I:41:PHE:N	2.20	0.57
1:O:59:PHE:C	1:O:59:PHE:CD2	2.77	0.57
1:G:85:ALA:HB2	1:G:108:LEU:HA	1.85	0.57
1:C:51:TRP:CZ3	1:C:107:LYS:HB2	2.40	0.57
1:F:143:LEU:HD13	1:F:192:ASN:HB2	1.86	0.57
1:J:177:HIS:ND1	1:J:178:PRO:HD2	2.19	0.57
1:N:85:ALA:HB2	1:N:108:LEU:HA	1.86	0.57
1:E:35:MET:O	1:E:36:GLU:C	2.41	0.57
1:C:59:PHE:C	1:C:59:PHE:CD2	2.77	0.57
1:C:85:ALA:HB2	1:C:108:LEU:HA	1.86	0.57
1:C:177:HIS:ND1	1:C:178:PRO:HD2	2.19	0.57
1:F:51:TRP:CD1	1:F:242:VAL:HG13	2.40	0.57
1:D:40:LEU:HD13	1:D:41:PHE:N	2.20	0.57
1:F:78:PRO:O	1:F:80:SER:N	2.38	0.57
1:I:220:CYS:SG	3:I:709:PBZ:H5	2.45	0.57
1:K:35:MET:O	1:K:36:GLU:C	2.43	0.57
1:O:59:PHE:HB2	1:O:90:ARG:HD3	1.87	0.57
1:H:177:HIS:ND1	1:H:178:PRO:HD2	2.19	0.57
1:M:35:MET:O	1:M:36:GLU:C	2.43	0.57
1:N:40:LEU:HD13	1:N:41:PHE:N	2.20	0.57
1:P:190:SER:O	3:P:716:PBZ:N3	2.38	0.57
1:F:35:MET:O	1:F:36:GLU:C	2.44	0.56
1:I:177:HIS:HE1	4:I:728:HOH:O	1.87	0.56
1:J:231:LEU:C	1:J:233:LYS:H	2.09	0.56
1:A:98:LEU:O	1:A:99:LEU:HB2	2.05	0.56
1:D:51:TRP:CZ3	1:D:107:LYS:HB2	2.39	0.56
1:D:201:CYS:HB2	1:D:210:GLN:HE21	1.69	0.56
1:E:59:PHE:HB2	1:E:90:ARG:HD3	1.87	0.56
1:F:59:PHE:C	1:F:59:PHE:CD2	2.78	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:GLN:N	4:G:719:HOH:O	2.18	0.56
1:J:191:CYS:HA	3:J:710:PBZ:HN32	1.70	0.56
1:K:186(A):GLN:HG2	1:L:57:HIS:CD2	2.41	0.56
1:L:136:CYS:HB3	1:L:200:ILE:O	2.05	0.56
1:N:35:MET:O	1:N:36:GLU:C	2.43	0.56
1:O:85:ALA:HB2	1:O:108:LEU:HA	1.87	0.56
1:P:48:HIS:CG	1:P:49:PRO:HD2	2.40	0.56
1:B:59:PHE:HB2	1:B:90:ARG:HD3	1.88	0.56
1:E:112:VAL:HG12	4:E:714:HOH:O	2.05	0.56
1:J:59:PHE:HB2	1:J:90:ARG:HD3	1.87	0.56
1:C:51:TRP:CD1	1:C:242:VAL:HG13	2.40	0.56
1:E:51:TRP:CZ3	1:E:107:LYS:HB2	2.40	0.56
1:I:128:CYS:HB3	1:I:129:PRO:CD	2.35	0.56
1:J:85:ALA:HB2	1:J:108:LEU:HA	1.88	0.56
1:C:40:LEU:HD13	1:C:41:PHE:N	2.21	0.56
1:G:127:GLN:HB2	1:K:208:TYR:OH	2.06	0.56
1:L:35:MET:HG2	1:L:41:PHE:CE1	2.40	0.56
1:E:136:CYS:HB3	1:E:200:ILE:O	2.06	0.56
1:J:35:MET:O	1:J:36:GLU:C	2.45	0.56
1:J:187:GLN:HA	4:J:729:HOH:O	2.06	0.56
1:A:48:HIS:CG	1:A:49:PRO:HD2	2.41	0.56
1:F:215:PHE:HA	3:F:706:PBZ:C6	2.36	0.56
1:H:103:LEU:HD23	1:H:103:LEU:H	1.70	0.56
1:A:49:PRO:O	1:A:112:VAL:HG22	2.06	0.56
1:A:50:GLN:HG3	1:A:111:SER:HA	1.86	0.56
1:J:48:HIS:CG	1:J:49:PRO:HD2	2.41	0.56
1:N:48:HIS:CG	1:N:49:PRO:HD2	2.41	0.56
1:O:136:CYS:HB3	1:O:200:ILE:O	2.05	0.56
1:B:35:MET:O	1:B:36:GLU:C	2.43	0.55
1:E:182:CYS:HB3	1:E:225:PRO:HB2	1.88	0.55
1:G:243:GLN:CG	1:K:244:ALA:H	2.16	0.55
1:K:59:PHE:HB2	1:K:90:ARG:HD3	1.88	0.55
1:L:59:PHE:HB2	1:L:90:ARG:HD3	1.87	0.55
1:L:235:THR:HG22	4:L:722:HOH:O	2.06	0.55
1:N:51:TRP:CD1	1:N:242:VAL:HG13	2.41	0.55
1:F:48:HIS:CG	1:F:49:PRO:HD2	2.41	0.55
1:L:85:ALA:HB2	1:L:108:LEU:HA	1.88	0.55
1:L:122:SER:HB3	4:L:730:HOH:O	2.06	0.55
1:A:142:GLY:N	1:A:194:ASP:OD1	2.38	0.55
1:P:50:GLN:HG3	1:P:111:SER:HA	1.89	0.55
1:D:35:MET:O	1:D:36:GLU:C	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:HIS:CG	1:E:49:PRO:HD2	2.40	0.55
1:G:115:SER:CA	1:N:90:ARG:NH2	2.68	0.55
1:J:40:LEU:HD13	1:J:41:PHE:N	2.21	0.55
1:J:142:GLY:N	1:J:194:ASP:OD1	2.39	0.55
1:O:192:ASN:HA	3:O:715:PBZ:HN11	1.72	0.55
1:O:220:CYS:SG	3:O:715:PBZ:H3	2.47	0.55
1:C:78:PRO:O	1:C:80:SER:N	2.40	0.55
1:N:50:GLN:HG3	1:N:111:SER:HA	1.89	0.55
1:N:177:HIS:ND1	1:N:178:PRO:HD2	2.22	0.55
1:B:48:HIS:CG	1:B:49:PRO:HD2	2.41	0.55
1:E:98:LEU:HG	1:E:99:LEU:HG	1.89	0.55
1:F:50:GLN:HG3	1:F:111:SER:HA	1.88	0.55
1:G:40:LEU:HD13	1:G:41:PHE:N	2.21	0.55
1:I:97:PRO:HB2	4:I:725:HOH:O	2.06	0.55
1:O:51:TRP:CZ3	1:O:107:LYS:HB2	2.42	0.55
1:A:78:PRO:O	1:A:80:SER:N	2.40	0.55
1:C:191:CYS:O	1:C:192:ASN:C	2.45	0.55
1:M:78:PRO:O	1:M:80:SER:N	2.40	0.55
1:N:23:SER:O	1:N:26:SER:OG	2.21	0.55
1:B:51:TRP:CZ3	1:B:107:LYS:HB2	2.42	0.55
1:G:35:MET:HG2	1:G:41:PHE:CE1	2.42	0.55
1:H:35:MET:HG2	1:H:41:PHE:CE1	2.42	0.55
1:H:51:TRP:CZ3	1:H:107:LYS:HB2	2.42	0.55
1:J:48:HIS:ND1	1:J:49:PRO:HD2	2.22	0.55
1:K:59:PHE:CD2	1:K:59:PHE:C	2.79	0.55
1:L:142:GLY:N	1:L:194:ASP:OD1	2.40	0.55
1:B:48:HIS:ND1	1:B:49:PRO:HD2	2.21	0.54
1:I:35:MET:O	1:I:36:GLU:C	2.45	0.54
1:G:48:HIS:ND1	1:G:49:PRO:HD2	2.23	0.54
1:G:243:GLN:CB	1:K:243:GLN:HG2	2.36	0.54
1:J:50:GLN:HG3	1:J:111:SER:HA	1.88	0.54
1:G:78:PRO:O	1:G:80:SER:N	2.40	0.54
1:J:28:PRO:HB2	1:J:119:ARG:N	2.20	0.54
1:L:35:MET:O	1:L:36:GLU:C	2.43	0.54
1:G:50:GLN:HG3	1:G:111:SER:HA	1.89	0.54
1:I:192:ASN:OD1	3:I:709:PBZ:H6	2.06	0.54
1:C:59:PHE:HB2	1:C:90:ARG:HD3	1.88	0.54
1:K:51:TRP:CZ3	1:K:107:LYS:HB2	2.41	0.54
1:P:45:VAL:HG11	1:P:209:LEU:HD22	1.89	0.54
1:A:51:TRP:CZ3	1:A:107:LYS:HB2	2.42	0.54
1:B:40:LEU:HD13	1:B:40:LEU:C	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ALA:HA	1:B:219:PRO:C	2.28	0.54
1:E:35:MET:HG2	1:E:41:PHE:CE1	2.42	0.54
1:E:78:PRO:O	1:E:80:SER:N	2.41	0.54
1:G:110:GLU:OE1	1:N:87:LEU:CG	2.51	0.54
1:P:125:SER:OG	4:P:724:HOH:O	1.96	0.54
1:C:35:MET:HG2	1:C:41:PHE:CE1	2.43	0.54
1:F:48:HIS:ND1	1:F:49:PRO:HD2	2.22	0.54
1:I:50:GLN:HG3	1:I:111:SER:HA	1.89	0.54
1:K:40:LEU:HD13	1:K:41:PHE:N	2.23	0.54
1:O:35:MET:HG2	1:O:41:PHE:CE1	2.43	0.54
1:D:190:SER:C	3:D:704:PBZ:N2	2.61	0.54
1:I:51:TRP:CZ3	1:I:107:LYS:HB2	2.43	0.54
1:O:50:GLN:HG3	1:O:111:SER:HA	1.90	0.54
1:E:48:HIS:HB3	1:E:51:TRP:HB2	1.90	0.54
1:F:98:LEU:HG	1:F:99:LEU:HG	1.89	0.54
1:N:98:LEU:HG	1:N:99:LEU:HG	1.90	0.54
1:A:28:PRO:HB2	1:A:119:ARG:N	2.23	0.53
1:D:48:HIS:CG	1:D:49:PRO:HD2	2.43	0.53
1:E:62:SER:CB	4:E:715:HOH:O	2.57	0.53
1:G:136:CYS:O	1:G:159:ASN:HA	2.07	0.53
1:F:177:HIS:ND1	1:F:178:PRO:HD2	2.23	0.53
1:L:40:LEU:HD13	1:L:41:PHE:N	2.24	0.53
1:M:48:HIS:CG	1:M:49:PRO:HD2	2.43	0.53
1:P:142:GLY:N	1:P:194:ASP:OD1	2.40	0.53
1:E:218:ALA:HA	1:E:219:PRO:C	2.29	0.53
1:F:40:LEU:HD13	1:F:41:PHE:N	2.23	0.53
1:L:182:CYS:HA	1:L:226:GLY:O	2.09	0.53
1:F:128:CYS:HB3	1:F:129:PRO:CD	2.38	0.53
1:J:231:LEU:C	1:J:233:LYS:N	2.60	0.53
1:M:50:GLN:HG3	1:M:111:SER:HA	1.89	0.53
1:O:98:LEU:HG	1:O:99:LEU:HG	1.90	0.53
1:P:51:TRP:CZ3	1:P:107:LYS:HB2	2.44	0.53
1:P:59:PHE:HB2	1:P:90:ARG:HD3	1.90	0.53
1:M:40:LEU:HD13	1:M:40:LEU:C	2.29	0.53
1:C:40:LEU:HD13	1:C:40:LEU:C	2.29	0.53
1:F:59:PHE:HB2	1:F:90:ARG:HD3	1.89	0.53
1:M:38:GLU:HG2	1:M:40:LEU:N	2.24	0.53
1:C:182:CYS:HB3	1:C:225:PRO:HB2	1.90	0.53
1:G:200:ILE:HA	1:G:208:TYR:O	2.08	0.53
1:I:28:PRO:HB2	1:I:119:ARG:N	2.23	0.53
1:J:186(A):GLN:HG2	1:K:57:HIS:CD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:MET:HG2	1:M:41:PHE:CE1	2.44	0.53
1:O:201:CYS:HB2	1:O:210:GLN:HE21	1.74	0.53
1:C:218:ALA:HA	1:C:219:PRO:C	2.30	0.53
1:E:142:GLY:N	1:E:194:ASP:OD1	2.39	0.53
1:G:218:ALA:HA	1:G:219:PRO:C	2.29	0.53
1:H:59:PHE:C	1:H:59:PHE:CD2	2.81	0.53
1:B:166:GLU:OE2	1:F:176:TYR:HE1	1.91	0.53
1:E:59:PHE:C	1:E:59:PHE:CD2	2.82	0.53
1:I:38:GLU:HG2	1:I:40:LEU:N	2.24	0.53
1:N:40:LEU:HD13	1:N:40:LEU:C	2.29	0.53
1:C:48:HIS:ND1	1:C:49:PRO:HD2	2.25	0.52
1:I:103:LEU:HD23	1:I:103:LEU:H	1.73	0.52
1:D:25:HIS:NE2	4:D:724:HOH:O	2.13	0.52
1:G:48:HIS:CG	1:G:49:PRO:HD2	2.44	0.52
1:G:234:PHE:HA	4:G:717:HOH:O	2.08	0.52
1:M:48:HIS:ND1	1:M:49:PRO:HD2	2.24	0.52
1:B:142:GLY:N	1:B:194:ASP:OD1	2.40	0.52
1:I:218:ALA:HA	1:I:219:PRO:C	2.29	0.52
1:L:50:GLN:HG3	1:L:111:SER:HA	1.89	0.52
1:P:197:GLY:O	1:P:212:LEU:HA	2.09	0.52
1:I:78:PRO:O	1:I:80:SER:N	2.43	0.52
1:A:218:ALA:HA	1:A:219:PRO:C	2.28	0.52
1:B:85:ALA:HB2	1:B:108:LEU:HA	1.91	0.52
1:G:142:GLY:N	1:G:194:ASP:OD1	2.41	0.52
1:G:243:GLN:HB3	1:K:243:GLN:CG	2.39	0.52
1:J:35:MET:HG2	1:J:41:PHE:CE1	2.45	0.52
1:C:98:LEU:O	1:C:99:LEU:HB2	2.10	0.52
1:K:25:HIS:NE2	4:K:719:HOH:O	2.26	0.52
1:K:98:LEU:HG	1:K:99:LEU:HG	1.92	0.52
1:M:59:PHE:HB2	1:M:90:ARG:HD3	1.89	0.52
1:N:98:LEU:O	1:N:99:LEU:HB2	2.09	0.52
1:K:48:HIS:CG	1:K:49:PRO:HD2	2.45	0.52
1:O:186(A):GLN:HG2	1:P:57:HIS:CG	2.45	0.52
1:E:40:LEU:HD13	1:E:41:PHE:N	2.24	0.52
1:L:48:HIS:CG	1:L:49:PRO:HD2	2.44	0.52
1:A:98:LEU:HG	1:A:99:LEU:HG	1.91	0.52
1:B:78:PRO:O	1:B:80:SER:N	2.43	0.52
1:B:197:GLY:O	1:B:212:LEU:HA	2.10	0.52
1:C:186(A):GLN:HG2	1:D:57:HIS:CD2	2.45	0.52
1:C:197:GLY:O	1:C:212:LEU:HA	2.10	0.52
1:G:51:TRP:CZ3	1:G:107:LYS:HB2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:HIS:HB3	1:I:51:TRP:HB2	1.92	0.52
1:P:27:GLN:N	4:P:730:HOH:O	2.34	0.52
1:D:78:PRO:O	1:D:80:SER:N	2.43	0.52
1:E:45:VAL:HG11	1:E:209:LEU:HD22	1.91	0.52
1:E:115:SER:HB3	4:E:726:HOH:O	2.10	0.52
1:G:197:GLY:O	1:G:212:LEU:HA	2.09	0.52
1:K:78:PRO:O	1:K:80:SER:N	2.43	0.52
1:N:78:PRO:O	1:N:80:SER:N	2.43	0.52
1:B:177:HIS:ND1	1:B:178:PRO:HD2	2.24	0.51
1:G:40:LEU:HD13	1:G:40:LEU:C	2.31	0.51
1:H:40:LEU:HD13	1:H:41:PHE:N	2.24	0.51
1:A:61:ASN:HA	4:A:721:HOH:O	2.11	0.51
1:I:197:GLY:O	1:I:212:LEU:HA	2.10	0.51
1:M:55:ALA:O	1:M:58:CYS:HB2	2.10	0.51
1:F:123:ILE:HG12	1:F:209:LEU:HD23	1.93	0.51
1:F:186(A):GLN:HG2	1:G:57:HIS:CD2	2.46	0.51
1:L:48:HIS:HB3	1:L:51:TRP:HB2	1.91	0.51
1:L:51:TRP:CZ3	1:L:107:LYS:HB2	2.45	0.51
1:B:98:LEU:O	1:B:99:LEU:HB2	2.10	0.51
1:G:103:LEU:H	1:G:103:LEU:HD23	1.74	0.51
1:J:51:TRP:CZ3	1:J:107:LYS:HB2	2.45	0.51
1:J:218:ALA:HA	1:J:219:PRO:C	2.30	0.51
1:K:28:PRO:HB2	1:K:119:ARG:N	2.23	0.51
1:K:41:PHE:CE2	1:K:42:CYS:HB2	2.46	0.51
1:P:136:CYS:HB3	1:P:200:ILE:O	2.10	0.51
1:A:112:VAL:HA	4:A:710:HOH:O	2.11	0.51
1:F:40:LEU:HD13	1:F:40:LEU:C	2.31	0.51
1:G:28:PRO:HB2	1:G:119:ARG:N	2.21	0.51
1:J:191:CYS:O	1:J:192:ASN:C	2.49	0.51
1:C:146:ASN:OD1	1:C:150:ARG:HB2	2.10	0.51
1:F:197:GLY:O	1:F:212:LEU:HA	2.10	0.51
1:H:78:PRO:O	1:H:80:SER:N	2.44	0.51
1:I:91:HIS:CG	1:I:92:PRO:HD2	2.46	0.51
1:J:78:PRO:O	1:J:80:SER:N	2.43	0.51
1:K:231:LEU:C	1:K:233:LYS:H	2.14	0.51
1:L:98:LEU:O	1:L:99:LEU:HB2	2.11	0.51
1:N:197:GLY:O	1:N:212:LEU:HA	2.10	0.51
1:O:40:LEU:HD13	1:O:41:PHE:N	2.25	0.51
1:D:98:LEU:O	1:D:99:LEU:HB2	2.09	0.51
1:H:197:GLY:O	1:H:212:LEU:HA	2.10	0.51
1:N:48:HIS:ND1	1:N:49:PRO:HD2	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:HIS:CE1	1:B:49:PRO:HD2	2.46	0.51
1:C:48:HIS:CG	1:C:49:PRO:HD2	2.45	0.51
1:C:166:GLU:OE2	1:E:176:TYR:CE1	2.55	0.51
1:D:91:HIS:CG	1:D:92:PRO:HD2	2.46	0.51
1:E:62:SER:HB2	4:E:715:HOH:O	2.10	0.51
1:H:37:ASN:HB2	4:H:726:HOH:O	2.09	0.51
1:K:48:HIS:HB3	1:K:51:TRP:HB2	1.92	0.51
1:L:98:LEU:HG	1:L:99:LEU:HG	1.92	0.51
1:O:186(A):GLN:HG2	1:P:57:HIS:CD2	2.46	0.51
1:C:28:PRO:HB2	1:C:119:ARG:N	2.26	0.51
1:I:48:HIS:CG	1:I:49:PRO:HD2	2.45	0.51
1:G:201:CYS:CB	1:G:210:GLN:HE21	2.24	0.51
1:H:216:GLY:HA3	3:H:708:PBZ:N2	2.26	0.50
1:L:45:VAL:HG11	1:L:209:LEU:HD22	1.94	0.50
1:J:98:LEU:O	1:J:99:LEU:HB2	2.11	0.50
1:N:103:LEU:HD23	1:N:103:LEU:N	2.23	0.50
1:A:48:HIS:HB3	1:A:51:TRP:HB2	1.93	0.50
1:J:197:GLY:O	1:J:212:LEU:HA	2.11	0.50
1:L:48:HIS:ND1	1:L:49:PRO:HD2	2.27	0.50
1:N:191:CYS:CB	1:N:220:CYS:HG	2.25	0.50
1:P:49:PRO:O	1:P:112:VAL:HG22	2.12	0.50
1:A:59:PHE:O	1:A:60:GLN:NE2	2.44	0.50
1:J:40:LEU:HD13	1:J:40:LEU:C	2.32	0.50
1:J:98:LEU:HG	1:J:99:LEU:HG	1.93	0.50
1:M:51:TRP:CZ3	1:M:107:LYS:HB2	2.46	0.50
1:N:189:ASP:HB2	4:N:717:HOH:O	2.11	0.50
1:O:48:HIS:CG	1:O:49:PRO:HD2	2.46	0.50
1:P:40:LEU:HD13	1:P:41:PHE:N	2.25	0.50
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.46	0.50
1:B:98:LEU:HG	1:B:99:LEU:HG	1.92	0.50
1:C:98:LEU:HG	1:C:99:LEU:HG	1.93	0.50
1:P:35:MET:HG2	1:P:41:PHE:CE1	2.47	0.50
1:P:48:HIS:ND1	1:P:49:PRO:HD2	2.26	0.50
1:F:49:PRO:O	1:F:112:VAL:HG22	2.12	0.50
1:H:142:GLY:N	1:H:194:ASP:OD1	2.41	0.50
1:N:191:CYS:HA	1:N:220:CYS:SG	2.52	0.50
1:P:191:CYS:SG	1:P:192:ASN:N	2.85	0.50
1:D:35:MET:HG2	1:D:41:PHE:CE1	2.47	0.50
1:H:49:PRO:O	1:H:112:VAL:HG22	2.11	0.50
1:K:38:GLU:HG2	1:K:40:LEU:N	2.27	0.50
1:L:200:ILE:HA	1:L:208:TYR:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HB2	1:B:174:PRO:HG3	1.94	0.50
1:B:215:PHE:HA	3:B:702:PBZ:C1	2.42	0.50
1:E:182:CYS:HA	1:E:226:GLY:O	2.12	0.50
1:I:40:LEU:HD13	1:I:40:LEU:C	2.32	0.50
1:J:123:ILE:HG12	1:J:209:LEU:HD23	1.94	0.50
1:M:98:LEU:HG	1:M:99:LEU:HG	1.93	0.50
1:N:51:TRP:CZ3	1:N:107:LYS:HB2	2.46	0.50
1:O:49:PRO:O	1:O:112:VAL:HG22	2.11	0.50
1:C:45:VAL:HG11	1:C:209:LEU:HD22	1.93	0.49
1:F:98:LEU:O	1:F:99:LEU:HB2	2.13	0.49
1:H:98:LEU:HG	1:H:99:LEU:HG	1.93	0.49
1:N:35:MET:HG2	1:N:41:PHE:CE1	2.47	0.49
1:A:78:PRO:C	1:A:80:SER:H	2.15	0.49
1:C:49:PRO:O	1:C:112:VAL:HG22	2.12	0.49
1:E:59:PHE:O	1:E:60:GLN:NE2	2.44	0.49
1:E:137:LEU:HD11	1:E:157:CYS:HB3	1.93	0.49
1:F:35:MET:HG2	1:F:41:PHE:CE1	2.47	0.49
1:H:48:HIS:CG	1:H:49:PRO:HD2	2.46	0.49
1:K:128:CYS:HB3	1:K:129:PRO:CD	2.42	0.49
1:A:48:HIS:ND1	1:A:49:PRO:HD2	2.26	0.49
1:C:165:GLU:HB3	1:E:165:GLU:HB3	1.94	0.49
1:G:49:PRO:O	1:G:112:VAL:HG22	2.11	0.49
1:K:45:VAL:HG11	1:K:209:LEU:HD22	1.93	0.49
1:K:91:HIS:CG	1:K:92:PRO:HD2	2.46	0.49
1:K:218:ALA:HA	1:K:219:PRO:C	2.33	0.49
1:M:166:GLU:O	1:M:167:VAL:C	2.48	0.49
1:N:218:ALA:HA	1:N:219:PRO:C	2.33	0.49
1:P:78:PRO:C	1:P:80:SER:H	2.14	0.49
1:A:48:HIS:NE2	4:A:723:HOH:O	2.35	0.49
1:F:78:PRO:C	1:F:80:SER:H	2.16	0.49
1:H:201:CYS:HB2	1:H:210:GLN:HE21	1.77	0.49
1:K:142:GLY:N	1:K:194:ASP:OD1	2.42	0.49
1:N:17:ILE:HG13	1:N:220:CYS:HB3	1.94	0.49
1:N:123:ILE:HG12	1:N:209:LEU:HD23	1.93	0.49
1:N:215:PHE:HA	3:N:714:PBZ:C6	2.43	0.49
1:A:128:CYS:O	1:A:129:PRO:C	2.47	0.49
1:F:51:TRP:CZ3	1:F:107:LYS:HB2	2.47	0.49
1:I:59:PHE:O	1:I:60:GLN:NE2	2.46	0.49
1:I:128:CYS:HB3	1:I:129:PRO:HD2	1.93	0.49
1:K:35:MET:HG2	1:K:41:PHE:CE1	2.48	0.49
1:O:170:LYS:HB2	1:P:174:PRO:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:98:LEU:O	1:P:99:LEU:HB2	2.12	0.49
1:C:61:ASN:O	4:C:728:HOH:O	2.19	0.49
1:K:40:LEU:HD13	1:K:40:LEU:C	2.33	0.49
1:L:28:PRO:HB2	1:L:119:ARG:N	2.25	0.49
1:D:45:VAL:HG11	1:D:209:LEU:HD22	1.95	0.49
1:D:231:LEU:C	1:D:233:LYS:H	2.15	0.49
1:F:128:CYS:HB3	1:F:129:PRO:HD2	1.95	0.49
1:F:218:ALA:HA	1:F:219:PRO:C	2.32	0.49
1:H:123:ILE:HG12	1:H:209:LEU:HD23	1.95	0.49
1:L:78:PRO:O	1:L:80:SER:N	2.46	0.49
1:A:165:GLU:HB3	1:G:165:GLU:HB3	1.94	0.49
1:B:48:HIS:CG	1:B:49:PRO:CD	2.96	0.49
1:D:142:GLY:N	1:D:194:ASP:OD1	2.42	0.49
1:G:190:SER:O	3:G:707:PBZ:N3	2.46	0.49
1:J:38:GLU:HG2	1:J:40:LEU:N	2.27	0.49
1:B:48:HIS:HB3	1:B:51:TRP:HB2	1.95	0.49
1:H:40:LEU:HD13	1:H:40:LEU:C	2.33	0.49
1:I:142:GLY:N	1:I:194:ASP:OD1	2.42	0.49
1:L:91:HIS:CG	1:L:92:PRO:HD2	2.48	0.49
1:J:49:PRO:O	1:J:112:VAL:HG22	2.12	0.49
1:P:137:LEU:HG	1:P:138:VAL:N	2.27	0.49
1:A:48:HIS:CG	1:A:49:PRO:CD	2.96	0.48
1:K:197:GLY:O	1:K:212:LEU:HA	2.13	0.48
1:M:200:ILE:HG23	1:M:208:TYR:O	2.13	0.48
1:G:27:GLN:C	4:G:719:HOH:O	2.51	0.48
1:J:48:HIS:CG	1:J:49:PRO:CD	2.96	0.48
1:J:137:LEU:HG	1:J:138:VAL:N	2.28	0.48
1:K:103:LEU:HD23	1:K:103:LEU:N	2.28	0.48
1:A:43:SER:OG	4:A:719:HOH:O	2.19	0.48
1:F:48:HIS:HB3	1:F:51:TRP:HB2	1.95	0.48
1:F:55:ALA:O	1:F:58:CYS:HB2	2.12	0.48
1:G:136:CYS:SG	1:G:201:CYS:SG	3.11	0.48
1:H:45:VAL:HG11	1:H:209:LEU:HD22	1.94	0.48
1:M:231:LEU:O	1:M:232:CYS:C	2.49	0.48
1:P:28:PRO:HB2	1:P:119:ARG:N	2.27	0.48
1:B:45:VAL:HG11	1:B:209:LEU:HD22	1.95	0.48
1:E:28:PRO:HB2	1:E:119:ARG:N	2.27	0.48
1:E:91:HIS:CG	1:E:92:PRO:HD2	2.48	0.48
1:H:28:PRO:HB2	1:H:119:ARG:N	2.26	0.48
1:O:218:ALA:HA	1:O:219:PRO:C	2.34	0.48
1:A:166:GLU:OE2	1:G:176:TYR:CE1	2.65	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HG	1:B:138:VAL:N	2.27	0.48
1:F:48:HIS:CG	1:F:49:PRO:CD	2.97	0.48
1:G:103:LEU:HB3	1:G:229:THR:HG21	1.96	0.48
1:B:123:ILE:HG12	1:B:209:LEU:HD23	1.96	0.48
1:D:103:LEU:HD23	1:D:103:LEU:N	2.28	0.48
1:E:40:LEU:HD13	1:E:40:LEU:C	2.34	0.48
1:F:48:HIS:CE1	1:F:49:PRO:HD2	2.49	0.48
1:H:48:HIS:HB3	1:H:51:TRP:HB2	1.96	0.48
1:L:218:ALA:HA	1:L:219:PRO:C	2.33	0.48
1:N:48:HIS:CG	1:N:49:PRO:CD	2.97	0.48
1:P:48:HIS:CG	1:P:49:PRO:CD	2.96	0.48
1:E:137:LEU:HG	1:E:138:VAL:N	2.28	0.48
1:I:98:LEU:O	1:I:99:LEU:HB2	2.14	0.48
1:L:40:LEU:HD13	1:L:40:LEU:C	2.33	0.48
1:O:177:HIS:HB3	1:O:180:MET:HE2	1.95	0.48
1:O:192:ASN:HA	3:O:715:PBZ:N1	2.28	0.48
1:D:28:PRO:HB2	1:D:119:ARG:N	2.27	0.48
1:D:48:HIS:ND1	1:D:49:PRO:HD2	2.29	0.48
1:F:87:LEU:C	1:F:87:LEU:HD23	2.33	0.48
1:L:23:SER:O	1:L:24:PRO:C	2.52	0.48
1:N:182:CYS:HA	1:N:226:GLY:O	2.14	0.48
1:O:197:GLY:O	1:O:212:LEU:HA	2.13	0.48
1:D:55:ALA:O	1:D:58:CYS:HB2	2.14	0.48
1:G:48:HIS:CG	1:G:49:PRO:CD	2.97	0.48
1:C:123:ILE:HG12	1:C:209:LEU:HD23	1.95	0.48
1:D:48:HIS:HB3	1:D:51:TRP:HB2	1.95	0.48
1:L:201:CYS:HB2	1:L:210:GLN:HE21	1.79	0.48
1:M:45:VAL:HG11	1:M:209:LEU:HD22	1.95	0.48
1:B:35:MET:HG2	1:B:41:PHE:CE1	2.49	0.47
1:C:158:VAL:HG22	1:C:159:ASN:N	2.29	0.47
1:I:98:LEU:HG	1:I:99:LEU:HG	1.96	0.47
1:I:186(A):GLN:HG2	1:J:57:HIS:CD2	2.49	0.47
1:A:45:VAL:HG11	1:A:209:LEU:HD22	1.95	0.47
1:G:48:HIS:CE1	1:G:49:PRO:HD2	2.49	0.47
1:J:231:LEU:O	1:J:233:LYS:N	2.47	0.47
1:K:59:PHE:O	1:K:60:GLN:NE2	2.46	0.47
1:L:123:ILE:HG12	1:L:209:LEU:HD23	1.95	0.47
1:M:54:SER:OG	1:M:55:ALA:N	2.45	0.47
1:O:78:PRO:O	1:O:80:SER:N	2.47	0.47
1:D:73:LEU:N	4:D:727:HOH:O	2.42	0.47
1:K:171:LEU:HD13	1:K:225:PRO:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:GLY:O	1:L:212:LEU:HA	2.13	0.47
1:N:59:PHE:CB	1:N:90:ARG:HD3	2.43	0.47
1:E:49:PRO:O	1:E:112:VAL:HG22	2.14	0.47
1:K:78:PRO:C	1:K:80:SER:H	2.18	0.47
1:B:28:PRO:HB2	1:B:119:ARG:N	2.26	0.47
1:D:137:LEU:HG	1:D:138:VAL:N	2.30	0.47
1:E:59:PHE:CB	1:E:90:ARG:HD3	2.44	0.47
1:E:191:CYS:SG	1:E:192:ASN:N	2.87	0.47
1:J:146:ASN:OD1	1:J:150:ARG:HB2	2.13	0.47
1:J:171:LEU:HD13	1:J:225:PRO:HD2	1.97	0.47
1:K:186(A):GLN:HE22	1:L:215:PHE:HB3	1.78	0.47
1:N:87:LEU:C	1:N:87:LEU:CD2	2.83	0.47
1:N:200:ILE:HA	1:N:208:TYR:O	2.14	0.47
1:O:171:LEU:HD13	1:O:225:PRO:HD2	1.95	0.47
1:D:40:LEU:HD13	1:D:40:LEU:C	2.34	0.47
1:F:142:GLY:N	1:F:194:ASP:OD1	2.42	0.47
1:L:231:LEU:C	1:L:233:LYS:H	2.18	0.47
1:A:123:ILE:HG12	1:A:209:LEU:HD23	1.97	0.47
1:B:123:ILE:HA	1:B:209:LEU:HB3	1.97	0.47
1:C:35:MET:HB3	1:C:36:GLU:H	1.48	0.47
1:C:78:PRO:C	1:C:80:SER:H	2.18	0.47
1:G:27:GLN:CA	4:G:719:HOH:O	2.62	0.47
1:G:243:GLN:HG2	1:K:243:GLN:CB	2.28	0.47
1:I:45:VAL:HG11	1:I:209:LEU:HD22	1.97	0.47
1:I:200:ILE:HA	1:I:208:TYR:O	2.15	0.47
1:J:103:LEU:HD23	1:J:103:LEU:N	2.29	0.47
1:L:22:CYS:SG	1:L:155:LEU:O	2.72	0.47
1:M:48:HIS:CE1	1:M:49:PRO:HD2	2.50	0.47
1:O:23:SER:O	1:O:24:PRO:C	2.53	0.47
1:O:45:VAL:HG11	1:O:209:LEU:HD22	1.97	0.47
1:P:103:LEU:HD23	1:P:103:LEU:N	2.28	0.47
1:A:197:GLY:O	1:A:212:LEU:HA	2.14	0.47
1:A:200:ILE:HA	1:A:208:TYR:O	2.15	0.47
1:A:231:LEU:C	1:A:233:LYS:N	2.64	0.47
1:D:123:ILE:HG12	1:D:209:LEU:HD23	1.96	0.47
1:G:91:HIS:CG	1:G:92:PRO:HD2	2.49	0.47
1:L:54:SER:OG	1:L:55:ALA:N	2.47	0.47
1:M:35:MET:HB3	1:M:36:GLU:H	1.46	0.47
1:O:48:HIS:HB3	1:O:51:TRP:HB2	1.96	0.47
1:A:171:LEU:HD13	1:A:225:PRO:HD2	1.95	0.47
1:A:201:CYS:CB	1:A:210:GLN:HE21	2.26	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:HIS:ND1	1:G:49:PRO:N	2.62	0.47
1:I:140:GLY:CA	4:I:723:HOH:O	2.63	0.47
1:O:28:PRO:HB2	1:O:119:ARG:N	2.25	0.47
1:P:98:LEU:HG	1:P:99:LEU:HG	1.97	0.47
1:C:59:PHE:O	1:C:60:GLN:NE2	2.45	0.47
1:D:218:ALA:HA	1:D:219:PRO:C	2.35	0.47
1:G:79:GLY:CA	4:G:714:HOH:O	2.62	0.47
1:J:48:HIS:CE1	1:J:49:PRO:HD2	2.49	0.47
1:O:40:LEU:HD13	1:O:40:LEU:C	2.36	0.47
1:O:59:PHE:O	1:O:60:GLN:NE2	2.48	0.47
1:P:171:LEU:HD13	1:P:225:PRO:HD2	1.97	0.47
1:P:181:PHE:HZ	1:P:199:LEU:HD23	1.79	0.47
1:D:176:TYR:CE1	1:H:166:GLU:OE2	2.66	0.46
1:G:171:LEU:HD13	1:G:225:PRO:HD2	1.95	0.46
1:H:129:PRO:HA	4:H:719:HOH:O	2.14	0.46
1:M:136:CYS:HB3	1:M:200:ILE:O	2.15	0.46
1:M:201:CYS:HB2	1:M:210:GLN:HE21	1.81	0.46
1:N:192:ASN:OD1	3:N:714:PBZ:H2	2.15	0.46
1:O:123:ILE:HG12	1:O:209:LEU:HD23	1.96	0.46
1:P:40:LEU:HD13	1:P:40:LEU:C	2.36	0.46
1:D:48:HIS:CG	1:D:49:PRO:CD	2.99	0.46
1:F:137:LEU:HG	1:F:138:VAL:N	2.28	0.46
1:G:98:LEU:HG	1:G:99:LEU:HG	1.96	0.46
1:I:141:TRP:N	4:I:723:HOH:O	2.27	0.46
1:B:201:CYS:HB2	1:B:210:GLN:NE2	2.24	0.46
1:C:91:HIS:CG	1:C:92:PRO:HD2	2.50	0.46
1:E:35:MET:HB3	1:E:36:GLU:H	1.45	0.46
1:E:48:HIS:ND1	1:E:49:PRO:HD2	2.29	0.46
1:E:175:LEU:HA	1:E:175:LEU:HD23	1.66	0.46
1:E:197:GLY:O	1:E:212:LEU:HA	2.15	0.46
1:F:28:PRO:HB2	1:F:119:ARG:N	2.28	0.46
1:L:48:HIS:CG	1:L:49:PRO:CD	2.98	0.46
1:M:61:ASN:ND2	4:M:739:HOH:O	2.47	0.46
1:M:158:VAL:HG22	1:M:159:ASN:N	2.31	0.46
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.67	0.46
1:B:78:PRO:C	1:B:80:SER:H	2.19	0.46
1:B:103:LEU:HB3	1:B:229:THR:HG21	1.97	0.46
1:H:158:VAL:HG22	1:H:159:ASN:N	2.30	0.46
1:J:69:GLY:CA	1:J:118:ILE:HG12	2.46	0.46
1:M:137:LEU:HD11	1:M:157:CYS:HB3	1.97	0.46
1:N:123:ILE:HA	1:N:209:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:142:GLY:N	1:O:194:ASP:OD1	2.45	0.46
1:D:78:PRO:C	1:D:80:SER:H	2.19	0.46
1:E:48:HIS:CG	1:E:49:PRO:CD	2.98	0.46
1:E:98:LEU:O	1:E:99:LEU:HB2	2.15	0.46
1:I:78:PRO:C	1:I:80:SER:H	2.19	0.46
1:I:123:ILE:HG12	1:I:209:LEU:HD23	1.97	0.46
1:I:171:LEU:HD13	1:I:225:PRO:HD2	1.97	0.46
1:J:48:HIS:HB3	1:J:51:TRP:HB2	1.96	0.46
1:M:91:HIS:CG	1:M:92:PRO:HD2	2.51	0.46
1:B:50:GLN:HG3	1:B:111:SER:CA	2.45	0.46
1:C:48:HIS:HB3	1:C:51:TRP:HB2	1.96	0.46
1:C:103:LEU:HB3	1:C:229:THR:HG21	1.97	0.46
1:F:103:LEU:HD23	1:F:103:LEU:N	2.28	0.46
1:H:123:ILE:HA	1:H:209:LEU:HB3	1.96	0.46
1:N:54:SER:OG	1:N:55:ALA:N	2.46	0.46
1:P:48:HIS:HB3	1:P:51:TRP:HB2	1.98	0.46
1:P:59:PHE:O	1:P:60:GLN:NE2	2.47	0.46
1:P:123:ILE:HG12	1:P:209:LEU:HD23	1.98	0.46
1:A:146:ASN:OD1	1:A:150:ARG:HB2	2.16	0.46
1:D:50:GLN:HG3	1:D:111:SER:CA	2.45	0.46
1:D:59:PHE:CB	1:D:90:ARG:HD3	2.46	0.46
1:F:182:CYS:HA	1:F:226:GLY:O	2.16	0.46
1:H:98:LEU:O	1:H:99:LEU:HB2	2.16	0.46
1:F:59:PHE:CB	1:F:90:ARG:HD3	2.46	0.46
1:F:177:HIS:HB3	1:F:180:MET:HE2	1.97	0.46
1:H:59:PHE:O	1:H:60:GLN:NE2	2.48	0.46
1:H:91:HIS:CG	1:H:92:PRO:HD2	2.51	0.46
1:I:59:PHE:CB	1:I:90:ARG:HD3	2.46	0.46
1:K:48:HIS:ND1	1:K:49:PRO:HD2	2.31	0.46
1:K:123:ILE:HG12	1:K:209:LEU:HD23	1.97	0.46
1:D:215:PHE:HA	3:D:704:PBZ:H6	1.97	0.46
1:G:69:GLY:CA	1:G:118:ILE:HG12	2.46	0.46
1:G:87:LEU:C	1:G:87:LEU:HD23	2.36	0.46
1:H:29:TRP:CE3	1:H:121:ILE:HB	2.50	0.46
1:J:78:PRO:C	1:J:80:SER:H	2.20	0.46
1:K:23:SER:O	1:K:24:PRO:C	2.54	0.46
1:L:22:CYS:SG	1:L:155:LEU:HG	2.56	0.46
1:N:78:PRO:C	1:N:80:SER:H	2.19	0.46
1:N:87:LEU:C	1:N:87:LEU:HD23	2.36	0.46
1:P:35:MET:HB3	1:P:36:GLU:H	1.46	0.46
1:P:231:LEU:C	1:P:233:LYS:N	2.70	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:SER:O	1:A:191:CYS:HB2	2.16	0.46
1:F:54:SER:OG	1:F:55:ALA:N	2.49	0.46
1:M:78:PRO:C	1:M:80:SER:H	2.19	0.46
1:M:197:GLY:O	1:M:212:LEU:HA	2.16	0.46
1:P:218:ALA:HA	1:P:219:PRO:C	2.35	0.46
1:B:170:LYS:NZ	4:B:707:HOH:O	2.31	0.45
1:F:23:SER:O	1:F:26:SER:OG	2.16	0.45
1:F:87:LEU:C	1:F:87:LEU:CD2	2.84	0.45
1:F:171:LEU:HD13	1:F:225:PRO:HD2	1.98	0.45
1:G:78:PRO:C	1:G:80:SER:H	2.19	0.45
1:L:231:LEU:C	1:L:233:LYS:N	2.68	0.45
1:M:123:ILE:HG12	1:M:209:LEU:HD23	1.98	0.45
1:B:49:PRO:O	1:B:112:VAL:HG22	2.16	0.45
1:C:48:HIS:CE1	1:C:49:PRO:HD2	2.51	0.45
1:D:158:VAL:HG22	1:D:159:ASN:N	2.31	0.45
1:D:231:LEU:C	1:D:233:LYS:N	2.69	0.45
1:E:123:ILE:HG12	1:E:209:LEU:HD23	1.98	0.45
1:F:91:HIS:CG	1:F:92:PRO:HD2	2.51	0.45
1:I:69:GLY:CA	1:I:118:ILE:HG12	2.47	0.45
1:M:171:LEU:HD13	1:M:225:PRO:HD2	1.99	0.45
1:M:186(A):GLN:HG2	1:N:57:HIS:CD2	2.51	0.45
1:O:137:LEU:HG	1:O:138:VAL:N	2.31	0.45
1:P:220:CYS:SG	3:P:716:PBZ:H5	2.56	0.45
1:D:23:SER:O	1:D:26:SER:OG	2.22	0.45
1:E:78:PRO:C	1:E:80:SER:H	2.19	0.45
1:F:158:VAL:HG22	1:F:159:ASN:N	2.32	0.45
1:H:231:LEU:C	1:H:233:LYS:H	2.19	0.45
1:K:128:CYS:HB3	1:K:129:PRO:HD2	1.98	0.45
1:M:48:HIS:CG	1:M:49:PRO:CD	2.99	0.45
1:A:23:SER:O	1:A:26:SER:OG	2.29	0.45
1:A:208:TYR:HE2	4:A:703:HOH:O	1.99	0.45
1:C:87:LEU:C	1:C:87:LEU:HD23	2.37	0.45
1:C:186(A):GLN:HE22	1:D:215:PHE:HB3	1.81	0.45
1:H:137:LEU:HG	1:H:138:VAL:N	2.31	0.45
1:H:171:LEU:HD13	1:H:225:PRO:HD2	1.99	0.45
1:J:123:ILE:HA	1:J:209:LEU:HB3	1.98	0.45
1:L:59:PHE:CB	1:L:90:ARG:HD3	2.46	0.45
1:L:103:LEU:HD23	1:L:103:LEU:N	2.31	0.45
1:M:48:HIS:HB3	1:M:51:TRP:HB2	1.98	0.45
1:M:142:GLY:N	1:M:194:ASP:OD1	2.44	0.45
1:M:218:ALA:HA	1:M:219:PRO:C	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:CYS:O	1:N:159:ASN:HA	2.16	0.45
1:N:171:LEU:HD13	1:N:225:PRO:HD2	1.98	0.45
1:E:243:GLN:HB3	1:E:244:ALA:H	1.62	0.45
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.71	0.45
1:H:91:HIS:O	1:H:92:PRO:C	2.55	0.45
1:F:69:GLY:CA	1:F:118:ILE:HG12	2.46	0.45
1:G:87:LEU:C	1:G:87:LEU:CD2	2.85	0.45
1:M:98:LEU:O	1:M:99:LEU:HB2	2.17	0.45
1:N:142:GLY:N	1:N:194:ASP:OD1	2.45	0.45
1:A:48:HIS:CE1	1:A:49:PRO:HD2	2.52	0.45
1:C:69:GLY:CA	1:C:118:ILE:HG12	2.47	0.45
1:D:69:GLY:CA	1:D:118:ILE:HG12	2.47	0.45
1:G:48:HIS:HB3	1:G:51:TRP:HB2	1.97	0.45
1:H:78:PRO:C	1:H:80:SER:H	2.19	0.45
1:H:163:VAL:HB	1:H:182:CYS:HB2	1.97	0.45
1:J:95:ASN:C	1:J:96:ARG:HG2	2.37	0.45
1:J:179:SER:HB2	1:J:234:PHE:HZ	1.82	0.45
1:K:201:CYS:HB2	1:K:210:GLN:HE21	1.82	0.45
1:L:177:HIS:CD2	1:L:179:SER:H	2.34	0.45
1:N:146:ASN:OD1	1:N:150:ARG:HB2	2.17	0.45
1:B:171:LEU:HD13	1:B:225:PRO:HD2	1.99	0.45
1:B:201:CYS:O	1:B:202:ASN:HB2	2.17	0.45
1:E:103:LEU:HD23	1:E:103:LEU:N	2.32	0.45
1:M:49:PRO:O	1:M:112:VAL:HG22	2.17	0.45
1:M:103:LEU:HD23	1:M:103:LEU:H	1.82	0.45
1:M:220:CYS:SG	3:M:713:PBZ:H3	2.56	0.45
1:O:146:ASN:OD1	1:O:150:ARG:HB2	2.16	0.45
1:P:127:GLN:HB2	4:P:733:HOH:O	2.17	0.45
1:C:59:PHE:CB	1:C:90:ARG:HD3	2.47	0.45
1:H:54:SER:OG	1:H:55:ALA:N	2.49	0.45
1:I:48:HIS:ND1	1:I:49:PRO:HD2	2.31	0.45
1:K:177:HIS:HB3	1:K:180:MET:HE2	1.99	0.45
1:N:137:LEU:HG	1:N:138:VAL:N	2.30	0.45
1:O:91:HIS:CG	1:O:92:PRO:HD2	2.52	0.45
1:A:57:HIS:CG	1:D:186(A):GLN:HG2	2.51	0.45
1:A:231:LEU:O	1:A:233:LYS:N	2.50	0.45
1:B:69:GLY:CA	1:B:118:ILE:HG12	2.47	0.45
1:B:186(A):GLN:HE22	1:C:215:PHE:HB2	1.77	0.45
1:C:171:LEU:HD13	1:C:225:PRO:HD2	1.99	0.45
1:E:200:ILE:HA	1:E:208:TYR:O	2.17	0.45
1:I:57:HIS:CD2	1:L:186(A):GLN:HG2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:SER:OG	1:K:55:ALA:N	2.51	0.45
1:M:91:HIS:O	1:M:92:PRO:C	2.55	0.45
1:N:91:HIS:CG	1:N:92:PRO:HD2	2.52	0.45
1:P:48:HIS:CE1	1:P:49:PRO:HD2	2.52	0.45
1:P:59:PHE:CB	1:P:90:ARG:HD3	2.47	0.45
1:P:201:CYS:HB2	1:P:210:GLN:HE21	1.82	0.45
1:B:48:HIS:ND1	1:B:49:PRO:CD	2.80	0.44
1:B:59:PHE:CB	1:B:90:ARG:HD3	2.46	0.44
1:B:201:CYS:CB	1:B:210:GLN:HE21	2.24	0.44
1:E:29:TRP:CE3	1:E:121:ILE:HB	2.53	0.44
1:E:195:SER:OG	3:E:705:PBZ:N1	2.39	0.44
1:F:45:VAL:HG11	1:F:209:LEU:HD22	1.97	0.44
1:G:158:VAL:HG22	1:G:159:ASN:N	2.32	0.44
1:H:69:GLY:CA	1:H:118:ILE:HG12	2.47	0.44
1:J:54:SER:OG	1:J:55:ALA:N	2.50	0.44
1:J:177:HIS:HB3	1:J:180:MET:HE2	1.98	0.44
1:K:35:MET:HB3	1:K:36:GLU:H	1.49	0.44
1:K:231:LEU:C	1:K:233:LYS:N	2.71	0.44
1:L:78:PRO:C	1:L:80:SER:H	2.21	0.44
1:M:87:LEU:C	1:M:87:LEU:HD23	2.37	0.44
1:N:48:HIS:CE1	1:N:49:PRO:HD2	2.52	0.44
1:O:48:HIS:ND1	1:O:49:PRO:HD2	2.32	0.44
1:C:56:ALA:C	1:C:58:CYS:H	2.21	0.44
1:E:112:VAL:HA	4:E:714:HOH:O	2.17	0.44
1:M:137:LEU:HG	1:M:138:VAL:N	2.31	0.44
1:B:48:HIS:ND1	1:B:49:PRO:N	2.66	0.44
1:B:181:PHE:HZ	1:B:199:LEU:HD23	1.83	0.44
1:C:50:GLN:HG3	1:C:111:SER:CA	2.47	0.44
1:D:197:GLY:O	1:D:212:LEU:HA	2.16	0.44
1:J:87:LEU:HD23	1:J:87:LEU:C	2.38	0.44
1:N:59:PHE:O	1:N:60:GLN:NE2	2.50	0.44
1:B:87:LEU:C	1:B:87:LEU:HD23	2.37	0.44
1:C:48:HIS:CG	1:C:49:PRO:CD	3.00	0.44
1:E:220:CYS:SG	3:E:705:PBZ:N3	2.90	0.44
1:G:59:PHE:CB	1:G:90:ARG:HD3	2.46	0.44
1:H:93:GLU:O	1:H:94:TYR:C	2.53	0.44
1:H:218:ALA:HA	1:H:219:PRO:C	2.38	0.44
1:J:59:PHE:CB	1:J:90:ARG:HD3	2.47	0.44
1:K:50:GLN:HG3	1:K:111:SER:CA	2.48	0.44
1:L:181:PHE:HZ	1:L:199:LEU:HD23	1.82	0.44
1:N:45:VAL:HG11	1:N:209:LEU:HD22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:GLU:O	1:G:94:TYR:C	2.53	0.44
1:I:181:PHE:HZ	1:I:199:LEU:HD23	1.83	0.44
1:K:103:LEU:HB3	1:K:229:THR:HG21	2.00	0.44
1:M:56:ALA:C	1:M:58:CYS:H	2.21	0.44
1:N:48:HIS:HB3	1:N:51:TRP:HB2	1.99	0.44
1:P:158:VAL:HG22	1:P:159:ASN:N	2.32	0.44
1:A:163:VAL:HG12	1:A:164:SER:N	2.31	0.44
1:A:166:GLU:O	1:A:167:VAL:C	2.54	0.44
1:B:87:LEU:C	1:B:87:LEU:CD2	2.86	0.44
1:C:166:GLU:O	1:C:167:VAL:C	2.56	0.44
1:C:181:PHE:HZ	1:C:199:LEU:HD23	1.82	0.44
1:G:98:LEU:O	1:G:99:LEU:HB2	2.17	0.44
1:I:49:PRO:O	1:I:112:VAL:HG22	2.18	0.44
1:I:200:ILE:HG23	1:I:208:TYR:O	2.18	0.44
1:O:158:VAL:HG22	1:O:159:ASN:N	2.33	0.44
1:A:103:LEU:HD23	1:A:103:LEU:N	2.33	0.44
1:A:180:MET:HB2	1:A:227:VAL:CG1	2.47	0.44
1:E:35:MET:HG2	1:E:41:PHE:CD1	2.53	0.44
1:F:35:MET:HB3	1:F:36:GLU:H	1.43	0.44
1:G:243:GLN:CG	1:K:244:ALA:HB2	2.34	0.44
1:J:158:VAL:HG22	1:J:159:ASN:N	2.32	0.44
1:J:165:GLU:CD	1:N:165:GLU:HB3	2.38	0.44
1:J:175:LEU:HD23	1:J:175:LEU:HA	1.76	0.44
1:K:69:GLY:CA	1:K:118:ILE:HG12	2.48	0.44
1:L:19:GLY:HA3	1:L:157:CYS:O	2.17	0.44
1:N:158:VAL:HG22	1:N:159:ASN:N	2.32	0.44
1:O:200:ILE:HA	1:O:208:TYR:O	2.18	0.44
1:C:123:ILE:HA	1:C:209:LEU:HB3	2.00	0.44
1:I:177:HIS:CE1	4:I:728:HOH:O	2.68	0.44
1:I:231:LEU:C	1:I:233:LYS:N	2.70	0.44
1:J:29:TRP:CE3	1:J:121:ILE:HB	2.53	0.44
1:L:35:MET:HG2	1:L:41:PHE:CD1	2.53	0.44
1:L:69:GLY:CA	1:L:118:ILE:HG12	2.48	0.44
1:P:175:LEU:HA	1:P:175:LEU:HD23	1.71	0.44
1:C:48:HIS:ND1	1:C:49:PRO:N	2.66	0.44
1:H:175:LEU:HD23	1:H:175:LEU:HA	1.74	0.44
1:K:32:ALA:C	1:K:33:LEU:HD12	2.38	0.44
1:M:28:PRO:HB2	1:M:119:ARG:N	2.30	0.44
1:N:49:PRO:O	1:N:112:VAL:HG22	2.18	0.44
1:O:139:SER:HA	1:O:156:GLN:O	2.18	0.44
1:O:243:GLN:HB3	1:O:244:ALA:H	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:HIS:CE1	1:D:49:PRO:HD2	2.53	0.43
1:F:200:ILE:HA	1:F:208:TYR:O	2.18	0.43
1:G:48:HIS:ND1	1:G:49:PRO:CD	2.80	0.43
1:H:166:GLU:O	1:H:167:VAL:C	2.54	0.43
1:J:42:CYS:HB3	1:J:43:SER:H	1.61	0.43
1:J:48:HIS:ND1	1:J:49:PRO:CD	2.81	0.43
1:J:111:SER:N	4:J:731:HOH:O	2.45	0.43
1:L:49:PRO:O	1:L:112:VAL:HG22	2.18	0.43
1:N:175:LEU:HD23	1:N:175:LEU:HA	1.72	0.43
1:O:35:MET:HB3	1:O:36:GLU:H	1.49	0.43
1:O:59:PHE:CB	1:O:90:ARG:HD3	2.48	0.43
1:P:48:HIS:ND1	1:P:49:PRO:N	2.65	0.43
1:A:159:ASN:HB3	1:K:116:ASP:OD1	2.18	0.43
1:D:171:LEU:HD13	1:D:225:PRO:HD2	2.00	0.43
1:D:190:SER:O	3:D:704:PBZ:N2	2.50	0.43
1:F:123:ILE:HA	1:F:209:LEU:HB3	1.99	0.43
1:G:123:ILE:HA	1:G:209:LEU:HB3	2.00	0.43
1:I:175:LEU:HD23	1:I:175:LEU:HA	1.68	0.43
1:I:231:LEU:C	1:I:233:LYS:H	2.21	0.43
1:K:48:HIS:CG	1:K:49:PRO:CD	3.01	0.43
1:K:87:LEU:C	1:K:87:LEU:HD23	2.39	0.43
1:L:48:HIS:ND1	1:L:49:PRO:N	2.66	0.43
1:M:59:PHE:CB	1:M:90:ARG:HD3	2.48	0.43
1:N:28:PRO:HB2	1:N:119:ARG:N	2.29	0.43
1:P:54:SER:OG	1:P:55:ALA:N	2.51	0.43
1:P:203:GLY:HA2	4:P:720:HOH:O	2.18	0.43
1:G:35:MET:HG2	1:G:41:PHE:CD1	2.54	0.43
1:H:231:LEU:C	1:H:233:LYS:N	2.72	0.43
1:I:166:GLU:OE2	1:O:176:TYR:HE1	2.02	0.43
1:K:87:LEU:C	1:K:87:LEU:CD2	2.87	0.43
1:L:35:MET:HB3	1:L:36:GLU:H	1.52	0.43
1:F:48:HIS:ND1	1:F:49:PRO:CD	2.82	0.43
1:F:201:CYS:O	1:F:202:ASN:HB2	2.18	0.43
1:J:45:VAL:HG11	1:J:209:LEU:HD22	2.00	0.43
1:O:191:CYS:HA	3:O:715:PBZ:C3	2.48	0.43
1:P:59:PHE:CD2	1:P:60:GLN:N	2.86	0.43
1:P:121:ILE:CG1	1:P:122:SER:N	2.81	0.43
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.77	0.43
1:A:158:VAL:HG22	1:A:159:ASN:N	2.33	0.43
1:C:29:TRP:CE3	1:C:121:ILE:HB	2.53	0.43
1:C:200:ILE:HA	1:C:208:TYR:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:SER:HB2	3:D:704:PBZ:N2	2.25	0.43
1:E:181:PHE:HZ	1:E:199:LEU:HD23	1.83	0.43
1:F:48:HIS:ND1	1:F:49:PRO:N	2.66	0.43
1:G:54:SER:OG	1:G:55:ALA:N	2.51	0.43
1:H:23:SER:O	1:H:24:PRO:C	2.56	0.43
1:H:35:MET:HG2	1:H:41:PHE:CD1	2.53	0.43
1:J:59:PHE:O	1:J:60:GLN:NE2	2.51	0.43
1:J:201:CYS:HB2	1:J:210:GLN:HE21	1.84	0.43
1:L:137:LEU:HG	1:L:138:VAL:N	2.33	0.43
1:M:200:ILE:HA	1:M:208:TYR:O	2.18	0.43
1:H:177:HIS:CD2	1:H:179:SER:H	2.37	0.43
1:L:48:HIS:CE1	1:L:49:PRO:HD2	2.54	0.43
1:N:35:MET:HB3	1:N:36:GLU:H	1.47	0.43
1:N:122:SER:CB	4:N:721:HOH:O	2.66	0.43
1:O:48:HIS:CG	1:O:49:PRO:CD	3.02	0.43
1:O:69:GLY:CA	1:O:118:ILE:HG12	2.49	0.43
1:O:123:ILE:HA	1:O:209:LEU:HB3	1.99	0.43
1:O:181:PHE:HZ	1:O:199:LEU:HD23	1.82	0.43
1:B:91:HIS:CG	1:B:92:PRO:HD2	2.54	0.43
1:G:123:ILE:HG12	1:G:209:LEU:HD23	1.99	0.43
3:H:708:PBZ:N1	4:H:710:HOH:O	2.37	0.43
1:I:22:CYS:HB2	1:I:155:LEU:O	2.18	0.43
1:I:137:LEU:HG	1:I:138:VAL:N	2.32	0.43
1:J:91:HIS:CG	1:J:92:PRO:HD2	2.54	0.43
1:K:91:HIS:O	1:K:92:PRO:C	2.57	0.43
1:N:69:GLY:CA	1:N:118:ILE:HG12	2.49	0.43
1:A:69:GLY:CA	1:A:118:ILE:HG12	2.49	0.43
1:B:231:LEU:C	1:B:233:LYS:N	2.71	0.43
1:C:103:LEU:HD23	1:C:103:LEU:N	2.31	0.43
1:D:181:PHE:HZ	1:D:199:LEU:HD23	1.82	0.43
1:E:69:GLY:CA	1:E:118:ILE:HG12	2.49	0.43
1:G:231:LEU:C	1:G:233:LYS:N	2.72	0.43
1:P:70:LEU:N	4:P:727:HOH:O	2.30	0.43
1:B:186(A):GLN:NE2	1:C:215:PHE:HB3	2.32	0.43
1:E:23:SER:O	1:E:24:PRO:C	2.55	0.43
1:E:123:ILE:HA	1:E:209:LEU:HB3	2.01	0.43
1:E:171:LEU:HD13	1:E:225:PRO:HD2	2.01	0.43
1:G:79:GLY:HA3	4:G:714:HOH:O	2.19	0.43
1:I:33:LEU:O	1:I:40:LEU:HD22	2.19	0.43
1:J:103:LEU:HB3	1:J:229:THR:HG21	2.01	0.43
1:P:69:GLY:CA	1:P:118:ILE:HG12	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:231:LEU:C	1:P:233:LYS:H	2.22	0.43
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.73	0.43
1:C:87:LEU:C	1:C:87:LEU:CD2	2.87	0.43
1:D:49:PRO:O	1:D:112:VAL:HG22	2.19	0.43
1:G:59:PHE:O	1:G:60:GLN:NE2	2.51	0.43
1:I:54:SER:OG	1:I:55:ALA:N	2.51	0.43
1:J:182:CYS:HA	1:J:226:GLY:O	2.18	0.43
1:J:200:ILE:HA	1:J:208:TYR:O	2.19	0.43
1:N:93:GLU:O	1:N:94:TYR:C	2.56	0.43
1:C:144:LEU:HB2	1:C:146:ASN:OD1	2.19	0.42
1:E:128:CYS:O	1:E:129:PRO:C	2.57	0.42
1:F:180:MET:HB2	1:F:227:VAL:CG1	2.49	0.42
1:I:103:LEU:HB3	1:I:229:THR:HG21	2.00	0.42
1:K:59:PHE:CB	1:K:90:ARG:HD3	2.47	0.42
1:K:158:VAL:HG22	1:K:159:ASN:N	2.33	0.42
1:K:175:LEU:HD23	1:K:175:LEU:HA	1.73	0.42
1:P:91:HIS:O	1:P:92:PRO:C	2.58	0.42
1:A:54:SER:OG	1:A:55:ALA:N	2.52	0.42
1:B:103:LEU:HD23	1:B:103:LEU:N	2.33	0.42
1:C:175:LEU:HA	1:C:175:LEU:HD23	1.74	0.42
1:E:231:LEU:C	1:E:233:LYS:N	2.72	0.42
1:I:48:HIS:CG	1:I:49:PRO:CD	3.02	0.42
1:J:91:HIS:O	1:J:92:PRO:C	2.57	0.42
1:K:182:CYS:N	4:K:714:HOH:O	2.36	0.42
1:L:171:LEU:HD13	1:L:225:PRO:HD2	2.01	0.42
1:O:78:PRO:C	1:O:80:SER:H	2.23	0.42
1:P:78:PRO:HA	4:P:735:HOH:O	2.12	0.42
1:C:23:SER:O	1:C:24:PRO:C	2.58	0.42
1:H:139:SER:HA	1:H:156:GLN:O	2.19	0.42
1:L:128:CYS:HB3	1:L:129:PRO:CD	2.50	0.42
1:P:189:ASP:CG	1:P:190:SER:N	2.73	0.42
1:B:165:GLU:HB3	1:F:165:GLU:HB3	2.01	0.42
1:G:69:GLY:N	1:G:118:ILE:HG12	2.34	0.42
1:I:180:MET:HB2	1:I:227:VAL:CG1	2.49	0.42
1:J:48:HIS:ND1	1:J:49:PRO:N	2.67	0.42
1:L:123:ILE:HA	1:L:209:LEU:HB3	2.00	0.42
1:M:35:MET:HG2	1:M:41:PHE:CD1	2.54	0.42
1:P:50:GLN:HG3	1:P:111:SER:CA	2.50	0.42
1:P:215:PHE:HB2	4:P:728:HOH:O	2.18	0.42
1:A:231:LEU:C	1:A:233:LYS:H	2.23	0.42
1:C:180:MET:HB2	1:C:227:VAL:CG1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:MET:HB3	1:G:36:GLU:H	1.52	0.42
1:G:103:LEU:HD23	1:G:103:LEU:N	2.34	0.42
1:G:137:LEU:HG	1:G:138:VAL:N	2.35	0.42
1:M:87:LEU:C	1:M:87:LEU:CD2	2.87	0.42
1:M:123:ILE:HD13	1:M:238:ILE:HD13	2.01	0.42
1:A:128:CYS:HB3	1:A:129:PRO:CD	2.48	0.42
1:C:177:HIS:HB3	1:C:180:MET:HE2	2.01	0.42
1:D:48:HIS:ND1	1:D:49:PRO:N	2.67	0.42
1:D:180:MET:HB2	1:D:227:VAL:CG1	2.50	0.42
1:J:87:LEU:C	1:J:87:LEU:CD2	2.87	0.42
1:M:23:SER:O	1:M:24:PRO:C	2.58	0.42
1:M:69:GLY:CA	1:M:118:ILE:HG12	2.49	0.42
1:O:94:TYR:HA	1:O:101:ASN:HB2	2.02	0.42
1:A:123:ILE:HA	1:A:209:LEU:HB3	2.02	0.42
1:B:54:SER:OG	1:B:55:ALA:N	2.52	0.42
1:B:97:PRO:O	1:B:98:LEU:C	2.58	0.42
1:E:158:VAL:HG22	1:E:159:ASN:N	2.34	0.42
1:E:180:MET:HB2	1:E:227:VAL:CG1	2.49	0.42
1:F:177:HIS:HB3	1:F:180:MET:CE	2.49	0.42
1:G:215:PHE:HA	3:G:707:PBZ:C6	2.49	0.42
1:H:190:SER:O	3:H:708:PBZ:N3	2.52	0.42
1:I:50:GLN:HG3	1:I:111:SER:CA	2.50	0.42
1:J:121:ILE:CG1	1:J:122:SER:N	2.82	0.42
1:A:48:HIS:ND1	1:A:49:PRO:N	2.68	0.42
1:A:137:LEU:HG	1:A:138:VAL:N	2.33	0.42
1:D:56:ALA:C	1:D:58:CYS:H	2.22	0.42
1:F:95:ASN:C	1:F:96:ARG:HG2	2.38	0.42
1:G:95:ASN:C	1:G:96:ARG:HG2	2.39	0.42
1:I:136:CYS:HB3	1:I:200:ILE:O	2.20	0.42
1:I:182:CYS:HA	1:I:226:GLY:O	2.20	0.42
1:J:50:GLN:HG3	1:J:111:SER:CA	2.49	0.42
1:N:136:CYS:HB3	1:N:200:ILE:O	2.19	0.42
1:P:33:LEU:O	1:P:40:LEU:HD22	2.20	0.42
1:B:200:ILE:HA	1:B:208:TYR:O	2.20	0.42
1:C:200:ILE:HG23	1:C:208:TYR:O	2.20	0.42
1:D:103:LEU:HB3	1:D:229:THR:HG21	2.02	0.42
1:D:175:LEU:HD23	1:D:175:LEU:HA	1.64	0.42
1:E:95:ASN:C	1:E:96:ARG:HG2	2.40	0.42
1:F:59:PHE:O	1:F:60:GLN:NE2	2.51	0.42
1:F:69:GLY:N	1:F:118:ILE:HG12	2.35	0.42
1:G:121:ILE:CG1	1:G:122:SER:N	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:MET:HG2	1:J:41:PHE:CD1	2.55	0.42
1:K:17:ILE:HG12	1:K:191:CYS:HB2	2.01	0.42
1:K:177:HIS:HB3	1:K:180:MET:CE	2.50	0.42
1:P:91:HIS:CG	1:P:92:PRO:HD2	2.54	0.42
1:A:191:CYS:O	1:A:192:ASN:C	2.58	0.42
1:B:35:MET:HG2	1:B:41:PHE:CD1	2.55	0.42
1:F:231:LEU:C	1:F:233:LYS:N	2.72	0.42
1:I:29:TRP:CE3	1:I:121:ILE:HB	2.54	0.42
1:L:93:GLU:O	1:L:94:TYR:C	2.54	0.42
1:O:180:MET:HB2	1:O:227:VAL:CG1	2.50	0.42
1:P:177:HIS:HB3	1:P:180:MET:HE2	2.01	0.42
1:A:231:LEU:O	1:A:232:CYS:C	2.54	0.41
1:D:231:LEU:O	1:D:233:LYS:N	2.53	0.41
1:E:103:LEU:HB3	1:E:229:THR:HG21	2.02	0.41
1:G:177:HIS:CD2	1:G:179:SER:H	2.38	0.41
1:I:93:GLU:O	1:I:94:TYR:C	2.56	0.41
1:I:166:GLU:O	1:I:167:VAL:C	2.57	0.41
1:I:179:SER:HB2	1:I:234:PHE:HZ	1.84	0.41
1:N:243:GLN:HB3	1:N:244:ALA:H	1.64	0.41
1:P:32:ALA:C	1:P:33:LEU:HD12	2.40	0.41
1:A:144:LEU:HB2	1:A:146:ASN:OD1	2.21	0.41
1:G:30:GLN:NE2	1:G:198:PRO:HG3	2.35	0.41
1:I:103:LEU:HD23	1:I:103:LEU:N	2.35	0.41
1:L:121:ILE:CG1	1:L:122:SER:N	2.82	0.41
1:N:48:HIS:ND1	1:N:49:PRO:N	2.69	0.41
1:O:191:CYS:SG	1:O:192:ASN:N	2.93	0.41
1:A:181:PHE:HZ	1:A:199:LEU:HD23	1.85	0.41
1:E:93:GLU:O	1:E:94:TYR:C	2.56	0.41
1:B:29:TRP:CE3	1:B:121:ILE:HB	2.56	0.41
1:D:123:ILE:HA	1:D:209:LEU:HB3	2.00	0.41
1:E:54:SER:OG	1:E:55:ALA:N	2.53	0.41
1:F:103:LEU:HB3	1:F:229:THR:HG21	2.02	0.41
1:G:139:SER:HA	1:G:156:GLN:O	2.21	0.41
1:G:208:TYR:CZ	1:K:125:SER:OG	2.64	0.41
1:J:23:SER:O	1:J:24:PRO:C	2.56	0.41
1:J:38:GLU:HG2	1:J:40:LEU:H	1.85	0.41
1:O:103:LEU:HD23	1:O:103:LEU:H	1.84	0.41
1:O:177:HIS:HB3	1:O:180:MET:CE	2.50	0.41
1:A:139:SER:HA	1:A:156:GLN:O	2.21	0.41
1:B:144:LEU:HB2	1:B:146:ASN:OD1	2.21	0.41
1:B:215:PHE:HA	3:B:702:PBZ:C2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:SER:OG	1:C:55:ALA:N	2.53	0.41
1:D:35:MET:HB3	1:D:36:GLU:H	1.51	0.41
1:D:87:LEU:C	1:D:87:LEU:HD23	2.40	0.41
1:E:23:SER:HA	1:E:24:PRO:HD3	1.95	0.41
1:H:48:HIS:ND1	1:H:49:PRO:HD2	2.35	0.41
1:I:123:ILE:HA	1:I:209:LEU:HB3	2.02	0.41
1:J:53:LEU:HD12	1:J:53:LEU:HA	1.77	0.41
1:J:189:ASP:CG	1:J:190:SER:N	2.73	0.41
1:L:69:GLY:N	1:L:118:ILE:HG12	2.36	0.41
1:N:231:LEU:C	1:N:233:LYS:N	2.74	0.41
1:A:23:SER:HB3	1:A:26:SER:HB3	2.03	0.41
1:D:23:SER:O	1:D:24:PRO:C	2.59	0.41
1:I:189:ASP:CG	1:I:190:SER:N	2.74	0.41
1:M:38:GLU:HG2	1:M:40:LEU:H	1.84	0.41
1:O:144:LEU:HB2	1:O:146:ASN:OD1	2.21	0.41
1:P:53:LEU:HD12	1:P:53:LEU:HA	1.79	0.41
1:P:123:ILE:HA	1:P:209:LEU:HB3	2.02	0.41
1:P:166:GLU:O	1:P:167:VAL:C	2.56	0.41
1:B:23:SER:O	1:B:24:PRO:C	2.59	0.41
1:E:186(A):GLN:HG2	1:F:57:HIS:CD2	2.55	0.41
1:H:48:HIS:CG	1:H:49:PRO:CD	3.03	0.41
1:H:177:HIS:HB3	1:H:180:MET:CE	2.51	0.41
1:J:96:ARG:HH12	1:O:233:LYS:NZ	2.19	0.41
1:J:200:ILE:HG23	1:J:208:TYR:O	2.21	0.41
1:L:175:LEU:HD23	1:L:175:LEU:HA	1.68	0.41
1:P:78:PRO:C	1:P:80:SER:N	2.74	0.41
1:D:33:LEU:O	1:D:40:LEU:HD22	2.20	0.41
1:D:200:ILE:HA	1:D:208:TYR:O	2.21	0.41
1:F:50:GLN:HG3	1:F:111:SER:CA	2.49	0.41
1:I:30:GLN:NE2	1:I:198:PRO:HG3	2.36	0.41
1:I:123:ILE:HD13	1:I:238:ILE:HD13	2.03	0.41
1:K:121:ILE:CG1	1:K:122:SER:N	2.83	0.41
3:L:712:PBZ:N1	4:L:732:HOH:O	2.37	0.41
1:M:95:ASN:C	1:M:96:ARG:HG2	2.41	0.41
1:N:200:ILE:HG23	1:N:208:TYR:O	2.20	0.41
1:O:177:HIS:CE1	1:O:178:PRO:HD2	2.55	0.41
1:P:48:HIS:ND1	1:P:49:PRO:CD	2.84	0.41
1:A:50:GLN:HG3	1:A:111:SER:CA	2.50	0.41
1:B:67:LEU:HA	1:B:67:LEU:HD23	1.87	0.41
1:B:95:ASN:C	1:B:96:ARG:HG2	2.39	0.41
1:C:95:ASN:C	1:C:96:ARG:HG2	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HG	1:C:138:VAL:N	2.36	0.41
1:D:190:SER:CB	3:D:704:PBZ:HN22	2.26	0.41
1:F:29:TRP:CE3	1:F:121:ILE:HB	2.56	0.41
1:H:123:ILE:HD13	1:H:238:ILE:HD13	2.02	0.41
1:J:60:GLN:HB2	1:J:63:TYR:CE2	2.56	0.41
1:J:128:CYS:HB3	1:J:129:PRO:CD	2.51	0.41
1:K:22:CYS:O	1:K:71:HIS:HE1	2.04	0.41
1:L:123:ILE:HD13	1:L:238:ILE:HD13	2.03	0.41
1:M:175:LEU:HA	1:M:175:LEU:HD23	1.66	0.41
1:O:50:GLN:HG3	1:O:111:SER:CA	2.51	0.41
1:P:123:ILE:HD13	1:P:238:ILE:HD13	2.03	0.41
1:C:146:ASN:OD1	1:C:150:ARG:CB	2.68	0.41
1:F:78:PRO:C	1:F:80:SER:N	2.75	0.41
1:I:48:HIS:CE1	1:I:49:PRO:HD2	2.56	0.41
1:L:48:HIS:ND1	1:L:49:PRO:CD	2.84	0.41
1:L:182:CYS:HB3	1:L:225:PRO:HB2	2.03	0.41
1:N:181:PHE:HZ	1:N:199:LEU:HD23	1.86	0.41
1:O:177:HIS:CD2	1:O:179:SER:H	2.39	0.41
1:A:176:TYR:HE1	1:G:166:GLU:OE2	2.03	0.40
1:D:69:GLY:N	1:D:118:ILE:HG12	2.37	0.40
1:H:103:LEU:HD23	1:H:103:LEU:N	2.34	0.40
1:J:180:MET:HB2	1:J:227:VAL:CG1	2.51	0.40
1:O:35:MET:HG2	1:O:41:PHE:CD1	2.56	0.40
1:P:29:TRP:CE3	1:P:121:ILE:HB	2.56	0.40
1:B:139:SER:HA	1:B:156:GLN:O	2.21	0.40
1:C:121:ILE:CG1	1:C:122:SER:N	2.85	0.40
1:C:231:LEU:C	1:C:233:LYS:N	2.73	0.40
1:D:29:TRP:CE3	1:D:121:ILE:HB	2.57	0.40
1:D:91:HIS:ND1	1:D:92:PRO:HD2	2.36	0.40
1:G:23:SER:O	1:G:24:PRO:C	2.59	0.40
1:H:200:ILE:HG23	1:H:208:TYR:O	2.21	0.40
1:K:165:GLU:HB3	1:M:165:GLU:HB3	2.02	0.40
1:M:50:GLN:HG3	1:M:111:SER:CA	2.52	0.40
1:M:177:HIS:CE1	1:M:178:PRO:HD2	2.57	0.40
1:A:94:TYR:HA	1:A:101:ASN:HB2	2.04	0.40
1:A:121:ILE:CG1	1:A:122:SER:N	2.84	0.40
1:C:177:HIS:HB3	1:C:180:MET:CE	2.51	0.40
1:C:189:ASP:CG	1:C:190:SER:N	2.75	0.40
1:D:87:LEU:C	1:D:87:LEU:CD2	2.89	0.40
1:D:93:GLU:O	1:D:94:TYR:C	2.57	0.40
1:E:177:HIS:HB3	1:E:180:MET:CE	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:LEU:O	1:E:232:CYS:C	2.53	0.40
1:F:67:LEU:HA	1:F:67:LEU:HD23	1.89	0.40
1:F:200:ILE:HG23	1:F:208:TYR:O	2.21	0.40
1:G:53:LEU:HA	1:G:53:LEU:HD12	1.77	0.40
1:H:17:ILE:HG13	1:H:220:CYS:HB3	2.03	0.40
1:I:51:TRP:CZ2	1:I:107:LYS:HD2	2.57	0.40
1:L:103:LEU:HB3	1:L:229:THR:HG21	2.04	0.40
1:M:97:PRO:O	1:M:98:LEU:C	2.60	0.40
1:P:200:ILE:HA	1:P:208:TYR:O	2.21	0.40
1:P:231:LEU:O	1:P:233:LYS:N	2.55	0.40
1:A:29:TRP:CE3	1:A:121:ILE:HB	2.56	0.40
1:C:33:LEU:O	1:C:40:LEU:HD22	2.22	0.40
1:C:48:HIS:ND1	1:C:49:PRO:CD	2.83	0.40
1:E:91:HIS:HA	1:E:92:PRO:HD3	2.00	0.40
1:F:163:VAL:HG12	1:F:164:SER:N	2.36	0.40
1:G:182:CYS:HB3	1:G:225:PRO:HB2	2.03	0.40
1:I:23:SER:O	1:I:24:PRO:C	2.60	0.40
1:L:146:ASN:OD1	1:L:150:ARG:HB2	2.21	0.40
1:M:48:HIS:ND1	1:M:49:PRO:N	2.69	0.40
1:M:103:LEU:HB3	1:M:229:THR:HG21	2.03	0.40
1:M:121:ILE:CG1	1:M:122:SER:N	2.84	0.40
1:M:189:ASP:CG	1:M:190:SER:N	2.75	0.40
1:N:143:LEU:HB2	1:N:191:CYS:SG	2.62	0.40
1:P:94:TYR:HA	1:P:101:ASN:HB2	2.03	0.40
1:A:78:PRO:C	1:A:80:SER:N	2.75	0.40
1:C:35:MET:HG2	1:C:41:PHE:CD1	2.56	0.40
1:E:48:HIS:ND1	1:E:49:PRO:N	2.70	0.40
1:G:29:TRP:CE3	1:G:121:ILE:HB	2.57	0.40
1:H:33:LEU:O	1:H:40:LEU:HD22	2.21	0.40
1:H:58:CYS:O	1:H:60:GLN:HG2	2.22	0.40
1:H:192:ASN:CG	3:H:708:PBZ:H6	2.42	0.40
1:I:231:LEU:O	1:I:233:LYS:N	2.54	0.40
1:J:94:TYR:HA	1:J:101:ASN:HB2	2.03	0.40
1:J:243:GLN:HB3	1:J:244:ALA:H	1.63	0.40
1:L:139:SER:HA	1:L:156:GLN:O	2.21	0.40
1:N:29:TRP:CE3	1:N:121:ILE:HB	2.56	0.40
1:N:111:SER:N	4:N:733:HOH:O	2.49	0.40
1:P:144:LEU:HB2	1:P:146:ASN:OD1	2.21	0.40

All (9) 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:H:119:ARG:NH1	4:F:731:HOH:O[1_565]	1.91	0.29
1:E:84:GLU:OE2	1:G:76:GLN:OE1[2_555]	2.01	0.19
1:B:75:ASP:O	1:C:146:ASN:CB[2_544]	2.02	0.18
1:I:37:ASN:OD1	4:K:720:HOH:O[2_454]	2.09	0.11
1:N:239:GLU:CG	4:L:740:HOH:O[1_545]	2.09	0.11
1:B:75:ASP:C	1:C:146:ASN:ND2[2_544]	2.10	0.10
1:B:75:ASP:O	1:C:146:ASN:ND2[2_544]	2.11	0.09
1:F:116:ASP:OD2	1:H:159:ASN:CG[1_545]	2.17	0.03
1:O:239:GLU:CG	4:C:723:HOH:O[1_455]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	6	30
1	B	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	8	37
1	C	221/223 (99%)	192 (87%)	25 (11%)	4 (2%)	8	37
1	D	221/223 (99%)	196 (89%)	21 (10%)	4 (2%)	8	37
1	E	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	8	37
1	F	221/223 (99%)	198 (90%)	19 (9%)	4 (2%)	8	37
1	G	221/223 (99%)	193 (87%)	24 (11%)	4 (2%)	8	37
1	H	221/223 (99%)	196 (89%)	19 (9%)	6 (3%)	5	26
1	I	221/223 (99%)	196 (89%)	20 (9%)	5 (2%)	6	30
1	J	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	8	37
1	K	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	8	37
1	L	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	6	30
1	M	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	8	37
1	N	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	8	37
1	O	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	6	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	8 37
All	All	3536/3568 (99%)	3115 (88%)	351 (10%)	70 (2%)	7 34

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	B	78	PRO
1	C	78	PRO
1	D	78	PRO
1	E	78	PRO
1	F	78	PRO
1	G	78	PRO
1	H	78	PRO
1	I	78	PRO
1	J	78	PRO
1	K	78	PRO
1	L	78	PRO
1	M	78	PRO
1	N	78	PRO
1	O	78	PRO
1	P	78	PRO
1	A	79	GLY
1	B	79	GLY
1	C	79	GLY
1	D	79	GLY
1	E	79	GLY
1	F	79	GLY
1	G	79	GLY
1	H	79	GLY
1	I	79	GLY
1	J	79	GLY
1	J	243	GLN
1	K	79	GLY
1	L	79	GLY
1	M	79	GLY
1	M	243	GLN
1	N	79	GLY
1	N	243	GLN
1	P	79	GLY
1	A	114	GLU
1	A	243	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	243	GLN
1	C	243	GLN
1	D	114	GLU
1	D	243	GLN
1	E	243	GLN
1	F	243	GLN
1	G	243	GLN
1	H	243	GLN
1	I	243	GLN
1	K	243	GLN
1	L	243	GLN
1	O	79	GLY
1	O	243	GLN
1	P	243	GLN
1	B	114	GLU
1	C	114	GLU
1	E	114	GLU
1	F	114	GLU
1	G	114	GLU
1	H	114	GLU
1	I	114	GLU
1	J	114	GLU
1	K	114	GLU
1	L	114	GLU
1	P	114	GLU
1	A	74	GLU
1	H	74	GLU
1	M	114	GLU
1	N	114	GLU
1	O	74	GLU
1	O	114	GLU
1	H	129	PRO
1	L	158	VAL
1	I	129	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	B	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	C	189/189 (100%)	176 (93%)	13 (7%)	15	48
1	D	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	E	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	F	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	G	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	H	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	I	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	J	189/189 (100%)	179 (95%)	10 (5%)	22	58
1	K	189/189 (100%)	179 (95%)	10 (5%)	22	58
1	L	189/189 (100%)	178 (94%)	11 (6%)	20	55
1	M	189/189 (100%)	180 (95%)	9 (5%)	25	62
1	N	189/189 (100%)	177 (94%)	12 (6%)	18	51
1	O	189/189 (100%)	179 (95%)	10 (5%)	22	58
1	P	189/189 (100%)	179 (95%)	10 (5%)	22	58
All	All	3024/3024 (100%)	2851 (94%)	173 (6%)	20	56

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	87	LEU
1	A	88	SER
1	A	122	SER
1	A	127	GLN
1	A	137	LEU
1	A	138	VAL
1	A	150	ARG
1	A	178	PRO
1	A	180	MET
1	A	190	SER
1	B	30	GLN
1	B	87	LEU
1	B	88	SER
1	B	127	GLN
1	B	137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	138	VAL
1	B	150	ARG
1	B	174	PRO
1	B	180	MET
1	B	190	SER
1	B	191	CYS
1	C	22	CYS
1	C	30	GLN
1	C	87	LEU
1	C	88	SER
1	C	127	GLN
1	C	136	CYS
1	C	137	LEU
1	C	138	VAL
1	C	150	ARG
1	C	174	PRO
1	C	180	MET
1	C	190	SER
1	C	201	CYS
1	D	30	GLN
1	D	87	LEU
1	D	88	SER
1	D	127	GLN
1	D	137	LEU
1	D	138	VAL
1	D	150	ARG
1	D	174	PRO
1	D	180	MET
1	D	190	SER
1	D	191	CYS
1	E	22	CYS
1	E	30	GLN
1	E	87	LEU
1	E	88	SER
1	E	127	GLN
1	E	137	LEU
1	E	138	VAL
1	E	150	ARG
1	E	174	PRO
1	E	180	MET
1	E	190	SER
1	F	22	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	30	GLN
1	F	87	LEU
1	F	88	SER
1	F	127	GLN
1	F	137	LEU
1	F	138	VAL
1	F	150	ARG
1	F	180	MET
1	F	190	SER
1	F	191	CYS
1	G	22	CYS
1	G	30	GLN
1	G	87	LEU
1	G	88	SER
1	G	122	SER
1	G	127	GLN
1	G	138	VAL
1	G	150	ARG
1	G	174	PRO
1	G	180	MET
1	G	190	SER
1	H	30	GLN
1	H	87	LEU
1	H	88	SER
1	H	127	GLN
1	H	137	LEU
1	H	138	VAL
1	H	150	ARG
1	H	174	PRO
1	H	178	PRO
1	H	180	MET
1	H	190	SER
1	I	30	GLN
1	I	87	LEU
1	I	88	SER
1	I	122	SER
1	I	127	GLN
1	I	137	LEU
1	I	138	VAL
1	I	150	ARG
1	I	174	PRO
1	I	180	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	190	SER
1	J	30	GLN
1	J	87	LEU
1	J	88	SER
1	J	127	GLN
1	J	137	LEU
1	J	138	VAL
1	J	150	ARG
1	J	174	PRO
1	J	180	MET
1	J	190	SER
1	K	30	GLN
1	K	87	LEU
1	K	88	SER
1	K	127	GLN
1	K	137	LEU
1	K	138	VAL
1	K	150	ARG
1	K	174	PRO
1	K	180	MET
1	K	190	SER
1	L	30	GLN
1	L	87	LEU
1	L	88	SER
1	L	127	GLN
1	L	137	LEU
1	L	138	VAL
1	L	150	ARG
1	L	174	PRO
1	L	178	PRO
1	L	180	MET
1	L	190	SER
1	M	30	GLN
1	M	87	LEU
1	M	88	SER
1	M	127	GLN
1	M	138	VAL
1	M	150	ARG
1	M	174	PRO
1	M	180	MET
1	M	190	SER
1	N	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	87	LEU
1	N	88	SER
1	N	122	SER
1	N	127	GLN
1	N	137	LEU
1	N	138	VAL
1	N	150	ARG
1	N	174	PRO
1	N	178	PRO
1	N	180	MET
1	N	190	SER
1	O	30	GLN
1	O	87	LEU
1	O	88	SER
1	O	127	GLN
1	O	137	LEU
1	O	138	VAL
1	O	150	ARG
1	O	174	PRO
1	O	180	MET
1	O	190	SER
1	P	30	GLN
1	P	87	LEU
1	P	88	SER
1	P	127	GLN
1	P	137	LEU
1	P	138	VAL
1	P	150	ARG
1	P	174	PRO
1	P	180	MET
1	P	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	30	GLN
1	A	50	GLN
1	A	61	ASN
1	A	159	ASN
1	A	177	HIS
1	A	202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	210	GLN
1	A	221	GLN
1	B	18	ASN
1	B	30	GLN
1	B	50	GLN
1	B	156	GLN
1	B	177	HIS
1	B	186(A)	GLN
1	B	202	ASN
1	B	210	GLN
1	B	221	GLN
1	C	18	ASN
1	C	30	GLN
1	C	50	GLN
1	C	156	GLN
1	C	177	HIS
1	C	186(A)	GLN
1	C	202	ASN
1	C	210	GLN
1	C	221	GLN
1	C	243	GLN
1	D	18	ASN
1	D	30	GLN
1	D	50	GLN
1	D	156	GLN
1	D	177	HIS
1	D	186(A)	GLN
1	D	202	ASN
1	D	210	GLN
1	E	18	ASN
1	E	30	GLN
1	E	76	GLN
1	E	81	GLN
1	E	156	GLN
1	E	177	HIS
1	E	202	ASN
1	E	210	GLN
1	F	18	ASN
1	F	30	GLN
1	F	50	GLN
1	F	156	GLN
1	F	177	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	202	ASN
1	F	210	GLN
1	F	221	GLN
1	F	243	GLN
1	G	18	ASN
1	G	30	GLN
1	G	50	GLN
1	G	156	GLN
1	G	177	HIS
1	G	186(A)	GLN
1	G	210	GLN
1	G	221	GLN
1	H	18	ASN
1	H	30	GLN
1	H	156	GLN
1	H	177	HIS
1	H	186(A)	GLN
1	H	202	ASN
1	H	210	GLN
1	I	18	ASN
1	I	30	GLN
1	I	50	GLN
1	I	156	GLN
1	I	177	HIS
1	I	186(A)	GLN
1	I	210	GLN
1	J	18	ASN
1	J	30	GLN
1	J	156	GLN
1	J	177	HIS
1	J	202	ASN
1	J	210	GLN
1	J	221	GLN
1	J	243	GLN
1	K	18	ASN
1	K	30	GLN
1	K	50	GLN
1	K	71	HIS
1	K	156	GLN
1	K	177	HIS
1	K	186(A)	GLN
1	K	202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	210	GLN
1	K	221	GLN
1	L	18	ASN
1	L	30	GLN
1	L	50	GLN
1	L	156	GLN
1	L	177	HIS
1	L	202	ASN
1	L	210	GLN
1	L	221	GLN
1	L	243	GLN
1	M	18	ASN
1	M	30	GLN
1	M	50	GLN
1	M	61	ASN
1	M	76	GLN
1	M	156	GLN
1	M	177	HIS
1	M	202	ASN
1	M	210	GLN
1	N	18	ASN
1	N	30	GLN
1	N	50	GLN
1	N	156	GLN
1	N	177	HIS
1	N	202	ASN
1	N	210	GLN
1	N	221	GLN
1	N	243	GLN
1	O	18	ASN
1	O	30	GLN
1	O	50	GLN
1	O	156	GLN
1	O	177	HIS
1	O	210	GLN
1	O	221	GLN
1	P	18	ASN
1	P	30	GLN
1	P	50	GLN
1	P	156	GLN
1	P	177	HIS
1	P	186(A)	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	202	ASN
1	P	210	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PBZ	C	703	-	10,10,10	1.96	4 (40%)	9,13,13	1.71	3 (33%)
3	PBZ	D	704	-	10,10,10	2.27	3 (30%)	9,13,13	1.30	1 (11%)
3	PBZ	F	706	-	10,10,10	1.59	2 (20%)	9,13,13	1.76	2 (22%)
3	PBZ	G	707	-	10,10,10	2.75	4 (40%)	9,13,13	1.72	3 (33%)
3	PBZ	J	710	-	10,10,10	1.81	2 (20%)	9,13,13	1.06	1 (11%)
3	PBZ	I	709	-	10,10,10	3.40	7 (70%)	9,13,13	0.81	0
3	PBZ	L	712	-	10,10,10	3.63	9 (90%)	9,13,13	0.78	0
3	PBZ	M	713	-	10,10,10	1.64	2 (20%)	9,13,13	1.75	3 (33%)
3	PBZ	N	714	-	10,10,10	3.27	5 (50%)	9,13,13	1.90	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PBZ	B	702	-	10,10,10	2.93	3 (30%)	9,13,13	1.40	1 (11%)
3	PBZ	P	716	-	10,10,10	3.50	8 (80%)	9,13,13	1.09	1 (11%)
3	PBZ	O	715	-	10,10,10	2.40	4 (40%)	9,13,13	1.99	5 (55%)
3	PBZ	K	711	-	10,10,10	1.91	2 (20%)	9,13,13	1.39	1 (11%)
3	PBZ	E	705	-	10,10,10	3.31	5 (50%)	9,13,13	1.33	1 (11%)
3	PBZ	A	701	-	10,10,10	4.32	7 (70%)	9,13,13	2.64	5 (55%)
3	PBZ	H	708	-	10,10,10	2.93	6 (60%)	9,13,13	1.36	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
3	PBZ	C	703	-	-	0/4/4/4	0/1/1/1
3	PBZ	D	704	-	-	3/4/4/4	0/1/1/1
3	PBZ	F	706	-	-	4/4/4/4	0/1/1/1
3	PBZ	G	707	-	-	2/4/4/4	0/1/1/1
3	PBZ	J	710	-	-	1/4/4/4	0/1/1/1
3	PBZ	I	709	-	-	2/4/4/4	0/1/1/1
3	PBZ	L	712	-	-	4/4/4/4	0/1/1/1
3	PBZ	M	713	-	-	0/4/4/4	0/1/1/1
3	PBZ	N	714	-	-	0/4/4/4	0/1/1/1
3	PBZ	B	702	-	-	2/4/4/4	0/1/1/1
3	PBZ	P	716	-	-	2/4/4/4	0/1/1/1
3	PBZ	O	715	-	-	4/4/4/4	0/1/1/1
3	PBZ	K	711	-	-	2/4/4/4	0/1/1/1
3	PBZ	E	705	-	-	0/4/4/4	0/1/1/1
3	PBZ	A	701	-	-	3/4/4/4	0/1/1/1
3	PBZ	H	708	-	-	2/4/4/4	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PBZ	C4-C7	9.24	1.64	1.47
3	A	701	PBZ	C5-C4	6.91	1.51	1.39
3	L	712	PBZ	C4-C7	6.88	1.59	1.47
3	E	705	PBZ	C4-C7	6.68	1.59	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	707	PBZ	C4-C7	6.30	1.58	1.47
3	B	702	PBZ	C5-C4	6.30	1.50	1.39
3	P	716	PBZ	C4-C7	6.12	1.58	1.47
3	P	716	PBZ	C5-C4	5.68	1.49	1.39
3	N	714	PBZ	C6-C5	5.63	1.49	1.38
3	H	708	PBZ	C2-C1	5.49	1.51	1.40
3	N	714	PBZ	C3-C4	5.30	1.48	1.39
3	E	705	PBZ	C5-C4	5.05	1.48	1.39
3	O	715	PBZ	C4-C7	5.05	1.56	1.47
3	N	714	PBZ	C6-C1	4.74	1.50	1.40
3	D	704	PBZ	C4-C7	4.67	1.55	1.47
3	I	709	PBZ	C3-C2	4.66	1.47	1.38
3	I	709	PBZ	C6-C5	4.62	1.47	1.38
3	L	712	PBZ	C5-C4	4.62	1.47	1.39
3	B	702	PBZ	C4-C7	4.55	1.55	1.47
3	I	709	PBZ	C5-C4	4.49	1.47	1.39
3	P	716	PBZ	C3-C4	4.46	1.46	1.39
3	I	709	PBZ	C2-C1	4.36	1.49	1.40
3	J	710	PBZ	C3-C2	3.90	1.45	1.38
3	H	708	PBZ	C7-N2	-3.89	1.23	1.33
3	E	705	PBZ	C1-N1	3.82	1.51	1.38
3	I	709	PBZ	C4-C7	3.73	1.54	1.47
3	K	711	PBZ	C3-C2	3.71	1.45	1.38
3	D	704	PBZ	C6-C5	3.70	1.45	1.38
3	L	712	PBZ	C6-C1	3.62	1.47	1.40
3	H	708	PBZ	C5-C4	3.56	1.45	1.39
3	F	706	PBZ	C6-C1	-3.49	1.32	1.40
3	A	701	PBZ	C6-C5	3.44	1.45	1.38
3	N	714	PBZ	C3-C2	3.43	1.45	1.38
3	O	715	PBZ	C6-C1	-3.43	1.32	1.40
3	M	713	PBZ	C6-C1	3.37	1.47	1.40
3	L	712	PBZ	C1-N1	3.30	1.49	1.38
3	A	701	PBZ	C7-N3	3.28	1.42	1.28
3	G	707	PBZ	C2-C1	3.27	1.47	1.40
3	P	716	PBZ	C3-C2	3.26	1.44	1.38
3	K	711	PBZ	C5-C4	-3.24	1.33	1.39
3	L	712	PBZ	C7-N3	3.17	1.41	1.28
3	E	705	PBZ	C7-N3	3.16	1.41	1.28
3	A	701	PBZ	C2-C1	-3.11	1.33	1.40
3	E	705	PBZ	C2-C1	3.05	1.46	1.40
3	O	715	PBZ	C3-C4	-3.05	1.34	1.39
3	D	704	PBZ	C2-C1	-3.04	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	PBZ	C3-C4	2.96	1.44	1.39
3	C	703	PBZ	C3-C2	2.93	1.44	1.38
3	A	701	PBZ	C7-N2	2.92	1.41	1.33
3	G	707	PBZ	C7-N2	2.89	1.41	1.33
3	L	712	PBZ	C7-N2	2.88	1.41	1.33
3	H	708	PBZ	C6-C5	2.87	1.44	1.38
3	C	703	PBZ	C6-C5	2.85	1.43	1.38
3	B	702	PBZ	C3-C2	2.84	1.43	1.38
3	I	709	PBZ	C6-C1	2.80	1.46	1.40
3	H	708	PBZ	C4-C7	2.80	1.52	1.47
3	L	712	PBZ	C2-C1	2.68	1.45	1.40
3	H	708	PBZ	C1-N1	2.64	1.47	1.38
3	P	716	PBZ	C7-N3	2.62	1.39	1.28
3	A	701	PBZ	C6-C1	2.58	1.45	1.40
3	M	713	PBZ	C3-C4	2.58	1.43	1.39
3	L	712	PBZ	C6-C5	2.57	1.43	1.38
3	F	706	PBZ	C3-C4	-2.57	1.34	1.39
3	I	709	PBZ	C3-C4	2.56	1.43	1.39
3	N	714	PBZ	C4-C7	2.48	1.51	1.47
3	G	707	PBZ	C5-C4	2.44	1.43	1.39
3	P	716	PBZ	C2-C1	2.39	1.45	1.40
3	C	703	PBZ	C5-C4	-2.34	1.35	1.39
3	L	712	PBZ	C3-C4	2.32	1.43	1.39
3	O	715	PBZ	C3-C2	2.29	1.42	1.38
3	P	716	PBZ	C6-C5	2.06	1.42	1.38
3	P	716	PBZ	C6-C1	2.04	1.44	1.40
3	J	710	PBZ	C5-C4	2.01	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	PBZ	C2-C1-N1	-4.80	111.97	120.91
3	A	701	PBZ	C5-C6-C1	-4.15	115.34	120.67
3	F	706	PBZ	C2-C3-C4	-3.54	116.66	120.78
3	N	714	PBZ	C6-C5-C4	-3.41	116.82	120.78
3	O	715	PBZ	C6-C5-C4	3.38	124.71	120.78
3	M	713	PBZ	C6-C5-C4	-3.15	117.11	120.78
3	N	714	PBZ	C2-C3-C4	2.96	124.22	120.78
3	G	707	PBZ	C4-C7-N2	2.95	122.50	118.05
3	B	702	PBZ	C4-C7-N2	2.95	122.50	118.05
3	G	707	PBZ	C6-C1-N1	-2.85	115.61	120.91
3	A	701	PBZ	C6-C1-N1	2.81	126.14	120.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	703	PBZ	C3-C2-C1	-2.78	117.10	120.67
3	N	714	PBZ	C5-C6-C1	2.65	124.08	120.67
3	M	713	PBZ	C3-C2-C1	-2.62	117.30	120.67
3	O	715	PBZ	C4-C7-N2	2.53	121.86	118.05
3	O	715	PBZ	C2-C3-C4	-2.45	117.93	120.78
3	A	701	PBZ	C6-C1-C2	2.41	121.88	118.15
3	O	715	PBZ	C5-C6-C1	-2.35	117.65	120.67
3	K	711	PBZ	C5-C6-C1	2.29	123.62	120.67
3	C	703	PBZ	C6-C5-C4	-2.28	118.12	120.78
3	J	710	PBZ	C2-C3-C4	-2.25	118.16	120.78
3	A	701	PBZ	C3-C2-C1	2.22	123.53	120.67
3	D	704	PBZ	C2-C1-N1	-2.20	116.81	120.91
3	F	706	PBZ	C5-C6-C1	-2.15	117.91	120.67
3	P	716	PBZ	C6-C1-C2	2.10	121.41	118.15
3	O	715	PBZ	C3-C2-C1	2.09	123.37	120.67
3	C	703	PBZ	C5-C6-C1	2.09	123.36	120.67
3	E	705	PBZ	C6-C5-C4	2.04	123.15	120.78
3	M	713	PBZ	C5-C4-C3	2.03	121.47	118.59
3	G	707	PBZ	C2-C1-N1	2.01	124.66	120.91

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	PBZ	C3-C4-C7-N2
3	D	704	PBZ	C5-C4-C7-N2
3	H	708	PBZ	C3-C4-C7-N2
3	H	708	PBZ	C5-C4-C7-N2
3	K	711	PBZ	C3-C4-C7-N2
3	K	711	PBZ	C5-C4-C7-N2
3	O	715	PBZ	C3-C4-C7-N2
3	O	715	PBZ	C5-C4-C7-N2
3	P	716	PBZ	C3-C4-C7-N2
3	P	716	PBZ	C5-C4-C7-N2
3	B	702	PBZ	C5-C4-C7-N3
3	I	709	PBZ	C5-C4-C7-N3
3	O	715	PBZ	C3-C4-C7-N3
3	O	715	PBZ	C5-C4-C7-N3
3	A	701	PBZ	C3-C4-C7-N2
3	A	701	PBZ	C5-C4-C7-N2
3	F	706	PBZ	C3-C4-C7-N2
3	F	706	PBZ	C5-C4-C7-N2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	707	PBZ	C5-C4-C7-N2
3	I	709	PBZ	C3-C4-C7-N2
3	J	710	PBZ	C3-C4-C7-N2
3	L	712	PBZ	C3-C4-C7-N2
3	L	712	PBZ	C5-C4-C7-N2
3	A	701	PBZ	C3-C4-C7-N3
3	B	702	PBZ	C3-C4-C7-N3
3	D	704	PBZ	C3-C4-C7-N3
3	F	706	PBZ	C3-C4-C7-N3
3	F	706	PBZ	C5-C4-C7-N3
3	G	707	PBZ	C3-C4-C7-N3
3	L	712	PBZ	C3-C4-C7-N3
3	L	712	PBZ	C5-C4-C7-N3

There are no ring outliers.

14 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	704	PBZ	7	0
3	F	706	PBZ	1	0
3	G	707	PBZ	2	0
3	J	710	PBZ	2	0
3	I	709	PBZ	2	0
3	L	712	PBZ	1	0
3	M	713	PBZ	2	0
3	N	714	PBZ	2	0
3	B	702	PBZ	2	0
3	P	716	PBZ	6	0
3	O	715	PBZ	8	0
3	E	705	PBZ	2	0
3	A	701	PBZ	2	0
3	H	708	PBZ	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	220/223 (98%)	-0.07	5 (2%)	60	31	9, 32, 56, 68	28 (12%)
1	B	222/223 (99%)	-0.17	7 (3%)	47	20	7, 30, 56, 65	20 (9%)
1	C	223/223 (100%)	-0.21	6 (2%)	54	26	7, 31, 56, 69	18 (8%)
1	D	222/223 (99%)	-0.10	3 (1%)	75	49	6, 30, 58, 67	22 (9%)
1	E	223/223 (100%)	-0.25	2 (0%)	84	63	7, 30, 55, 65	24 (10%)
1	F	223/223 (100%)	-0.22	3 (1%)	77	51	4, 27, 54, 64	17 (7%)
1	G	223/223 (100%)	-0.04	5 (2%)	62	33	5, 31, 58, 67	20 (8%)
1	H	223/223 (100%)	-0.05	6 (2%)	54	26	9, 31, 56, 68	30 (13%)
1	I	223/223 (100%)	-0.03	4 (1%)	68	40	10, 32, 56, 65	30 (13%)
1	J	223/223 (100%)	-0.15	4 (1%)	68	40	7, 32, 58, 65	18 (8%)
1	K	222/223 (99%)	-0.11	3 (1%)	75	49	5, 31, 56, 64	22 (9%)
1	L	223/223 (100%)	-0.13	4 (1%)	68	40	5, 32, 57, 67	20 (8%)
1	M	223/223 (100%)	-0.29	3 (1%)	77	51	6, 27, 54, 62	16 (7%)
1	N	223/223 (100%)	-0.17	7 (3%)	49	21	4, 29, 56, 68	18 (8%)
1	O	223/223 (100%)	-0.29	2 (0%)	84	63	6, 27, 55, 63	19 (8%)
1	P	223/223 (100%)	-0.01	5 (2%)	62	33	8, 32, 57, 65	23 (10%)
All	All	3562/3568 (99%)	-0.14	69 (1%)	66	37	4, 30, 57, 69	345 (9%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	190	SER	6.0
1	C	190	SER	4.5
1	H	190	SER	4.3
1	H	76	GLN	4.2
1	E	145	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	244	ALA	4.0
1	J	244	ALA	3.9
1	P	45	VAL	3.9
1	A	190	SER	3.8
1	B	45	VAL	3.8
1	L	190	SER	3.7
1	N	147	GLY	3.4
1	P	74(A)	ALA	3.4
1	N	75	ASP	3.4
1	F	244	ALA	3.4
1	C	74(A)	ALA	3.4
1	I	190	SER	3.4
1	K	45	VAL	3.3
1	H	45	VAL	3.2
1	B	190	SER	3.2
1	C	146	ASN	3.1
1	H	75	ASP	3.1
1	J	146	ASN	3.1
1	F	36	GLU	3.1
1	O	45	VAL	3.0
1	C	45	VAL	3.0
1	I	244	ALA	2.9
1	M	190	SER	2.9
1	B	146	ASN	2.8
1	H	244	ALA	2.8
1	G	78	PRO	2.8
1	O	190	SER	2.8
1	P	117	THR	2.8
1	G	45	VAL	2.7
1	F	190	SER	2.6
1	D	190	SER	2.6
1	B	244	ALA	2.5
1	B	147	GLY	2.5
1	A	244	ALA	2.5
1	B	36	GLU	2.5
1	C	243	GLN	2.5
1	J	243	GLN	2.5
1	B	145	ALA	2.4
1	D	62	SER	2.4
1	M	45	VAL	2.4
1	N	219	PRO	2.4
1	P	145	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	79	GLY	2.4
1	N	45	VAL	2.4
1	J	45	VAL	2.4
1	A	92	PRO	2.4
1	L	74(A)	ALA	2.4
1	M	244	ALA	2.3
1	E	75	ASP	2.3
1	A	146	ASN	2.3
1	D	133	GLY	2.3
1	N	244	ALA	2.3
1	H	74(A)	ALA	2.3
1	I	208	TYR	2.2
1	G	190	SER	2.2
1	N	125	SER	2.2
1	P	190	SER	2.2
1	G	75	ASP	2.2
1	N	190	SER	2.2
1	A	75	ASP	2.1
1	K	109	ASP	2.1
1	I	152	PRO	2.1
1	G	18	ASN	2.0
1	C	75	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	PBZ	G	707	10/10	0.85	0.31	62,65,66,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PBZ	L	712	10/10	0.86	0.25	35,37,42,45	0
3	PBZ	N	714	10/10	0.86	0.28	33,39,41,45	0
3	PBZ	M	713	10/10	0.87	0.24	24,26,28,33	0
3	PBZ	P	716	10/10	0.87	0.25	25,33,34,36	0
3	PBZ	E	705	10/10	0.88	0.23	14,30,31,32	0
3	PBZ	B	702	10/10	0.88	0.28	40,47,50,53	0
3	PBZ	I	709	10/10	0.89	0.27	45,46,48,50	0
3	PBZ	J	710	10/10	0.90	0.24	38,39,42,42	0
3	PBZ	K	711	10/10	0.91	0.23	32,36,39,42	0
3	PBZ	F	706	10/10	0.91	0.23	22,26,28,28	0
3	PBZ	C	703	10/10	0.91	0.23	34,39,41,42	0
3	PBZ	D	704	10/10	0.91	0.21	17,21,22,24	0
3	PBZ	O	715	10/10	0.91	0.23	37,39,46,48	0
2	CO	A	1	1/1	0.91	0.09	62,62,62,62	0
3	PBZ	H	708	10/10	0.92	0.21	27,31,34,36	0
3	PBZ	A	701	10/10	0.93	0.19	14,19,26,33	0
2	CO	E	2	1/1	0.97	0.06	35,35,35,35	0
2	CO	I	3	1/1	0.97	0.04	63,63,63,63	0
2	CO	M	4	1/1	0.99	0.07	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.