



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 7OK9 / pdb_00007ok9
Title : Crystal structure of Penicillin-Binding Protein 1 (PBP1) from *Staphylococcus aureus* in complex with pentaglycine
Authors : Martinez Caballero, S.; Hermoso, J.A.
Deposited on : 2021-05-17
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

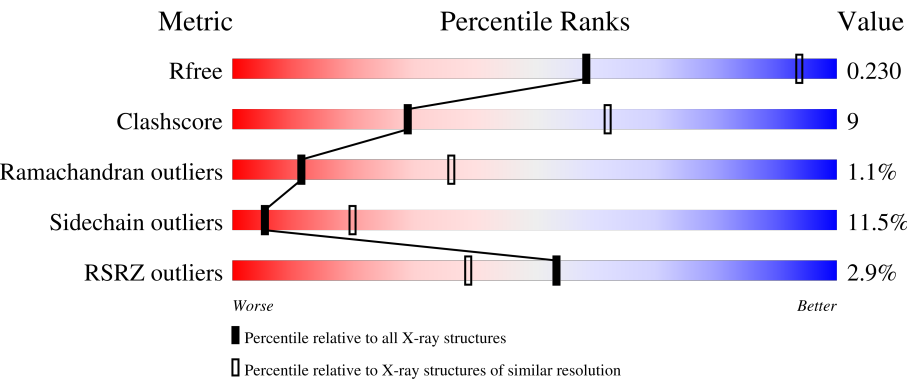
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.36 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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

Mol	Chain	Length	Quality of chain
1	A	650	2% 59%18%20%
1	B	650	2% 60%16%19%
1	C	650	2% 59%17%20%
1	D	650	4% 57%16%24%
1	E	650	2% 60%17%19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	650	
1	G	650	
1	H	650	
1	I	650	
1	J	650	
1	K	650	
1	L	650	
2	P	5	
2	Q	5	
2	R	5	
2	S	5	
2	T	5	
2	U	5	
2	V	5	
2	W	5	
2	X	5	
2	Y	5	

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
4	CL	D	802	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47917 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 Penicillin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4113	2613	707	777	16			
1	B	525	Total	C	N	O	S	0	0	0
			4138	2628	712	782	16			
1	C	522	Total	C	N	O	S	0	0	0
			4114	2614	708	776	16			
1	D	496	Total	C	N	O	S	0	0	0
			3913	2489	668	740	16			
1	E	524	Total	C	N	O	S	0	0	0
			4129	2623	711	779	16			
1	F	523	Total	C	N	O	S	0	0	0
			4122	2618	710	778	16			
1	G	520	Total	C	N	O	S	0	0	0
			4098	2604	705	773	16			
1	H	465	Total	C	N	O	S	0	0	0
			3661	2326	626	694	15			
1	I	519	Total	C	N	O	S	0	0	0
			4089	2598	703	772	16			
1	J	518	Total	C	N	O	S	0	0	0
			4080	2592	701	771	16			
1	K	462	Total	C	N	O	S	0	0	0
			3629	2306	619	690	14			
1	L	462	Total	C	N	O	S	0	0	0
			3646	2318	622	691	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	cloning artifact	UNP A0A0H2WVW5
B	64	MET	-	cloning artifact	UNP A0A0H2WVW5
C	64	MET	-	cloning artifact	UNP A0A0H2WVW5
D	64	MET	-	cloning artifact	UNP A0A0H2WVW5
E	64	MET	-	cloning artifact	UNP A0A0H2WVW5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	64	MET	-	cloning artifact	UNP A0A0H2WVW5
G	64	MET	-	cloning artifact	UNP A0A0H2WVW5
H	64	MET	-	cloning artifact	UNP A0A0H2WVW5
I	64	MET	-	cloning artifact	UNP A0A0H2WVW5
J	64	MET	-	cloning artifact	UNP A0A0H2WVW5
K	64	MET	-	cloning artifact	UNP A0A0H2WVW5
L	64	MET	-	cloning artifact	UNP A0A0H2WVW5

- Molecule 2 is a protein called pentaglycine.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			21	10	5	6			
2	Q	5	Total	C	N	O	0	0	0
			21	10	5	6			
2	R	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	S	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	T	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	U	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	V	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	W	4	Total	C	N	O	0	0	1
			13	6	4	3			
2	X	4	Total	C	N	O	0	0	1
			13	6	4	3			
2	Y	4	Total	C	N	O	0	0	1
			13	6	4	3			

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cd	0	0
			1	1		
3	B	1	Total	Cd	0	0
			1	1		
3	C	1	Total	Cd	0	0
			1	1		
3	D	1	Total	Cd	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cd	0	0
			1	1		
3	F	1	Total	Cd	0	0
			1	1		
3	G	1	Total	Cd	0	0
			1	1		
3	H	1	Total	Cd	0	0
			1	1		
3	I	1	Total	Cd	0	0
			1	1		
3	J	1	Total	Cd	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

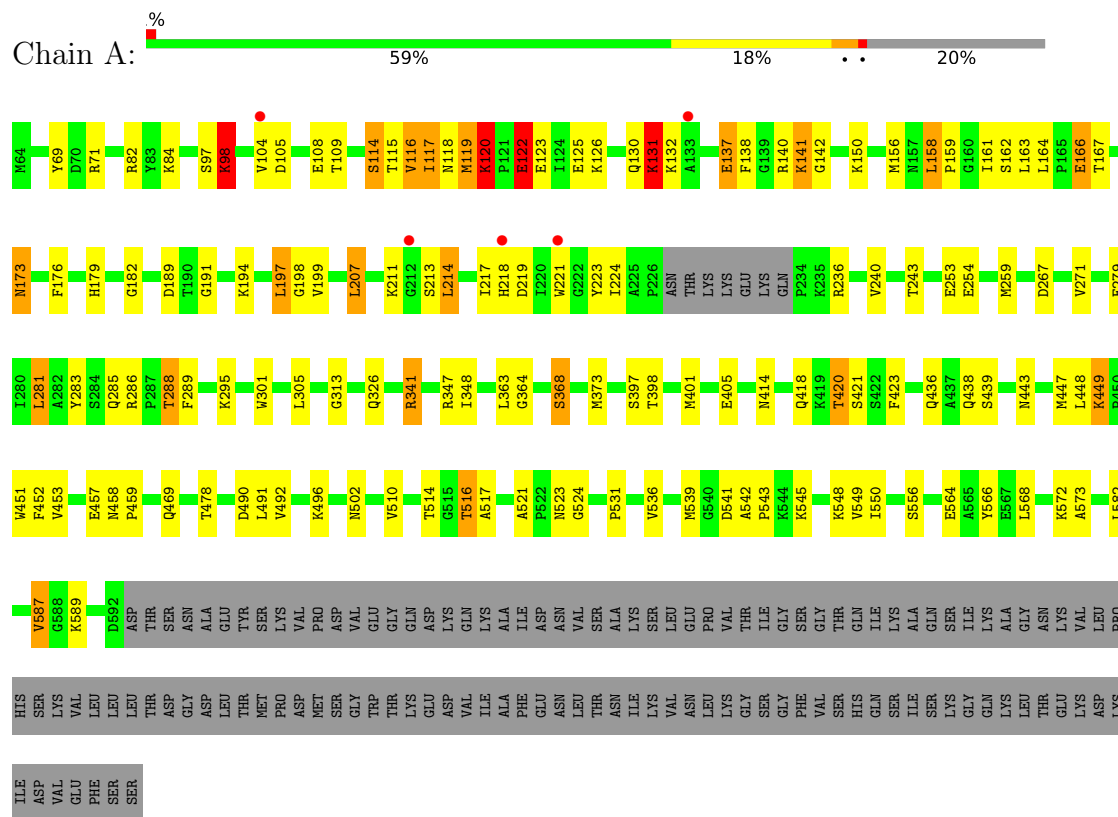
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	F	2	Total	O	0	0
			2	2		
5	H	1	Total	O	0	0
			1	1		
5	J	1	Total	O	0	0
			1	1		

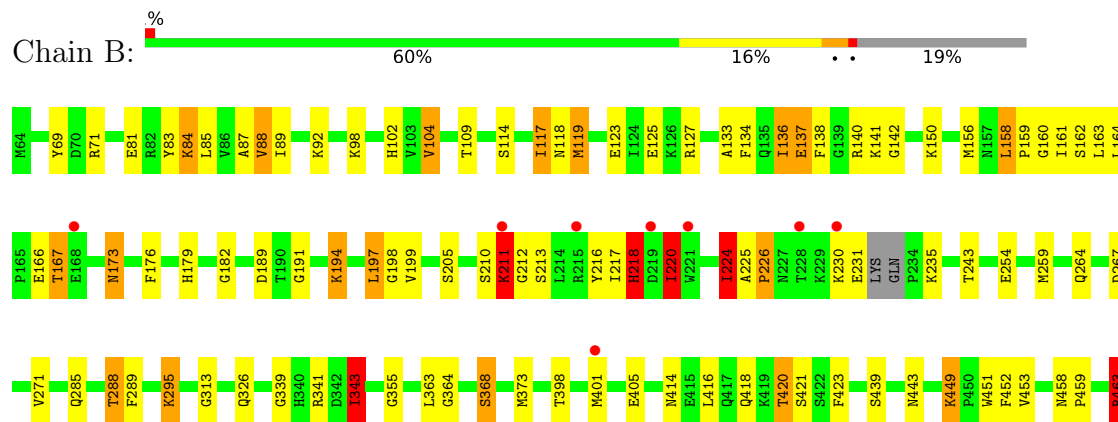
3 Residue-property plots [i](#)

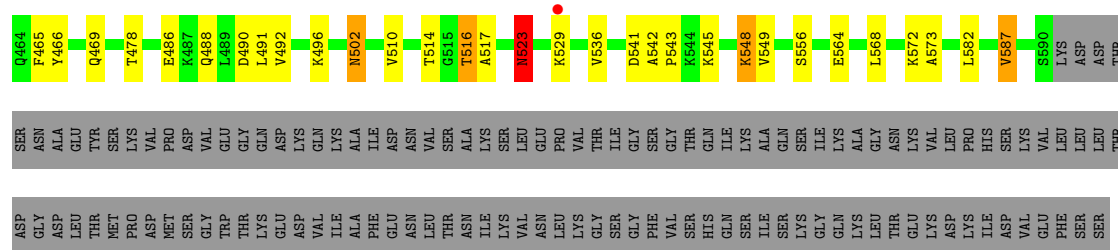
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Penicillin-binding protein 1

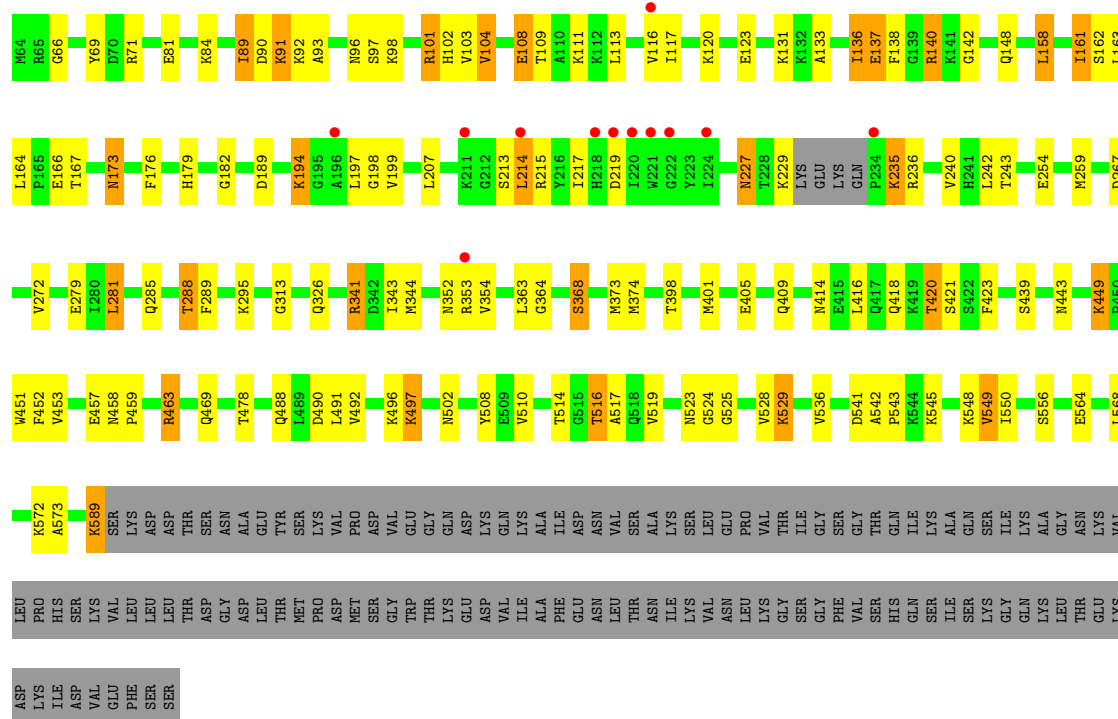


• Molecule 1: Penicillin-binding protein 1

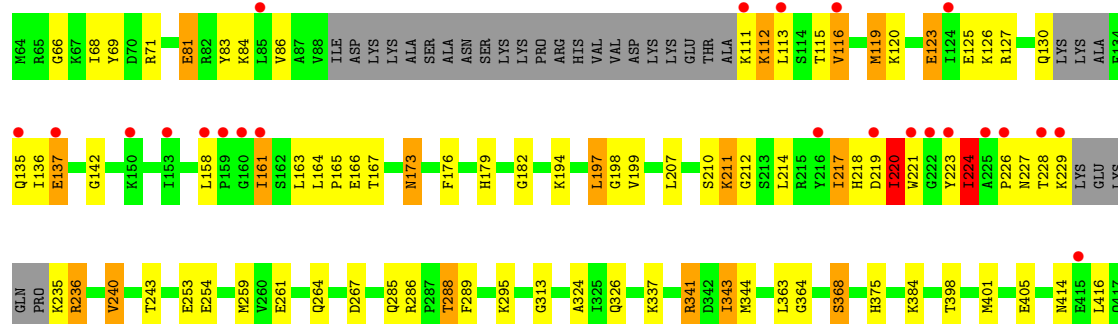


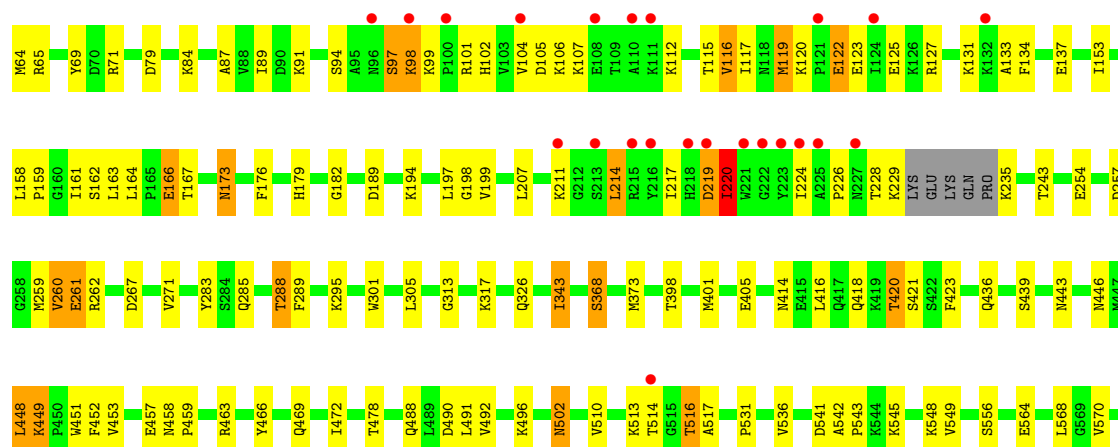


• Molecule 1: Penicillin-binding protein 1

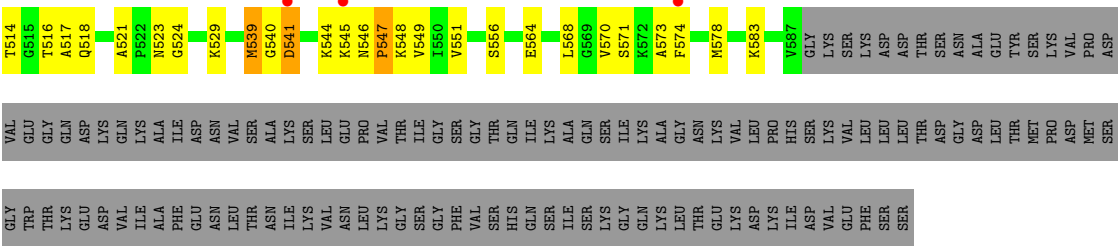


• Molecule 1: Penicillin-binding protein 1

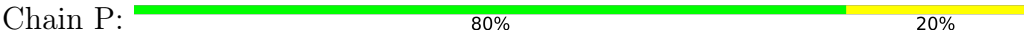








● Molecule 2: pentaglycine



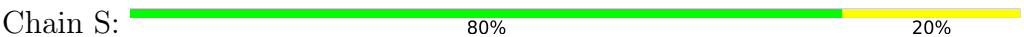
● Molecule 2: pentaglycine



● Molecule 2: pentaglycine



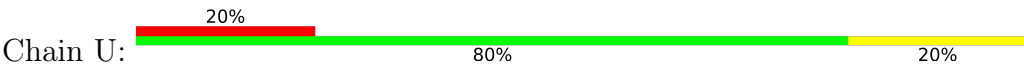
● Molecule 2: pentaglycine



● Molecule 2: pentaglycine



● Molecule 2: pentaglycine

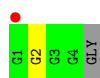




- Molecule 2: pentaglycine



- Molecule 2: pentaglycine



- Molecule 2: pentaglycine



- Molecule 2: pentaglycine



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	313.99Å 198.19Å 220.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.36 49.32 – 3.36	Depositor EDS
% Data completeness (in resolution range)	44.1 (49.32-3.36) 44.1 (49.32-3.36)	Depositor EDS
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.230 , 0.267 (Not available) , 0.230	Depositor DCC
R_{free} test set	4313 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47917	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL

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	1.03	3/4203 (0.1%)	1.23	4/5652 (0.1%)
1	B	1.03	6/4228 (0.1%)	1.22	4/5685 (0.1%)
1	C	1.04	4/4204 (0.1%)	1.22	8/5654 (0.1%)
1	D	1.03	7/3998 (0.2%)	1.22	6/5378 (0.1%)
1	E	1.03	5/4219 (0.1%)	1.21	2/5673 (0.0%)
1	F	1.04	5/4211 (0.1%)	1.21	4/5662 (0.1%)
1	G	1.02	5/4188 (0.1%)	1.21	2/5633 (0.0%)
1	H	1.06	8/3743 (0.2%)	1.21	7/5037 (0.1%)
1	I	1.02	5/4178 (0.1%)	1.20	7/5619 (0.1%)
1	J	1.04	8/4169 (0.2%)	1.22	3/5608 (0.1%)
1	K	1.03	5/3708 (0.1%)	1.18	6/4989 (0.1%)
1	L	1.02	4/3728 (0.1%)	1.18	3/5017 (0.1%)
2	P	1.21	0/20	1.81	0/22
2	Q	1.42	0/20	2.13	0/22
2	R	1.44	0/16	0.98	0/19
2	S	1.81	0/16	1.62	1/19 (5.3%)
2	T	2.25	1/16 (6.2%)	1.22	0/19
2	U	1.27	0/16	1.22	0/19
2	V	1.34	0/16	1.68	1/19 (5.3%)
2	W	1.23	0/12	2.63	2/14 (14.3%)
2	X	1.34	0/12	1.36	0/14
2	Y	1.47	0/12	0.73	0/14
All	All	1.03	66/48933 (0.1%)	1.21	60/65788 (0.1%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	ALA	C-O	7.23	1.32	1.24
1	H	85	LEU	C-O	-6.94	1.15	1.24
1	B	69	TYR	C-O	6.27	1.31	1.23
1	J	586	ASN	C-O	6.25	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	69	TYR	C-O	6.12	1.31	1.23
1	I	69	TYR	C-O	6.08	1.31	1.23
1	J	343	ILE	C-O	6.07	1.30	1.24
1	C	69	TYR	C-O	6.04	1.31	1.23
1	E	254	GLU	C-O	6.01	1.31	1.24
1	G	69	TYR	C-O	5.99	1.31	1.23
1	D	69	TYR	C-O	5.89	1.31	1.23
1	J	148	GLN	C-O	5.88	1.31	1.24
1	J	254	GLU	C-O	5.85	1.30	1.24
1	A	254	GLU	C-O	5.83	1.30	1.24
1	F	254	GLU	C-O	5.78	1.30	1.24
1	A	69	TYR	C-O	5.75	1.31	1.23
1	E	69	TYR	C-O	5.71	1.31	1.23
1	H	254	GLU	C-O	5.71	1.30	1.24
1	L	254	GLU	C-O	5.71	1.30	1.24
1	J	69	TYR	C-O	5.67	1.31	1.23
1	C	254	GLU	C-O	5.61	1.30	1.24
1	I	254	GLU	C-O	5.60	1.30	1.24
1	B	343	ILE	C-O	5.59	1.29	1.24
1	G	254	GLU	C-O	5.58	1.30	1.24
1	L	69	TYR	C-O	5.57	1.30	1.23
1	J	87	ALA	C-O	5.56	1.30	1.24
1	K	500	ALA	C-O	5.55	1.31	1.24
1	C	207	LEU	C-O	5.52	1.30	1.24
1	H	586	ASN	C-O	5.49	1.31	1.23
1	H	144	ASN	C-O	5.48	1.30	1.23
1	B	254	GLU	C-O	5.46	1.30	1.24
1	H	420	THR	C-O	5.42	1.30	1.24
1	H	343	ILE	C-O	5.40	1.29	1.24
1	B	264	GLN	N-CA	5.40	1.50	1.46
1	K	207	LEU	C-O	5.39	1.30	1.24
1	H	86	VAL	C-O	5.38	1.30	1.23
1	J	420	THR	C-O	5.38	1.30	1.24
1	L	420	THR	C-O	5.35	1.30	1.24
1	I	420	THR	C-O	5.33	1.30	1.24
1	I	264	GLN	N-CA	5.31	1.50	1.46
1	B	87	ALA	C-O	5.29	1.29	1.24
1	E	420	THR	C-O	5.28	1.30	1.24
1	B	420	THR	C-O	5.28	1.30	1.24
1	F	420	THR	C-O	5.28	1.30	1.24
1	A	420	THR	C-O	5.24	1.30	1.24
1	C	420	THR	C-O	5.24	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	343	ILE	C-O	5.24	1.29	1.24
1	D	586	ASN	C-O	5.23	1.30	1.23
1	G	420	THR	C-O	5.22	1.30	1.24
1	D	254	GLU	C-O	5.22	1.30	1.24
1	K	420	THR	C-O	5.21	1.30	1.24
1	D	264	GLN	N-CA	5.17	1.50	1.46
1	E	264	GLN	N-CA	5.17	1.50	1.46
1	G	207	LEU	C-O	5.17	1.30	1.24
1	L	264	GLN	N-CA	5.17	1.50	1.46
1	J	264	GLN	N-CA	5.13	1.50	1.46
1	F	207	LEU	C-O	5.13	1.29	1.24
1	H	264	GLN	N-CA	5.11	1.50	1.46
1	K	586	ASN	C-O	5.08	1.30	1.23
1	I	207	LEU	C-O	5.08	1.29	1.24
1	D	324	ALA	C-O	5.07	1.29	1.24
1	G	586	ASN	C-O	5.06	1.30	1.23
2	T	2	GLY	N-CA	5.05	1.50	1.45
1	E	207	LEU	C-O	5.03	1.29	1.24
1	K	371	THR	C-O	5.02	1.29	1.24
1	D	420	THR	C-O	5.02	1.30	1.24

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	523	ASN	CA-C-O	-11.09	112.79	119.55
1	C	354	VAL	N-CA-C	-10.54	103.36	111.90
1	J	587	VAL	CA-C-O	-9.92	110.09	120.71
1	H	587	VAL	CA-C-O	-9.89	110.13	120.71
1	K	409	GLN	CB-CG-CD	-7.28	100.23	112.60
1	H	218	HIS	CB-CA-C	7.22	118.68	109.80
1	C	421	SER	CA-C-O	-7.05	113.08	120.55
1	K	421	SER	CA-C-O	-7.02	113.11	120.55
1	F	421	SER	CA-C-O	-7.00	113.13	120.55
1	D	86	VAL	CA-C-O	-6.96	114.73	121.63
1	D	421	SER	CA-C-O	-6.93	113.20	120.55
1	B	421	SER	CA-C-O	-6.93	113.21	120.55
1	A	120	LYS	CA-C-O	-6.91	114.80	119.29
1	J	421	SER	CA-C-O	-6.89	113.25	120.55
1	I	421	SER	CA-C-O	-6.87	113.26	120.55
1	H	421	SER	CA-C-O	-6.86	113.28	120.55
1	G	421	SER	CA-C-O	-6.85	113.29	120.55
1	E	421	SER	CA-C-O	-6.85	113.29	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	421	SER	CA-C-O	-6.84	113.30	120.55
1	A	421	SER	CA-C-O	-6.78	113.37	120.55
1	I	141	LYS	N-CA-C	6.71	120.34	111.75
1	K	261	GLU	N-CA-C	-6.45	103.54	111.40
2	W	2	GLY	CA-C-O	-6.40	118.06	122.22
2	W	2	GLY	N-CA-C	-6.24	106.02	111.95
1	A	122	GLU	CB-CG-CD	5.85	122.55	112.60
1	C	352	ASN	N-CA-C	-5.75	106.26	113.28
1	F	219	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	548	LYS	N-CA-C	-5.55	106.18	113.12
1	H	523	ASN	O-C-N	5.45	125.61	120.71
1	K	200	GLU	CA-CB-CG	-5.44	103.22	114.10
1	H	523	ASN	CA-C-O	-5.39	116.26	119.55
1	I	548	LYS	N-CA-C	-5.38	106.40	113.12
1	I	220	ILE	N-CA-C	-5.38	106.62	112.80
1	J	496	LYS	N-CA-C	-5.36	106.68	113.43
1	I	102	HIS	CA-C-O	-5.32	115.39	121.40
2	S	2	GLY	N-CA-C	-5.31	105.49	112.81
1	K	514	THR	CA-C-O	-5.30	115.93	121.55
1	F	514	THR	CA-C-O	-5.29	115.94	121.55
1	F	548	LYS	N-CA-C	-5.28	106.52	113.12
1	H	514	THR	CA-C-O	-5.26	115.98	121.55
1	H	548	LYS	N-CA-C	-5.25	106.55	113.12
1	A	514	THR	CA-C-O	-5.25	115.99	121.55
1	D	514	THR	CA-C-O	-5.24	116.00	121.55
1	B	463	ARG	CB-CG-CD	5.19	123.24	111.30
1	B	514	THR	CA-C-O	-5.19	116.05	121.55
2	V	2	GLY	N-CA-C	-5.18	104.74	111.52
1	L	514	THR	CA-C-O	-5.17	116.07	121.55
1	C	514	THR	CA-C-O	-5.17	116.08	121.55
1	C	104	VAL	N-CA-C	-5.15	106.78	111.67
1	K	217	ILE	CA-C-O	-5.14	115.92	121.27
1	L	541	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	104	VAL	CA-C-O	-5.14	115.30	120.69
1	E	159	PRO	CA-C-O	-5.13	114.92	120.92
1	G	514	THR	CA-C-O	-5.10	116.14	121.55
1	D	523	ASN	O-C-N	5.09	125.30	120.71
1	C	102	HIS	CA-C-O	-5.09	115.65	121.40
1	C	463	ARG	CB-CG-CD	5.05	122.91	111.30
1	I	106	LYS	CA-C-N	5.05	127.31	120.65
1	I	106	LYS	C-N-CA	5.05	127.31	120.65
1	D	548	LYS	N-CA-C	-5.00	106.87	113.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4113	0	4100	102	0
1	B	4138	0	4128	83	0
1	C	4114	0	4104	68	0
1	D	3913	0	3877	74	0
1	E	4129	0	4122	70	0
1	F	4122	0	4114	74	0
1	G	4098	0	4084	82	0
1	H	3661	0	3597	54	0
1	I	4089	0	4075	62	0
1	J	4080	0	4062	62	0
1	K	3629	0	3570	53	0
1	L	3646	0	3579	77	0
2	P	21	0	17	1	0
2	Q	21	0	17	0	0
2	R	17	0	14	0	0
2	S	17	0	14	0	0
2	T	17	0	14	0	0
2	U	17	0	14	0	0
2	V	17	0	14	1	0
2	W	13	0	11	0	0
2	X	13	0	11	1	0
2	Y	13	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	D	1	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	H	1	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	2	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
All	All	47917	0	47549	830	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (830) 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:D:66:GLY:HA2	1:D:236:ARG:NH2	1.40	1.36
1:A:539:MET:HE1	1:A:550:ILE:CG2	1.62	1.26
1:D:84:LYS:CE	1:D:137:GLU:HG2	1.71	1.17
1:F:439:SER:HB2	1:F:448:LEU:CD1	1.80	1.11
1:L:429:VAL:HG21	1:L:434:MET:HE3	1.28	1.11
1:G:581:THR:O	1:G:585:LEU:HD22	1.49	1.10
1:F:439:SER:HB2	1:F:448:LEU:HD12	1.32	1.09
1:D:84:LYS:HE2	1:D:137:GLU:CG	1.81	1.09
1:H:164:LEU:HD22	1:H:165:PRO:HD2	1.17	1.09
1:A:539:MET:CE	1:A:550:ILE:HG23	1.82	1.09
1:A:539:MET:CE	1:A:550:ILE:CG2	2.31	1.08
1:D:84:LYS:HE2	1:D:137:GLU:HG2	1.09	1.03
1:B:136:ILE:HD13	1:B:137:GLU:O	1.59	1.01
1:A:539:MET:HE1	1:A:550:ILE:HG21	1.42	0.96
1:F:439:SER:CB	1:F:448:LEU:HD12	1.97	0.94
1:D:66:GLY:HA2	1:D:236:ARG:HH21	1.32	0.91
1:C:161:ILE:HD12	1:C:161:ILE:O	1.72	0.90
1:D:66:GLY:HA2	1:D:236:ARG:HH22	1.25	0.90
1:G:584:TYR:CD1	1:G:585:LEU:HD13	2.08	0.89
1:D:66:GLY:CA	1:D:236:ARG:NH2	2.33	0.88
1:L:394:PHE:CE1	1:L:434:MET:HE2	2.09	0.88
1:C:109:THR:HG23	1:C:158:LEU:HD22	1.57	0.87
1:J:119:MET:HE2	1:J:141:LYS:HE2	1.54	0.87
1:J:259:MET:HE1	1:J:572:LYS:HB2	1.57	0.86
1:E:259:MET:HE1	1:E:572:LYS:HB2	1.57	0.86
1:C:259:MET:HE1	1:C:572:LYS:HB2	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:MET:HE1	1:H:572:LYS:HB2	1.57	0.85
1:I:259:MET:HE1	1:I:572:LYS:HB2	1.57	0.85
1:A:120:LYS:HB3	1:A:122:GLU:OE2	1.76	0.85
1:L:425:GLN:OE1	1:L:518:GLN:HG3	1.77	0.85
1:D:259:MET:HE1	1:D:572:LYS:HB2	1.57	0.84
1:G:259:MET:HE1	1:G:572:LYS:HB2	1.57	0.84
1:A:259:MET:HE1	1:A:572:LYS:HB2	1.57	0.84
1:B:259:MET:HE1	1:B:572:LYS:HB2	1.57	0.83
1:J:109:THR:HG23	1:J:158:LEU:HD22	1.57	0.83
1:J:117:ILE:HD11	1:J:141:LYS:HB2	1.60	0.82
1:A:539:MET:HE3	1:A:550:ILE:HG23	1.62	0.80
1:A:116:VAL:O	1:A:117:ILE:HG22	1.81	0.80
1:F:343:ILE:HD11	1:F:416:LEU:HA	1.64	0.79
1:L:214:LEU:HB2	1:L:228:THR:HG21	1.64	0.79
1:B:136:ILE:CD1	1:B:137:GLU:O	2.32	0.77
1:G:584:TYR:HD1	1:G:585:LEU:HD13	1.48	0.76
1:L:217:ILE:HD11	1:L:401:MET:HE1	1.67	0.76
1:D:84:LYS:HE2	1:D:137:GLU:CD	2.11	0.76
1:G:551:VAL:CG1	1:G:574:PHE:CE2	2.69	0.75
1:F:271:VAL:HG22	1:F:283:TYR:HD1	1.52	0.75
1:L:343:ILE:HD11	1:L:416:LEU:HA	1.70	0.74
1:L:217:ILE:HG23	1:L:466:TYR:HB2	1.70	0.74
1:G:271:VAL:HG22	1:G:283:TYR:HD1	1.52	0.74
1:A:301:TRP:CE3	1:B:194:LYS:HD2	2.22	0.74
1:D:214:LEU:HB2	1:D:227:ASN:HB2	1.69	0.73
1:A:271:VAL:HG22	1:A:283:TYR:HD1	1.53	0.73
1:E:260:VAL:O	1:E:264:GLN:NE2	2.22	0.73
1:L:260:VAL:O	1:L:264:GLN:NE2	2.22	0.72
1:G:462:LYS:HE3	1:G:462:LYS:HA	1.72	0.71
1:D:344:MET:HE2	1:D:416:LEU:HB2	1.73	0.71
1:J:343:ILE:HD11	1:J:416:LEU:HA	1.72	0.71
1:B:343:ILE:HD11	1:B:416:LEU:HA	1.71	0.71
1:J:119:MET:HE2	1:J:141:LYS:CE	2.21	0.70
1:L:394:PHE:HE1	1:L:434:MET:HE2	1.50	0.70
1:C:344:MET:HE2	1:C:416:LEU:HB2	1.74	0.70
1:H:344:MET:HE2	1:H:416:LEU:HB2	1.74	0.70
1:A:117:ILE:HG13	1:A:118:ASN:H	1.57	0.70
1:A:118:ASN:ND2	1:A:141:LYS:HG2	2.07	0.69
1:A:114:SER:O	1:A:119:MET:HB3	1.92	0.69
1:J:194:LYS:HD2	1:L:301:TRP:CE3	2.28	0.69
1:G:581:THR:HG22	1:G:585:LEU:CD2	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HA	1:B:523:ASN:OD1	1.92	0.68
1:C:136:ILE:HD12	1:C:137:GLU:H	1.58	0.68
1:D:84:LYS:HE3	1:D:137:GLU:HG2	1.68	0.68
1:A:221:TRP:HE1	1:B:225:ALA:HB3	1.57	0.67
1:L:217:ILE:CG2	1:L:466:TYR:HB2	2.25	0.67
1:I:321:LEU:HD11	1:I:325:ILE:HD11	1.77	0.67
1:J:194:LYS:HD2	1:L:301:TRP:CD2	2.29	0.67
1:F:531:PRO:HD3	1:I:134:PHE:CD2	2.30	0.67
1:B:486:GLU:CD	1:B:545:LYS:HD2	2.21	0.66
1:A:120:LYS:HB2	1:A:123:GLU:HB2	1.76	0.66
1:G:112:LYS:O	1:G:115:THR:HG22	1.94	0.66
1:A:104:VAL:HG22	1:A:159:PRO:HG3	1.77	0.65
1:G:551:VAL:CG1	1:G:574:PHE:CD2	2.79	0.65
1:L:429:VAL:CG2	1:L:434:MET:HE3	2.17	0.65
1:K:420:THR:HA	1:K:423:PHE:CZ	2.32	0.65
1:A:420:THR:HA	1:A:423:PHE:CZ	2.32	0.65
1:B:420:THR:HA	1:B:423:PHE:CZ	2.32	0.65
1:C:519:VAL:O	1:C:528:VAL:HG12	1.97	0.65
1:L:439:SER:O	1:L:443:ASN:ND2	2.30	0.65
1:A:539:MET:CE	1:A:550:ILE:HG21	2.14	0.65
1:C:420:THR:HA	1:C:423:PHE:CZ	2.32	0.65
1:F:217:ILE:HA	1:F:224:ILE:HG12	1.76	0.65
1:F:420:THR:HA	1:F:423:PHE:CZ	2.32	0.65
1:I:420:THR:HA	1:I:423:PHE:CZ	2.32	0.65
1:J:420:THR:HA	1:J:423:PHE:CZ	2.32	0.65
1:D:420:THR:HA	1:D:423:PHE:CZ	2.32	0.65
1:G:420:THR:HA	1:G:423:PHE:CZ	2.31	0.65
1:H:420:THR:HA	1:H:423:PHE:CZ	2.32	0.65
1:D:84:LYS:HE2	1:D:137:GLU:OE1	1.97	0.64
1:E:420:THR:HA	1:E:423:PHE:CZ	2.32	0.64
1:A:439:SER:O	1:A:443:ASN:ND2	2.30	0.64
1:F:443:ASN:OD1	1:F:448:LEU:HD11	1.98	0.64
1:H:164:LEU:HD22	1:H:165:PRO:CD	2.11	0.64
1:B:439:SER:O	1:B:443:ASN:ND2	2.30	0.64
1:G:439:SER:O	1:G:443:ASN:ND2	2.30	0.64
1:K:260:VAL:HA	1:K:265:PRO:HD2	1.79	0.64
1:L:420:THR:HA	1:L:423:PHE:CZ	2.32	0.64
1:E:343:ILE:HD11	1:E:416:LEU:HA	1.79	0.63
1:E:439:SER:O	1:E:443:ASN:ND2	2.30	0.63
1:G:116:VAL:HG13	1:G:117:ILE:H	1.61	0.63
1:H:71:ARG:NH1	1:H:243:THR:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:ASN:HD21	1:H:465:PHE:HE2	1.46	0.63
1:A:207:LEU:HD11	1:A:240:VAL:HG23	1.81	0.63
1:L:425:GLN:OE1	1:L:518:GLN:CG	2.46	0.63
1:E:212:GLY:O	1:E:214:LEU:HD22	1.99	0.62
1:J:285:GLN:O	1:J:288:THR:HB	1.99	0.62
1:A:214:LEU:HD11	1:H:214:LEU:HD11	1.81	0.62
1:C:439:SER:O	1:C:443:ASN:ND2	2.30	0.62
1:D:439:SER:O	1:D:443:ASN:ND2	2.30	0.62
1:K:71:ARG:NH1	1:K:243:THR:O	2.32	0.62
1:L:64:MET:HG3	1:L:236:ARG:NH1	2.14	0.62
1:L:217:ILE:CG2	1:L:465:PHE:O	2.47	0.62
1:L:342:ASP:O	1:L:342:ASP:OD1	2.18	0.62
1:A:105:ASP:OD2	1:A:108:GLU:HG2	2.00	0.62
1:G:116:VAL:HG13	1:G:117:ILE:N	2.13	0.62
1:B:285:GLN:O	1:B:288:THR:HB	2.00	0.62
1:G:503:TYR:CE2	1:G:538:PHE:CD2	2.88	0.62
1:I:285:GLN:O	1:I:288:THR:HB	2.00	0.62
1:C:71:ARG:NH1	1:C:243:THR:O	2.32	0.62
1:I:71:ARG:NH1	1:I:243:THR:O	2.32	0.62
1:F:285:GLN:O	1:F:288:THR:HB	1.99	0.62
1:K:439:SER:O	1:K:443:ASN:ND2	2.30	0.62
1:D:68:ILE:HG12	1:D:240:VAL:HG13	1.81	0.62
1:D:285:GLN:O	1:D:288:THR:HB	1.99	0.62
1:L:138:PHE:HB2	1:L:142:GLY:HA3	1.82	0.62
1:K:285:GLN:O	1:K:288:THR:HB	1.99	0.62
1:F:71:ARG:NH1	1:F:243:THR:O	2.33	0.61
1:L:285:GLN:O	1:L:288:THR:HB	1.99	0.61
1:D:71:ARG:NH1	1:D:243:THR:O	2.32	0.61
1:C:285:GLN:O	1:C:288:THR:HB	2.00	0.61
1:H:285:GLN:O	1:H:288:THR:HB	1.99	0.61
1:B:216:TYR:HE1	1:B:463:ARG:NH1	1.98	0.61
1:C:213:SER:O	1:C:214:LEU:C	2.44	0.61
1:A:285:GLN:O	1:A:288:THR:HB	2.00	0.61
1:B:71:ARG:NH1	1:B:243:THR:O	2.33	0.61
1:A:71:ARG:NH1	1:A:243:THR:O	2.32	0.61
1:E:71:ARG:NH1	1:E:243:THR:O	2.33	0.61
1:L:316:PHE:HD2	1:L:434:MET:HE1	1.66	0.61
1:A:116:VAL:O	1:A:117:ILE:CG2	2.49	0.60
1:I:321:LEU:HD13	1:I:485:VAL:HG22	1.83	0.60
1:A:301:TRP:CD2	1:B:194:LYS:HD2	2.35	0.60
1:G:285:GLN:O	1:G:288:THR:HB	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:439:SER:O	1:H:443:ASN:ND2	2.30	0.60
1:J:439:SER:O	1:J:443:ASN:ND2	2.30	0.60
1:G:71:ARG:NH1	1:G:243:THR:O	2.32	0.60
1:F:119:MET:HE1	1:F:127:ARG:NE	2.16	0.60
1:F:439:SER:CB	1:F:448:LEU:CD1	2.66	0.60
1:A:564:GLU:HG3	1:A:568:LEU:HD12	1.84	0.60
1:E:564:GLU:HG3	1:E:568:LEU:HD12	1.84	0.60
1:E:211:LYS:HG2	1:E:228:THR:HB	1.84	0.60
1:J:564:GLU:HG3	1:J:568:LEU:HD12	1.84	0.59
1:C:508:TYR:OH	1:C:589:LYS:NZ	2.30	0.59
1:B:564:GLU:HG3	1:B:568:LEU:HD12	1.84	0.59
1:I:564:GLU:HG3	1:I:568:LEU:HD12	1.84	0.59
1:J:119:MET:HE1	1:J:127:ARG:NE	2.17	0.59
1:A:105:ASP:OD2	1:A:108:GLU:CG	2.50	0.59
1:E:214:LEU:HB2	1:E:227:ASN:HD21	1.67	0.59
1:D:564:GLU:HG3	1:D:568:LEU:HD12	1.84	0.59
1:F:564:GLU:HG3	1:F:568:LEU:HD12	1.85	0.59
1:C:564:GLU:HG3	1:C:568:LEU:HD12	1.83	0.59
1:I:119:MET:HE1	1:I:127:ARG:NE	2.18	0.59
1:I:146:THR:HG22	1:I:149:ASP:OD2	2.02	0.59
1:J:252:VAL:O	1:J:256:LEU:HD13	2.01	0.59
1:H:564:GLU:HG3	1:H:568:LEU:HD12	1.84	0.59
1:L:429:VAL:HG21	1:L:434:MET:CE	2.18	0.59
1:A:138:PHE:O	1:A:141:LYS:HE2	2.03	0.59
1:C:161:ILE:HD12	1:C:161:ILE:C	2.28	0.59
1:G:119:MET:HE1	1:G:127:ARG:NE	2.18	0.59
1:J:71:ARG:NH1	1:J:243:THR:O	2.32	0.58
1:G:564:GLU:HG3	1:G:568:LEU:HD12	1.84	0.58
1:L:564:GLU:HG3	1:L:568:LEU:HD12	1.84	0.58
1:E:119:MET:HE1	1:E:127:ARG:NE	2.18	0.58
1:B:109:THR:HG23	1:B:158:LEU:HD23	1.84	0.58
1:D:220:ILE:HG12	1:D:401:MET:HA	1.86	0.58
1:H:164:LEU:CD2	1:H:165:PRO:HD2	2.12	0.58
1:H:281:LEU:HD13	1:H:281:LEU:N	2.18	0.58
1:A:207:LEU:CD1	1:A:240:VAL:HG23	2.33	0.58
1:D:66:GLY:CA	1:D:236:ARG:HH22	2.06	0.58
1:K:331:ASP:HB3	1:K:334:LYS:HB2	1.86	0.58
1:B:119:MET:HE1	1:B:127:ARG:NE	2.19	0.58
1:A:281:LEU:HD13	1:A:281:LEU:N	2.19	0.57
1:C:137:GLU:HG2	1:C:138:PHE:N	2.19	0.57
1:J:88:VAL:CG1	1:J:101:ARG:O	2.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:LEU:HD13	1:C:281:LEU:N	2.19	0.57
1:A:582:LEU:HB3	1:A:587:VAL:CG2	2.34	0.57
1:J:138:PHE:HB2	1:J:142:GLY:HA3	1.87	0.57
1:G:352:ASN:HB2	1:I:105:ASP:HB2	1.86	0.57
1:K:164:LEU:HD23	1:K:165:PRO:O	2.04	0.57
1:K:564:GLU:HG3	1:K:568:LEU:HD12	1.85	0.57
1:K:513:LYS:NZ	1:K:514:THR:HG22	2.19	0.57
1:K:582:LEU:HB3	1:K:587:VAL:CG2	2.35	0.57
1:D:164:LEU:HD23	1:D:165:PRO:O	2.04	0.57
1:B:582:LEU:HB3	1:B:587:VAL:CG2	2.35	0.56
1:G:551:VAL:HG11	1:G:574:PHE:CD2	2.40	0.56
1:A:523:ASN:ND2	1:B:167:THR:OG1	2.39	0.56
1:G:105:ASP:O	1:G:109:THR:HG23	2.06	0.56
1:I:259:MET:HE1	1:I:572:LYS:CB	2.33	0.56
1:I:109:THR:HG23	1:I:158:LEU:HD23	1.86	0.56
1:A:109:THR:HG23	1:A:158:LEU:HD23	1.87	0.56
1:G:584:TYR:CD1	1:G:585:LEU:CD1	2.87	0.56
1:I:582:LEU:HB3	1:I:587:VAL:CG2	2.35	0.56
1:A:115:THR:O	1:A:119:MET:HE2	2.06	0.56
1:A:219:ASP:OD1	1:B:225:ALA:HB2	2.05	0.56
1:E:582:LEU:HB3	1:E:587:VAL:CG2	2.34	0.56
1:F:220:ILE:HG12	1:F:401:MET:HA	1.85	0.56
1:G:115:THR:CG2	1:G:156:MET:HE1	2.36	0.56
1:J:88:VAL:HG11	1:J:101:ARG:O	2.05	0.56
1:C:259:MET:HE1	1:C:572:LYS:CB	2.33	0.56
1:D:375:HIS:CE1	4:D:802:CL:CL	2.96	0.56
1:B:205:SER:HB3	1:B:226:PRO:HG3	1.88	0.55
1:H:164:LEU:HD13	1:H:165:PRO:O	2.06	0.55
1:H:259:MET:HE1	1:H:572:LYS:CB	2.34	0.55
1:K:502:ASN:OD1	1:K:502:ASN:N	2.38	0.55
1:D:221:TRP:HH2	1:H:214:LEU:HD12	1.70	0.55
1:J:313:GLY:HA3	1:J:517:ALA:HB2	1.89	0.55
1:E:105:ASP:O	1:E:109:THR:HG23	2.04	0.55
1:G:551:VAL:HG11	1:G:574:PHE:CE2	2.42	0.55
1:D:66:GLY:CA	1:D:236:ARG:HH21	2.08	0.55
1:F:502:ASN:OD1	1:F:502:ASN:N	2.39	0.55
1:E:259:MET:HE1	1:E:572:LYS:CB	2.33	0.55
1:H:341:ARG:C	1:H:343:ILE:HD12	2.32	0.55
1:C:341:ARG:C	1:C:343:ILE:HD12	2.32	0.55
1:G:503:TYR:CD2	1:G:538:PHE:CD2	2.95	0.55
1:A:259:MET:HE1	1:A:572:LYS:CB	2.33	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ARG:C	1:D:343:ILE:HD12	2.32	0.55
1:I:529:LYS:HE3	1:I:530:GLY:H	1.72	0.55
1:B:88:VAL:HG13	1:B:160:GLY:HA2	1.89	0.55
1:C:93:ALA:O	1:C:101:ARG:NH1	2.40	0.55
1:J:89:ILE:HD11	1:J:133:ALA:HB3	1.89	0.54
1:A:448:LEU:HD12	1:A:448:LEU:N	2.22	0.54
1:F:472:ILE:H	1:J:464:GLN:HE21	1.54	0.54
1:L:434:MET:HB3	1:L:539:MET:HE1	1.89	0.54
1:E:502:ASN:OD1	1:E:502:ASN:N	2.39	0.54
1:E:96:ASN:O	1:E:98:LYS:HD3	2.08	0.54
1:G:259:MET:HE1	1:G:572:LYS:CB	2.33	0.54
1:E:89:ILE:HD11	1:E:133:ALA:HB3	1.88	0.54
1:H:281:LEU:N	1:H:281:LEU:CD1	2.70	0.54
1:B:89:ILE:HD11	1:B:133:ALA:HB3	1.89	0.54
1:E:546:ASN:OD1	1:E:546:ASN:O	2.26	0.54
1:B:156:MET:HB3	1:B:158:LEU:HD13	1.90	0.54
1:E:285:GLN:O	1:E:288:THR:HB	2.07	0.54
1:F:89:ILE:HD11	1:F:133:ALA:HB3	1.89	0.54
1:G:271:VAL:HG22	1:G:283:TYR:CD1	2.40	0.54
1:L:502:ASN:HD22	1:L:568:LEU:HA	1.73	0.54
1:C:549:VAL:CG1	1:C:550:ILE:N	2.70	0.53
1:F:472:ILE:H	1:J:464:GLN:NE2	2.05	0.53
1:B:88:VAL:HG22	1:B:102:HIS:HA	1.89	0.53
1:D:259:MET:HE1	1:D:572:LYS:CB	2.33	0.53
1:K:549:VAL:CG1	1:K:550:ILE:N	2.70	0.53
1:L:217:ILE:HG23	1:L:465:PHE:O	2.08	0.53
1:C:103:VAL:O	1:C:103:VAL:HG13	2.07	0.53
1:L:377:GLN:HE22	1:L:418:GLN:HB3	1.74	0.53
1:B:502:ASN:OD1	1:B:502:ASN:N	2.39	0.53
1:C:281:LEU:N	1:C:281:LEU:CD1	2.71	0.53
1:G:503:TYR:CE2	1:G:538:PHE:CG	2.96	0.53
1:I:156:MET:HB3	1:I:158:LEU:HD13	1.90	0.53
1:A:281:LEU:N	1:A:281:LEU:CD1	2.70	0.53
1:L:425:GLN:HE22	1:L:517:ALA:HB1	1.74	0.53
1:J:259:MET:HE1	1:J:572:LYS:CB	2.33	0.53
1:B:220:ILE:HG12	1:B:401:MET:HA	1.91	0.53
1:F:217:ILE:HB	1:F:466:TYR:HB2	1.91	0.53
1:I:89:ILE:HD11	1:I:133:ALA:HB3	1.91	0.52
1:F:84:LYS:HB2	1:F:166:GLU:OE2	2.09	0.52
1:F:516:THR:HB	2:X:1:GLY:HA2	1.90	0.52
1:K:502:ASN:HD22	1:K:568:LEU:HA	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:C	1:A:117:ILE:HG22	2.35	0.52
1:F:271:VAL:HG21	1:F:305:LEU:HD13	1.92	0.52
1:K:260:VAL:HG23	1:K:265:PRO:HD2	1.91	0.52
1:B:85:LEU:CD2	1:B:117:ILE:HD11	2.40	0.52
1:C:138:PHE:HB2	1:C:142:GLY:HA3	1.91	0.52
1:D:221:TRP:CH2	1:H:214:LEU:HD12	2.44	0.52
1:E:138:PHE:HB2	1:E:142:GLY:HA3	1.91	0.52
1:B:343:ILE:HD13	1:B:343:ILE:O	2.10	0.52
1:G:551:VAL:CG1	1:G:574:PHE:HE2	2.21	0.52
1:A:117:ILE:HG13	1:A:118:ASN:N	2.23	0.52
1:B:216:TYR:CE1	1:B:463:ARG:NH1	2.77	0.52
1:F:112:LYS:O	1:F:115:THR:HG22	2.10	0.52
1:F:446:ASN:HD22	1:F:472:ILE:HG21	1.75	0.52
1:I:104:VAL:HG22	1:I:159:PRO:HG3	1.92	0.52
1:I:259:MET:SD	1:I:573:ALA:HB2	2.50	0.52
1:B:259:MET:HE1	1:B:572:LYS:CB	2.33	0.52
1:G:502:ASN:HD22	1:G:568:LEU:HA	1.75	0.52
1:C:259:MET:SD	1:C:573:ALA:HB2	2.50	0.51
1:F:94:SER:O	1:F:97:SER:N	2.43	0.51
1:J:343:ILE:HD13	1:J:343:ILE:O	2.11	0.51
1:A:271:VAL:HG21	1:A:305:LEU:HD13	1.92	0.51
1:D:259:MET:SD	1:D:573:ALA:HB2	2.51	0.51
1:E:259:MET:SD	1:E:573:ALA:HB2	2.50	0.51
1:A:156:MET:HB3	1:A:158:LEU:HD13	1.93	0.51
1:D:502:ASN:HD22	1:D:568:LEU:HA	1.76	0.51
1:G:551:VAL:HG13	1:G:574:PHE:CD2	2.44	0.51
1:H:259:MET:SD	1:H:573:ALA:HB2	2.50	0.51
1:J:190:THR:OG1	1:J:192:GLU:HG2	2.11	0.51
1:K:313:GLY:HA3	1:K:517:ALA:HB2	1.93	0.51
1:D:119:MET:HE2	1:D:123:GLU:HG2	1.91	0.51
1:G:259:MET:SD	1:G:573:ALA:HB2	2.50	0.51
1:A:126:LYS:O	1:A:130:GLN:HG3	2.11	0.51
1:A:313:GLY:HA3	1:A:517:ALA:HB2	1.93	0.51
1:H:502:ASN:HD22	1:H:568:LEU:HA	1.75	0.51
1:A:130:GLN:HB3	1:A:131:LYS:HE2	1.93	0.51
1:B:259:MET:SD	1:B:573:ALA:HB2	2.50	0.51
1:E:502:ASN:HD22	1:E:568:LEU:HA	1.75	0.51
1:G:116:VAL:CG1	1:G:117:ILE:H	2.23	0.51
1:G:502:ASN:OD1	1:G:502:ASN:N	2.39	0.51
1:J:259:MET:SD	1:J:573:ALA:HB2	2.50	0.51
1:B:502:ASN:HD22	1:B:568:LEU:HA	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HH11	1:C:227:ASN:HD22	1.59	0.51
1:G:271:VAL:HG21	1:G:305:LEU:HD13	1.93	0.51
1:F:439:SER:HB2	1:F:448:LEU:HD11	1.85	0.50
1:G:180:LEU:HD23	1:G:244:ILE:HD11	1.92	0.50
1:B:313:GLY:HA3	1:B:517:ALA:HB2	1.94	0.50
1:I:313:GLY:HA3	1:I:517:ALA:HB2	1.92	0.50
1:D:313:GLY:HA3	1:D:517:ALA:HB2	1.93	0.50
1:G:313:GLY:HA3	1:G:517:ALA:HB2	1.93	0.50
1:L:259:MET:SD	1:L:573:ALA:HB2	2.52	0.50
1:B:217:ILE:HB	1:B:466:TYR:HB2	1.93	0.50
1:F:259:MET:SD	1:F:573:ALA:HB2	2.51	0.50
1:F:313:GLY:HA3	1:F:517:ALA:HB2	1.94	0.50
1:F:502:ASN:HD22	1:F:568:LEU:HA	1.75	0.50
1:H:502:ASN:OD1	1:H:502:ASN:N	2.39	0.50
1:A:259:MET:SD	1:A:573:ALA:HB2	2.50	0.50
1:E:190:THR:OG1	1:E:192:GLU:HG2	2.10	0.50
1:D:344:MET:HE2	1:D:416:LEU:CB	2.41	0.50
1:I:502:ASN:HD22	1:I:568:LEU:HA	1.76	0.50
1:C:344:MET:HE2	1:C:416:LEU:CB	2.42	0.50
1:A:115:THR:CG2	1:A:156:MET:HE1	2.42	0.50
1:E:313:GLY:HA3	1:E:517:ALA:HB2	1.94	0.50
1:G:261:GLU:OE1	1:G:262:ARG:N	2.45	0.50
1:G:507:GLY:HA3	1:G:589:LYS:CE	2.41	0.50
1:K:138:PHE:HB2	1:K:142:GLY:HA3	1.94	0.50
1:L:299:LYS:HB2	1:L:299:LYS:NZ	2.25	0.50
1:A:118:ASN:HD22	1:A:141:LYS:HB3	1.77	0.49
1:B:217:ILE:HG23	1:B:224:ILE:HG21	1.94	0.49
1:C:182:GLY:HA3	1:C:197:LEU:O	2.12	0.49
1:D:182:GLY:HA3	1:D:197:LEU:O	2.12	0.49
1:E:217:ILE:HB	1:E:466:TYR:HB2	1.94	0.49
1:I:182:GLY:HA3	1:I:197:LEU:O	2.12	0.49
1:F:271:VAL:HG22	1:F:283:TYR:CD1	2.40	0.49
1:H:182:GLY:HA3	1:H:197:LEU:O	2.13	0.49
1:L:313:GLY:HA3	1:L:517:ALA:HB2	1.93	0.49
1:B:182:GLY:HA3	1:B:197:LEU:O	2.12	0.49
1:C:313:GLY:HA3	1:C:517:ALA:HB2	1.93	0.49
1:E:182:GLY:HA3	1:E:197:LEU:O	2.12	0.49
1:E:104:VAL:HG22	1:E:159:PRO:HG3	1.94	0.49
1:E:261:GLU:OE1	1:E:262:ARG:N	2.45	0.49
1:E:582:LEU:HB3	1:E:587:VAL:HG21	1.93	0.49
1:H:344:MET:HE2	1:H:416:LEU:CB	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:LEU:CD1	1:I:485:VAL:HG22	2.42	0.49
1:K:273:MET:CE	1:K:450:PRO:HB3	2.42	0.49
1:K:398:THR:HG23	1:K:405:GLU:OE2	2.13	0.49
1:E:549:VAL:HG23	1:E:578:MET:CE	2.43	0.49
1:F:182:GLY:HA3	1:F:197:LEU:O	2.12	0.49
1:F:531:PRO:HG3	1:I:134:PHE:CD1	2.47	0.49
1:H:398:THR:HG23	1:H:405:GLU:OE2	2.13	0.49
1:J:117:ILE:HD11	1:J:141:LYS:CB	2.38	0.49
1:J:182:GLY:HA3	1:J:197:LEU:O	2.13	0.49
1:C:398:THR:HG23	1:C:405:GLU:OE2	2.13	0.49
1:K:182:GLY:HA3	1:K:197:LEU:O	2.13	0.49
1:B:486:GLU:CD	1:B:545:LYS:CD	2.86	0.49
1:E:216:TYR:HE1	1:E:463:ARG:NH1	2.11	0.49
1:G:182:GLY:HA3	1:G:197:LEU:O	2.12	0.49
1:I:398:THR:HG23	1:I:405:GLU:OE2	2.13	0.49
1:L:182:GLY:HA3	1:L:197:LEU:O	2.12	0.49
1:A:182:GLY:HA3	1:A:197:LEU:O	2.13	0.49
1:B:136:ILE:HD13	1:B:137:GLU:N	2.27	0.49
1:B:138:PHE:HB2	1:B:142:GLY:HA3	1.94	0.49
1:F:317:LYS:HD2	1:F:513:LYS:NZ	2.28	0.49
1:G:138:PHE:HB2	1:G:142:GLY:HA3	1.94	0.49
1:A:207:LEU:HD11	1:A:240:VAL:CG2	2.43	0.49
1:A:279:GLU:O	1:A:281:LEU:HD13	2.13	0.49
1:F:261:GLU:OE1	1:F:262:ARG:N	2.45	0.49
1:G:398:THR:HG23	1:G:405:GLU:OE2	2.13	0.49
1:I:321:LEU:CD1	1:I:325:ILE:HD11	2.41	0.49
1:A:582:LEU:HB3	1:A:587:VAL:HG21	1.94	0.49
1:B:104:VAL:HG13	1:B:159:PRO:HG3	1.94	0.49
1:B:213:SER:HA	1:B:226:PRO:HB2	1.94	0.48
1:C:66:GLY:HA2	1:C:236:ARG:HH22	1.78	0.48
1:C:279:GLU:O	1:C:281:LEU:HD13	2.13	0.48
1:H:313:GLY:HA3	1:H:517:ALA:HB2	1.93	0.48
1:I:138:PHE:HB2	1:I:142:GLY:HA3	1.94	0.48
1:L:217:ILE:HG22	1:L:465:PHE:O	2.12	0.48
1:E:220:ILE:HG22	1:E:224:ILE:HD11	1.95	0.48
1:H:190:THR:OG1	1:H:192:GLU:HG2	2.12	0.48
1:I:549:VAL:HG23	1:I:578:MET:CE	2.44	0.48
1:B:398:THR:HG22	1:B:405:GLU:OE2	2.13	0.48
1:B:218:HIS:ND1	1:H:221:TRP:O	2.45	0.48
1:E:491:LEU:O	1:E:492:VAL:C	2.56	0.48
1:H:279:GLU:O	1:H:281:LEU:HD13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:491:LEU:O	1:L:492:VAL:C	2.57	0.48
1:B:491:LEU:O	1:B:492:VAL:C	2.56	0.48
1:B:582:LEU:HB3	1:B:587:VAL:HG21	1.95	0.48
1:F:463:ARG:HD2	1:J:473:ALA:O	2.13	0.48
1:H:82:ARG:NH1	1:H:144:ASN:OD1	2.46	0.48
1:J:217:ILE:HD12	1:J:223:TYR:CD2	2.49	0.48
1:K:347:ARG:HE	1:K:353:ARG:HH22	1.62	0.48
1:K:549:VAL:HG13	1:K:550:ILE:N	2.29	0.48
1:D:398:THR:HG22	1:D:405:GLU:OE2	2.13	0.48
1:E:398:THR:HG22	1:E:405:GLU:OE2	2.13	0.48
1:G:491:LEU:O	1:G:492:VAL:C	2.57	0.48
1:I:473:ALA:O	1:L:463:ARG:HD2	2.14	0.48
1:J:398:THR:HG23	1:J:405:GLU:OE2	2.13	0.48
1:A:267:ASP:HB3	1:A:556:SER:HB3	1.96	0.48
1:F:398:THR:HG22	1:F:405:GLU:OE2	2.13	0.48
1:J:119:MET:HE2	1:J:141:LYS:CD	2.44	0.48
1:B:267:ASP:HB3	1:B:556:SER:HB3	1.96	0.48
1:A:542:ALA:HA	1:A:543:PRO:C	2.39	0.47
1:E:339:GLY:HA2	1:E:355:GLY:HA3	1.95	0.47
1:K:513:LYS:HZ2	1:K:514:THR:HG22	1.79	0.47
1:A:398:THR:HG22	1:A:405:GLU:OE2	2.13	0.47
1:F:267:ASP:HB3	1:F:556:SER:HB3	1.96	0.47
1:F:542:ALA:HA	1:F:543:PRO:C	2.39	0.47
1:I:582:LEU:HB3	1:I:587:VAL:HG21	1.95	0.47
1:C:491:LEU:O	1:C:492:VAL:C	2.57	0.47
1:E:217:ILE:HD12	1:E:466:TYR:HB3	1.96	0.47
1:F:491:LEU:O	1:F:492:VAL:C	2.57	0.47
1:J:173:ASN:HB2	1:J:176:PHE:CB	2.44	0.47
1:D:210:SER:O	1:D:212:GLY:N	2.47	0.47
1:H:491:LEU:O	1:H:492:VAL:C	2.56	0.47
1:H:542:ALA:HA	1:H:543:PRO:C	2.39	0.47
1:I:371:THR:HA	1:I:374:MET:HE3	1.96	0.47
1:L:81:GLU:OE1	1:L:83:TYR:CZ	2.67	0.47
1:L:173:ASN:HB2	1:L:176:PHE:CB	2.44	0.47
1:B:542:ALA:HA	1:B:543:PRO:C	2.39	0.47
1:D:491:LEU:O	1:D:492:VAL:C	2.57	0.47
1:G:104:VAL:HG22	1:G:159:PRO:HG3	1.96	0.47
1:G:507:GLY:HA3	1:G:589:LYS:HE3	1.97	0.47
1:I:491:LEU:O	1:I:492:VAL:C	2.57	0.47
1:L:398:THR:HG23	1:L:405:GLU:OE2	2.13	0.47
1:A:217:ILE:HD12	1:A:223:TYR:CD2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:PHE:CD1	1:C:452:PHE:N	2.83	0.47
1:C:549:VAL:HG13	1:C:550:ILE:N	2.29	0.47
1:E:94:SER:O	1:E:97:SER:N	2.41	0.47
1:G:173:ASN:HB2	1:G:176:PHE:CB	2.45	0.47
1:J:104:VAL:HG22	1:J:159:PRO:HG3	1.96	0.47
1:A:491:LEU:O	1:A:492:VAL:C	2.57	0.47
1:B:210:SER:O	1:B:212:GLY:N	2.48	0.47
1:B:217:ILE:HD12	1:B:466:TYR:HB3	1.97	0.47
1:C:194:LYS:HB3	1:K:301:TRP:CE2	2.49	0.47
1:D:161:ILE:HD13	1:D:161:ILE:HA	1.84	0.47
1:D:452:PHE:CD1	1:D:452:PHE:N	2.83	0.47
1:E:220:ILE:HG12	1:E:401:MET:HA	1.97	0.47
1:F:452:PHE:CD1	1:F:452:PHE:N	2.83	0.47
1:G:116:VAL:CG1	1:G:117:ILE:N	2.77	0.47
1:G:551:VAL:CG1	1:G:578:MET:HE2	2.44	0.47
1:G:581:THR:C	1:G:585:LEU:HD22	2.33	0.47
1:I:173:ASN:HB2	1:I:176:PHE:CB	2.45	0.47
1:J:88:VAL:CG1	1:J:160:GLY:HA2	2.45	0.47
1:K:491:LEU:O	1:K:492:VAL:C	2.57	0.47
1:L:267:ASP:HB3	1:L:556:SER:HB3	1.97	0.47
1:A:173:ASN:HB2	1:A:176:PHE:CB	2.45	0.47
1:C:363:LEU:O	1:C:364:GLY:C	2.58	0.47
1:D:542:ALA:HA	1:D:543:PRO:C	2.39	0.47
1:E:452:PHE:CD1	1:E:452:PHE:N	2.83	0.47
1:K:217:ILE:HB	1:K:466:TYR:HB2	1.96	0.47
1:K:267:ASP:HB3	1:K:556:SER:HB3	1.97	0.47
1:L:296:ASP:O	1:L:299:LYS:NZ	2.44	0.47
1:A:253:GLU:OE1	1:A:286:ARG:NH2	2.44	0.47
1:A:452:PHE:N	1:A:452:PHE:CD1	2.83	0.47
1:C:173:ASN:HB2	1:C:176:PHE:CB	2.45	0.47
1:C:542:ALA:HA	1:C:543:PRO:C	2.40	0.47
1:G:267:ASP:HB3	1:G:556:SER:HB3	1.97	0.47
1:J:452:PHE:N	1:J:452:PHE:CD1	2.83	0.47
1:K:452:PHE:N	1:K:452:PHE:CD1	2.83	0.47
1:K:582:LEU:HB3	1:K:587:VAL:HG21	1.96	0.47
1:A:84:LYS:O	1:A:163:LEU:HA	2.14	0.47
1:C:103:VAL:HG23	1:C:109:THR:HG21	1.97	0.47
1:D:217:ILE:HB	1:D:466:TYR:HB2	1.96	0.47
1:H:173:ASN:HB2	1:H:176:PHE:CB	2.45	0.47
1:I:339:GLY:HA2	1:I:355:GLY:HA3	1.96	0.47
1:L:156:MET:HB3	1:L:158:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:HB2	1:B:176:PHE:CB	2.45	0.46
1:C:267:ASP:HB3	1:C:556:SER:HB3	1.97	0.46
1:E:216:TYR:CE1	1:E:463:ARG:NH1	2.83	0.46
1:E:267:ASP:HB3	1:E:556:SER:HB3	1.97	0.46
1:E:542:ALA:HA	1:E:543:PRO:C	2.39	0.46
1:F:84:LYS:O	1:F:163:LEU:HA	2.15	0.46
1:F:104:VAL:HG22	1:F:159:PRO:HG3	1.96	0.46
1:G:551:VAL:HG12	1:G:578:MET:HE2	1.97	0.46
1:I:542:ALA:HA	1:I:543:PRO:C	2.39	0.46
1:L:442:PHE:HB3	1:L:547:PRO:HG3	1.97	0.46
1:B:363:LEU:O	1:B:364:GLY:C	2.58	0.46
1:E:173:ASN:HB2	1:E:176:PHE:CB	2.45	0.46
1:G:542:ALA:HA	1:G:543:PRO:C	2.39	0.46
1:I:84:LYS:O	1:I:163:LEU:HA	2.15	0.46
1:I:452:PHE:N	1:I:452:PHE:CD1	2.83	0.46
1:K:173:ASN:HB2	1:K:176:PHE:CB	2.46	0.46
1:E:210:SER:O	1:E:212:GLY:N	2.48	0.46
1:G:89:ILE:HD11	1:G:133:ALA:HB3	1.98	0.46
1:A:114:SER:CA	1:A:119:MET:HB3	2.46	0.46
1:B:84:LYS:O	1:B:163:LEU:HA	2.15	0.46
1:D:84:LYS:HG3	1:D:142:GLY:O	2.15	0.46
1:E:363:LEU:O	1:E:364:GLY:C	2.58	0.46
1:G:84:LYS:O	1:G:163:LEU:HA	2.15	0.46
1:J:88:VAL:HG12	1:J:160:GLY:HA2	1.96	0.46
1:J:516:THR:HB	2:Y:1:GLY:HA2	1.97	0.46
1:A:137:GLU:OE2	1:A:137:GLU:C	2.59	0.46
1:G:503:TYR:CE2	1:G:538:PHE:HB2	2.50	0.46
1:K:340:HIS:CD2	1:K:347:ARG:NH1	2.83	0.46
1:B:398:THR:HG22	1:B:405:GLU:CD	2.41	0.46
1:D:398:THR:HG22	1:D:405:GLU:CD	2.41	0.46
1:F:217:ILE:HD12	1:F:466:TYR:HB3	1.97	0.46
1:H:197:LEU:HD23	1:H:198:GLY:N	2.31	0.46
1:D:115:THR:HG23	1:D:116:VAL:HG23	1.98	0.46
1:F:439:SER:OG	1:F:448:LEU:HD12	2.15	0.46
1:H:267:ASP:HB3	1:H:556:SER:HB3	1.97	0.46
1:K:521:ALA:HB3	1:K:524:GLY:O	2.16	0.46
1:C:213:SER:O	1:C:214:LEU:O	2.32	0.46
1:D:267:ASP:HB3	1:D:556:SER:HB3	1.97	0.46
1:D:363:LEU:O	1:D:364:GLY:C	2.58	0.46
1:E:84:LYS:O	1:E:163:LEU:HA	2.15	0.46
1:E:197:LEU:HD23	1:E:198:GLY:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:452:PHE:N	1:H:452:PHE:CD1	2.83	0.46
1:A:363:LEU:O	1:A:364:GLY:C	2.58	0.46
1:A:398:THR:HG22	1:A:405:GLU:CD	2.41	0.46
1:B:452:PHE:N	1:B:452:PHE:CD1	2.83	0.46
1:C:84:LYS:O	1:C:163:LEU:HA	2.16	0.46
1:C:140:ARG:HD2	1:C:140:ARG:HA	1.60	0.46
1:I:197:LEU:HD23	1:I:198:GLY:N	2.31	0.46
1:K:84:LYS:O	1:K:163:LEU:HA	2.15	0.46
1:K:210:SER:O	1:K:212:GLY:N	2.48	0.46
1:A:120:LYS:HE3	1:A:123:GLU:CB	2.45	0.46
1:C:108:GLU:C	1:C:108:GLU:OE1	2.58	0.46
1:C:161:ILE:C	1:C:161:ILE:CD1	2.89	0.46
1:D:68:ILE:HG12	1:D:240:VAL:CG1	2.46	0.46
1:K:197:LEU:HD23	1:K:198:GLY:N	2.31	0.46
1:C:235:LYS:HB3	1:C:235:LYS:HE3	1.58	0.45
1:D:173:ASN:HB2	1:D:176:PHE:CB	2.46	0.45
1:E:398:THR:HG22	1:E:405:GLU:CD	2.41	0.45
1:G:452:PHE:CD1	1:G:452:PHE:N	2.83	0.45
1:G:503:TYR:CE2	1:G:538:PHE:CB	2.99	0.45
1:J:94:SER:OG	1:J:101:ARG:N	2.44	0.45
1:J:197:LEU:HD23	1:J:198:GLY:N	2.31	0.45
1:L:452:PHE:CD1	1:L:452:PHE:N	2.83	0.45
1:A:114:SER:C	1:A:119:MET:HB3	2.41	0.45
1:A:132:LYS:HD3	1:A:132:LYS:HA	1.69	0.45
1:B:218:HIS:HB3	1:H:223:TYR:CZ	2.51	0.45
1:H:81:GLU:OE2	1:H:165:PRO:HB2	2.16	0.45
1:J:84:LYS:O	1:J:163:LEU:HA	2.15	0.45
1:L:503:TYR:CE2	1:L:571:SER:OG	2.69	0.45
1:F:398:THR:HG22	1:F:405:GLU:CD	2.41	0.45
1:H:326:GLN:CD	1:H:478:THR:HG23	2.42	0.45
1:E:326:GLN:CD	1:E:478:THR:HG23	2.42	0.45
1:H:375:HIS:ND1	4:H:802:CL:CL	2.77	0.45
1:I:267:ASP:HB3	1:I:556:SER:HB3	1.98	0.45
1:F:516:THR:HG23	1:F:536:VAL:HG12	1.98	0.45
1:G:197:LEU:HD23	1:G:198:GLY:N	2.31	0.45
1:K:519:VAL:HG21	1:K:557:LEU:HD13	1.98	0.45
1:K:582:LEU:HB3	1:K:587:VAL:HG22	1.99	0.45
1:A:197:LEU:HD23	1:A:198:GLY:N	2.31	0.45
1:B:326:GLN:CD	1:B:478:THR:HG23	2.42	0.45
1:D:502:ASN:ND2	1:D:568:LEU:HA	2.32	0.45
1:F:173:ASN:HB2	1:F:176:PHE:CB	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLN:CD	1:F:478:THR:HG23	2.42	0.45
1:G:326:GLN:CD	1:G:478:THR:HG23	2.42	0.45
1:H:363:LEU:O	1:H:364:GLY:C	2.58	0.45
1:J:326:GLN:CD	1:J:478:THR:HG23	2.42	0.45
1:A:271:VAL:HG22	1:A:283:TYR:CD1	2.41	0.45
1:A:447:MET:C	1:A:448:LEU:HD12	2.41	0.45
1:A:448:LEU:N	1:A:448:LEU:CD1	2.79	0.45
1:B:502:ASN:ND2	1:B:568:LEU:HA	2.32	0.45
1:C:197:LEU:HD23	1:C:198:GLY:N	2.31	0.45
1:D:112:LYS:HB2	1:D:112:LYS:HE3	1.79	0.45
1:H:341:ARG:O	1:H:343:ILE:HD12	2.17	0.45
1:I:326:GLN:CD	1:I:478:THR:HG23	2.42	0.45
1:L:503:TYR:CZ	1:L:571:SER:OG	2.70	0.45
1:B:197:LEU:HD23	1:B:198:GLY:N	2.31	0.45
1:J:267:ASP:HB3	1:J:556:SER:HB3	1.97	0.45
1:F:301:TRP:CD2	1:I:194:LYS:HD3	2.52	0.45
1:F:502:ASN:ND2	1:F:568:LEU:HA	2.32	0.45
1:A:326:GLN:CD	1:A:478:THR:HG23	2.42	0.45
1:A:582:LEU:HB3	1:A:587:VAL:HG22	1.99	0.45
1:D:197:LEU:HD23	1:D:198:GLY:N	2.31	0.45
1:D:326:GLN:CD	1:D:478:THR:HG23	2.42	0.45
1:L:502:ASN:ND2	1:L:568:LEU:HA	2.31	0.45
1:B:516:THR:HG23	1:B:536:VAL:HG12	1.99	0.44
1:C:326:GLN:CD	1:C:478:THR:HG23	2.42	0.44
1:I:502:ASN:OD1	1:I:502:ASN:N	2.39	0.44
1:K:502:ASN:ND2	1:K:568:LEU:HA	2.32	0.44
1:L:197:LEU:HD23	1:L:198:GLY:N	2.32	0.44
1:L:326:GLN:CD	1:L:478:THR:HG23	2.42	0.44
1:L:502:ASN:OD1	1:L:502:ASN:N	2.38	0.44
1:C:136:ILE:HD12	1:C:137:GLU:N	2.29	0.44
1:F:64:MET:HE2	1:F:65:ARG:O	2.17	0.44
1:F:197:LEU:HD23	1:F:198:GLY:N	2.31	0.44
1:G:502:ASN:ND2	1:G:568:LEU:HA	2.32	0.44
1:I:502:ASN:ND2	1:I:568:LEU:HA	2.32	0.44
1:J:88:VAL:HG12	1:J:160:GLY:CA	2.47	0.44
1:J:386:LYS:NZ	1:J:390:GLU:OE2	2.48	0.44
1:E:117:ILE:HD11	1:E:141:LYS:CB	2.47	0.44
1:G:581:THR:CG2	1:G:585:LEU:CD2	2.95	0.44
1:I:549:VAL:HG23	1:I:578:MET:HE1	1.98	0.44
1:L:217:ILE:CG2	1:L:465:PHE:C	2.90	0.44
1:C:272:VAL:HG13	1:C:549:VAL:HG11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:502:ASN:ND2	1:H:568:LEU:HA	2.32	0.44
1:J:88:VAL:HG13	1:J:102:HIS:HA	2.00	0.44
1:K:516:THR:HG23	1:K:536:VAL:HG12	2.00	0.44
1:A:438:GLN:HG2	1:A:539:MET:HE2	1.98	0.44
1:J:138:PHE:O	1:J:141:LYS:HG2	2.18	0.44
1:L:539:MET:HE2	1:L:539:MET:HB2	1.75	0.44
1:A:115:THR:HG21	1:A:156:MET:CE	2.48	0.44
1:A:523:ASN:OD1	1:B:191:GLY:HA3	2.17	0.44
1:I:71:ARG:HH22	1:I:281:LEU:HD22	1.83	0.44
1:K:342:ASP:OD1	1:K:342:ASP:O	2.35	0.44
1:L:140:ARG:HH11	1:L:141:LYS:H	1.65	0.44
1:A:115:THR:HG21	1:A:156:MET:HE1	1.98	0.44
1:G:94:SER:OG	1:G:101:ARG:N	2.43	0.44
1:J:192:GLU:HG3	1:L:301:TRP:HZ2	1.83	0.44
1:K:272:VAL:HG13	1:K:549:VAL:HG11	2.00	0.44
1:D:516:THR:HG23	1:D:536:VAL:HG12	2.00	0.44
1:F:214:LEU:H	1:F:226:PRO:HB2	1.82	0.44
1:J:491:LEU:O	1:J:492:VAL:C	2.61	0.44
1:C:401:MET:HB2	1:C:452:PHE:CE1	2.53	0.43
1:F:134:PHE:CD2	1:I:531:PRO:HD3	2.53	0.43
1:D:84:LYS:O	1:D:163:LEU:HA	2.18	0.43
1:J:194:LYS:HB3	1:L:301:TRP:CE2	2.52	0.43
1:K:574:PHE:HE1	1:K:578:MET:HE2	1.83	0.43
1:L:401:MET:HB2	1:L:452:PHE:CE1	2.53	0.43
1:B:582:LEU:HB3	1:B:587:VAL:HG22	1.99	0.43
1:E:117:ILE:HD11	1:E:141:LYS:HB2	2.00	0.43
1:E:210:SER:OG	1:E:211:LYS:N	2.51	0.43
1:K:519:VAL:HG21	1:K:557:LEU:CD1	2.48	0.43
1:L:253:GLU:OE1	1:L:286:ARG:NH2	2.44	0.43
1:A:217:ILE:HD12	1:A:223:TYR:HD2	1.83	0.43
1:B:220:ILE:H	1:B:220:ILE:HG13	1.53	0.43
1:C:341:ARG:O	1:C:343:ILE:HD12	2.18	0.43
1:L:217:ILE:CG2	1:L:466:TYR:CB	2.94	0.43
1:A:117:ILE:O	1:A:119:MET:HG3	2.18	0.43
1:D:375:HIS:ND1	4:D:802:CL:CL	2.88	0.43
1:E:549:VAL:HG23	1:E:578:MET:HE1	2.00	0.43
1:J:401:MET:HB2	1:J:452:PHE:CE1	2.54	0.43
1:L:217:ILE:HG21	1:L:466:TYR:CB	2.48	0.43
1:L:272:VAL:HG22	1:L:551:VAL:HG22	2.00	0.43
1:A:173:ASN:HB2	1:A:176:PHE:HB2	2.01	0.43
1:A:516:THR:HG23	1:A:536:VAL:HG12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:MET:HE1	1:A:550:ILE:HG22	1.83	0.43
1:B:210:SER:OG	1:B:211:LYS:N	2.51	0.43
1:H:516:THR:HG23	1:H:536:VAL:HG12	1.99	0.43
1:L:224:ILE:H	1:L:224:ILE:HG13	1.44	0.43
1:F:259:MET:HE1	1:F:570:VAL:HA	2.00	0.43
1:F:401:MET:HB2	1:F:452:PHE:CE1	2.54	0.43
1:I:582:LEU:HB3	1:I:587:VAL:HG22	1.99	0.43
1:L:173:ASN:HB2	1:L:176:PHE:HB2	2.01	0.43
1:A:191:GLY:HA3	1:B:523:ASN:ND2	2.34	0.43
1:B:401:MET:HB2	1:B:452:PHE:CE1	2.54	0.43
1:E:109:THR:HG22	1:E:158:LEU:CD2	2.48	0.43
1:E:217:ILE:HG13	1:E:465:PHE:HB3	2.01	0.43
1:E:502:ASN:ND2	1:E:568:LEU:HA	2.32	0.43
1:F:194:LYS:HD3	1:I:301:TRP:CZ3	2.53	0.43
1:G:538:PHE:HE1	1:G:540:GLY:HA3	1.84	0.43
1:K:401:MET:HB2	1:K:452:PHE:CE1	2.54	0.43
1:K:451:TRP:CD1	1:K:451:TRP:N	2.87	0.43
1:B:343:ILE:HD13	1:B:343:ILE:C	2.44	0.43
1:D:253:GLU:OE1	1:D:286:ARG:NH2	2.44	0.43
1:H:401:MET:HB2	1:H:452:PHE:CE1	2.54	0.43
1:A:150:LYS:HA	1:A:163:LEU:HD13	2.01	0.43
1:C:91:LYS:H	1:C:91:LYS:HG2	1.62	0.43
1:D:451:TRP:CD1	1:D:451:TRP:N	2.87	0.43
1:E:103:VAL:HG21	1:E:128:LEU:HD22	2.01	0.43
1:E:582:LEU:HB3	1:E:587:VAL:HG22	2.00	0.43
1:F:220:ILE:H	1:F:220:ILE:HG13	1.54	0.43
1:G:401:MET:HB2	1:G:452:PHE:CE1	2.54	0.43
1:L:451:TRP:CD1	1:L:451:TRP:N	2.87	0.43
1:A:341:ARG:HD3	1:A:341:ARG:HA	1.72	0.42
1:C:89:ILE:HD11	1:C:133:ALA:HB3	2.00	0.42
1:C:516:THR:HG23	1:C:536:VAL:HG12	2.00	0.42
1:D:210:SER:OG	1:D:211:LYS:N	2.51	0.42
1:D:223:TYR:C	1:D:224:ILE:HG13	2.43	0.42
1:G:516:THR:HG23	1:G:536:VAL:HG12	2.00	0.42
1:A:114:SER:HA	1:A:119:MET:HB3	2.01	0.42
1:A:401:MET:HB2	1:A:452:PHE:CE1	2.54	0.42
1:E:344:MET:HE3	1:E:344:MET:HB3	1.71	0.42
1:G:109:THR:HG22	1:G:158:LEU:CD2	2.49	0.42
1:G:240:VAL:HG12	1:G:242:LEU:CD1	2.49	0.42
1:G:451:TRP:CD1	1:G:451:TRP:N	2.87	0.42
1:I:373:MET:HB3	1:I:422:SER:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE1	1:B:83:TYR:CZ	2.73	0.42
1:B:173:ASN:HB2	1:B:176:PHE:HB2	2.01	0.42
1:D:217:ILE:HA	1:D:224:ILE:HG21	2.00	0.42
1:F:64:MET:HE3	1:F:79:ASP:HB2	2.01	0.42
1:F:257:ASP:O	1:F:260:VAL:CG2	2.67	0.42
1:F:451:TRP:CD1	1:F:451:TRP:N	2.87	0.42
1:I:173:ASN:HB2	1:I:176:PHE:HB2	2.01	0.42
1:A:98:LYS:H	1:A:98:LYS:HG3	1.67	0.42
1:C:451:TRP:CD1	1:C:451:TRP:N	2.87	0.42
1:D:112:LYS:O	1:D:115:THR:HG22	2.19	0.42
1:F:116:VAL:HG21	1:F:153:ILE:HG12	2.01	0.42
1:F:122:GLU:H	1:F:122:GLU:HG3	1.68	0.42
1:H:173:ASN:HB2	1:H:176:PHE:HB2	2.01	0.42
1:K:210:SER:OG	1:K:211:LYS:N	2.51	0.42
1:B:85:LEU:HD22	1:B:117:ILE:HD11	2.00	0.42
1:B:451:TRP:CD1	1:B:451:TRP:N	2.87	0.42
1:D:401:MET:HB2	1:D:452:PHE:CE1	2.54	0.42
1:F:257:ASP:O	1:F:260:VAL:HG23	2.19	0.42
1:J:449:LYS:O	1:J:451:TRP:HD1	2.03	0.42
1:L:429:VAL:HG11	1:L:434:MET:CE	2.49	0.42
1:C:198:GLY:O	1:C:199:VAL:C	2.63	0.42
1:H:449:LYS:O	1:H:451:TRP:HD1	2.03	0.42
1:K:326:GLN:CD	1:K:478:THR:HG23	2.44	0.42
1:D:341:ARG:O	1:D:343:ILE:HD12	2.19	0.42
1:J:173:ASN:HB2	1:J:176:PHE:HB2	2.01	0.42
1:J:192:GLU:HG3	1:L:301:TRP:CZ2	2.54	0.42
1:L:198:GLY:O	1:L:199:VAL:C	2.63	0.42
1:B:127:ARG:HB3	1:B:136:ILE:HD12	2.02	0.42
1:E:451:TRP:CD1	1:E:451:TRP:N	2.87	0.42
1:H:150:LYS:HE2	1:H:150:LYS:HB3	1.75	0.42
1:I:253:GLU:OE1	1:I:286:ARG:NH2	2.44	0.42
1:B:198:GLY:O	1:B:199:VAL:C	2.63	0.42
1:B:217:ILE:HG13	1:B:465:PHE:HB3	2.02	0.42
1:C:173:ASN:HB2	1:C:176:PHE:HB2	2.01	0.42
1:C:242:LEU:CD1	1:C:242:LEU:N	2.83	0.42
1:E:401:MET:HB2	1:E:452:PHE:CE1	2.54	0.42
1:G:198:GLY:O	1:G:199:VAL:C	2.63	0.42
1:J:451:TRP:CD1	1:J:451:TRP:N	2.87	0.42
1:L:414:ASN:O	1:L:418:GLN:HG3	2.20	0.42
1:D:220:ILE:H	1:D:220:ILE:HG13	1.59	0.42
1:I:401:MET:HB2	1:I:452:PHE:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ARG:HG2	1:E:226:PRO:HA	2.02	0.41
1:G:449:LYS:O	1:G:451:TRP:HD1	2.03	0.41
1:H:414:ASN:O	1:H:418:GLN:HG3	2.20	0.41
1:A:458:ASN:OD1	1:A:459:PRO:HD2	2.20	0.41
1:D:449:LYS:O	1:D:451:TRP:HD1	2.03	0.41
1:E:173:ASN:HB2	1:E:176:PHE:HB2	2.02	0.41
1:E:414:ASN:O	1:E:418:GLN:HG3	2.21	0.41
1:G:551:VAL:HG13	1:G:574:PHE:HD2	1.84	0.41
1:I:314:SER:OG	2:V:1:GLY:N	2.53	0.41
1:I:414:ASN:O	1:I:418:GLN:HG3	2.21	0.41
1:I:458:ASN:OD1	1:I:459:PRO:HD2	2.20	0.41
1:L:449:LYS:O	1:L:451:TRP:HD1	2.03	0.41
1:A:398:THR:OG1	1:A:436:GLN:NE2	2.54	0.41
1:A:451:TRP:CD1	1:A:451:TRP:N	2.87	0.41
1:C:458:ASN:OD1	1:C:459:PRO:HD2	2.20	0.41
1:D:198:GLY:O	1:D:199:VAL:C	2.63	0.41
1:E:198:GLY:O	1:E:199:VAL:C	2.63	0.41
1:G:242:LEU:CD1	1:G:242:LEU:N	2.83	0.41
1:G:458:ASN:OD1	1:G:459:PRO:HD2	2.20	0.41
1:I:198:GLY:O	1:I:199:VAL:C	2.63	0.41
1:J:117:ILE:HD13	1:J:141:LYS:O	2.20	0.41
1:K:198:GLY:O	1:K:199:VAL:C	2.63	0.41
1:L:540:GLY:HA3	1:L:574:PHE:CE2	2.55	0.41
1:B:458:ASN:OD1	1:B:459:PRO:HD2	2.20	0.41
1:C:343:ILE:HD13	1:C:374:MET:CE	2.50	0.41
1:C:449:LYS:O	1:C:451:TRP:HD1	2.03	0.41
1:D:414:ASN:O	1:D:418:GLN:HG3	2.20	0.41
1:H:451:TRP:CD1	1:H:451:TRP:N	2.87	0.41
1:H:458:ASN:OD1	1:H:459:PRO:HD2	2.20	0.41
1:A:566:TYR:CE1	2:P:4:GLY:HA3	2.56	0.41
1:C:289:PHE:HB2	1:C:295:LYS:O	2.21	0.41
1:D:289:PHE:HB2	1:D:295:LYS:O	2.21	0.41
1:F:91:LYS:HA	1:F:102:HIS:ND1	2.35	0.41
1:F:94:SER:OG	1:F:101:ARG:N	2.43	0.41
1:F:198:GLY:O	1:F:199:VAL:C	2.63	0.41
1:G:173:ASN:HB2	1:G:176:PHE:HB2	2.01	0.41
1:G:344:MET:HE3	1:G:344:MET:HB3	1.90	0.41
1:G:507:GLY:HA3	1:G:589:LYS:HE2	2.03	0.41
1:I:289:PHE:HB2	1:I:295:LYS:O	2.21	0.41
1:I:449:LYS:O	1:I:451:TRP:HD1	2.03	0.41
1:I:451:TRP:N	1:I:451:TRP:CD1	2.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:521:ALA:HB3	1:I:524:GLY:O	2.20	0.41
1:J:343:ILE:HD13	1:J:343:ILE:C	2.45	0.41
1:L:521:ALA:HB3	1:L:524:GLY:O	2.21	0.41
1:A:138:PHE:HB2	1:A:142:GLY:HA3	2.02	0.41
1:A:198:GLY:O	1:A:199:VAL:C	2.63	0.41
1:A:414:ASN:O	1:A:418:GLN:HG3	2.21	0.41
1:B:150:LYS:HA	1:B:163:LEU:HD13	2.01	0.41
1:B:339:GLY:HA2	1:B:355:GLY:HA3	2.03	0.41
1:B:414:ASN:O	1:B:418:GLN:HG3	2.20	0.41
1:D:488:GLN:O	1:D:492:VAL:HG23	2.21	0.41
1:F:414:ASN:O	1:F:418:GLN:HG3	2.20	0.41
1:H:154:GLU:HB2	1:H:155:LYS:NZ	2.35	0.41
1:I:488:GLN:O	1:I:492:VAL:HG23	2.21	0.41
1:J:339:GLY:HA2	1:J:355:GLY:HA3	2.01	0.41
1:A:449:LYS:O	1:A:451:TRP:HD1	2.03	0.41
1:C:488:GLN:O	1:C:492:VAL:HG23	2.21	0.41
1:D:207:LEU:HD21	1:D:240:VAL:HG12	2.03	0.41
1:D:502:ASN:OD1	1:D:502:ASN:N	2.39	0.41
1:F:458:ASN:OD1	1:F:459:PRO:HD2	2.21	0.41
1:G:253:GLU:OE1	1:G:286:ARG:NH2	2.44	0.41
1:H:198:GLY:O	1:H:199:VAL:C	2.63	0.41
1:L:259:MET:HE1	1:L:570:VAL:HA	2.01	0.41
1:A:289:PHE:HB2	1:A:295:LYS:O	2.21	0.41
1:B:289:PHE:HB2	1:B:295:LYS:O	2.21	0.41
1:B:488:GLN:O	1:B:492:VAL:HG23	2.21	0.41
1:E:150:LYS:HA	1:E:163:LEU:HD13	2.03	0.41
1:F:289:PHE:HB2	1:F:295:LYS:O	2.21	0.41
1:F:398:THR:OG1	1:F:436:GLN:NE2	2.54	0.41
1:G:581:THR:O	1:G:585:LEU:CD2	2.42	0.41
1:J:198:GLY:O	1:J:199:VAL:C	2.63	0.41
1:J:414:ASN:O	1:J:418:GLN:HG3	2.20	0.41
1:K:289:PHE:HB2	1:K:295:LYS:O	2.21	0.41
1:K:414:ASN:O	1:K:418:GLN:HG3	2.20	0.41
1:A:521:ALA:HB3	1:A:524:GLY:O	2.21	0.41
1:E:94:SER:OG	1:E:101:ARG:N	2.43	0.41
1:F:449:LYS:O	1:F:451:TRP:HD1	2.03	0.41
1:K:173:ASN:HB2	1:K:176:PHE:HB2	2.02	0.41
1:L:81:GLU:CD	1:L:83:TYR:HH	2.29	0.41
1:A:531:PRO:HD3	1:B:134:PHE:CD2	2.56	0.40
1:D:458:ASN:OD1	1:D:459:PRO:HD2	2.20	0.40
1:H:488:GLN:O	1:H:492:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:GLU:HG2	1:L:523:ASN:HD22	1.85	0.40
1:B:449:LYS:O	1:B:451:TRP:HD1	2.03	0.40
1:C:497:LYS:HE2	1:C:497:LYS:HB3	1.72	0.40
1:J:289:PHE:HB2	1:J:295:LYS:O	2.21	0.40
1:K:449:LYS:O	1:K:451:TRP:HD1	2.03	0.40
1:K:488:GLN:O	1:K:492:VAL:HG23	2.21	0.40
1:L:436:GLN:O	1:L:439:SER:OG	2.36	0.40
1:L:458:ASN:OD1	1:L:459:PRO:HD2	2.21	0.40
1:C:414:ASN:O	1:C:418:GLN:HG3	2.21	0.40
1:C:529:LYS:HE2	1:C:529:LYS:HB2	1.91	0.40
1:D:81:GLU:OE1	1:D:83:TYR:CZ	2.75	0.40
1:E:118:ASN:C	1:E:141:LYS:HE2	2.47	0.40
1:E:488:GLN:O	1:E:492:VAL:HG23	2.21	0.40
1:L:220:ILE:HG12	1:L:224:ILE:HG12	2.03	0.40
1:C:240:VAL:HG12	1:C:242:LEU:CD1	2.52	0.40
1:G:91:LYS:HA	1:G:102:HIS:ND1	2.36	0.40
1:G:206:TYR:OH	1:G:223:TYR:O	2.40	0.40
1:I:148:GLN:H	1:I:148:GLN:HG3	1.73	0.40
1:K:458:ASN:OD1	1:K:459:PRO:HD2	2.22	0.40
1:B:118:ASN:C	1:B:141:LYS:HE2	2.46	0.40
1:D:173:ASN:HB2	1:D:176:PHE:HB2	2.02	0.40
1:E:220:ILE:H	1:E:220:ILE:HG13	1.55	0.40
1:F:488:GLN:O	1:F:492:VAL:HG23	2.21	0.40
1:G:414:ASN:O	1:G:418:GLN:HG3	2.21	0.40
1:L:71:ARG:HG3	1:L:72:ASN:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/650 (80%)	468 (90%)	43 (8%)	7 (1%)	9	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	521/650 (80%)	473 (91%)	40 (8%)	8 (2%)	8	29
1	C	518/650 (80%)	467 (90%)	46 (9%)	5 (1%)	12	38
1	D	488/650 (75%)	438 (90%)	40 (8%)	10 (2%)	6	24
1	E	520/650 (80%)	473 (91%)	39 (8%)	8 (2%)	8	29
1	F	519/650 (80%)	479 (92%)	36 (7%)	4 (1%)	16	44
1	G	516/650 (79%)	472 (92%)	40 (8%)	4 (1%)	16	44
1	H	457/650 (70%)	416 (91%)	38 (8%)	3 (1%)	18	46
1	I	515/650 (79%)	472 (92%)	40 (8%)	3 (1%)	21	49
1	J	514/650 (79%)	465 (90%)	43 (8%)	6 (1%)	10	33
1	K	452/650 (70%)	409 (90%)	39 (9%)	4 (1%)	14	41
1	L	452/650 (70%)	414 (92%)	37 (8%)	1 (0%)	43	70
2	P	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	R	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
2	S	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	T	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
2	U	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
2	V	3/5 (60%)	3 (100%)	0	0	100	100
2	W	2/5 (40%)	2 (100%)	0	0	100	100
2	X	2/5 (40%)	2 (100%)	0	0	100	100
2	Y	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	6017/7850 (77%)	5465 (91%)	487 (8%)	65 (1%)	11	36

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	B	211	LYS
1	B	218	HIS
1	D	211	LYS
1	E	98	LYS
1	E	211	LYS
1	E	218	HIS
1	I	223	TYR
1	J	218	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	211	LYS
1	A	117	ILE
1	B	226	PRO
1	C	214	LEU
1	C	524	GLY
1	D	116	VAL
1	D	228	THR
1	E	226	PRO
1	F	98	LYS
1	F	228	THR
1	F	368	SER
1	G	132	LYS
1	G	211	LYS
1	H	368	SER
1	J	524	GLY
1	A	368	SER
1	B	368	SER
1	B	523	ASN
1	C	368	SER
1	D	368	SER
1	E	368	SER
1	G	98	LYS
1	H	211	LYS
1	I	98	LYS
1	J	213	SER
1	K	218	HIS
1	A	98	LYS
1	A	131	LYS
1	A	213	SER
1	B	98	LYS
1	B	220	ILE
1	C	98	LYS
1	D	135	GLN
1	D	218	HIS
1	D	226	PRO
1	E	97	SER
1	F	220	ILE
1	H	213	SER
1	I	211	LYS
1	J	98	LYS
1	J	224	ILE
1	J	525	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	231	GLU
2	U	3	GLY
1	B	224	ILE
1	D	136	ILE
1	G	368	SER
1	L	547	PRO
2	T	3	GLY
1	C	525	GLY
1	K	226	PRO
1	D	224	ILE
1	E	220	ILE
1	E	525	GLY
1	A	224	ILE
1	D	220	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	439/552 (80%)	388 (88%)	51 (12%)	5	20
1	B	442/552 (80%)	390 (88%)	52 (12%)	5	19
1	C	439/552 (80%)	378 (86%)	61 (14%)	3	14
1	D	417/552 (76%)	370 (89%)	47 (11%)	5	20
1	E	441/552 (80%)	393 (89%)	48 (11%)	6	22
1	F	440/552 (80%)	390 (89%)	50 (11%)	5	20
1	G	437/552 (79%)	390 (89%)	47 (11%)	6	22
1	H	387/552 (70%)	347 (90%)	40 (10%)	7	25
1	I	436/552 (79%)	388 (89%)	48 (11%)	6	22
1	J	435/552 (79%)	385 (88%)	50 (12%)	5	20
1	K	384/552 (70%)	339 (88%)	45 (12%)	5	19
1	L	386/552 (70%)	338 (88%)	48 (12%)	4	18
All	All	5083/6624 (77%)	4496 (88%)	587 (12%)	5	20

All (587) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	97	SER
1	A	98	LYS
1	A	114	SER
1	A	116	VAL
1	A	119	MET
1	A	120	LYS
1	A	122	GLU
1	A	125	GLU
1	A	131	LYS
1	A	137	GLU
1	A	140	ARG
1	A	141	LYS
1	A	158	LEU
1	A	161	ILE
1	A	162	SER
1	A	164	LEU
1	A	166	GLU
1	A	167	THR
1	A	173	ASN
1	A	179	HIS
1	A	189	ASP
1	A	194	LYS
1	A	197	LEU
1	A	207	LEU
1	A	211	LYS
1	A	214	LEU
1	A	236	ARG
1	A	281	LEU
1	A	288	THR
1	A	341	ARG
1	A	347	ARG
1	A	348	ILE
1	A	368	SER
1	A	373	MET
1	A	397	SER
1	A	449	LYS
1	A	453	VAL
1	A	457	GLU
1	A	469	GLN
1	A	490	ASP
1	A	496	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	502	ASN
1	A	510	VAL
1	A	516	THR
1	A	541	ASP
1	A	545	LYS
1	A	548	LYS
1	A	549	VAL
1	A	587	VAL
1	A	589	LYS
1	B	84	LYS
1	B	88	VAL
1	B	92	LYS
1	B	104	VAL
1	B	114	SER
1	B	117	ILE
1	B	119	MET
1	B	123	GLU
1	B	125	GLU
1	B	136	ILE
1	B	137	GLU
1	B	140	ARG
1	B	158	LEU
1	B	161	ILE
1	B	162	SER
1	B	164	LEU
1	B	166	GLU
1	B	167	THR
1	B	173	ASN
1	B	179	HIS
1	B	189	ASP
1	B	194	LYS
1	B	197	LEU
1	B	211	LYS
1	B	218	HIS
1	B	220	ILE
1	B	224	ILE
1	B	230	LYS
1	B	231	GLU
1	B	235	LYS
1	B	271	VAL
1	B	288	THR
1	B	295	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	ARG
1	B	343	ILE
1	B	368	SER
1	B	373	MET
1	B	449	LYS
1	B	453	VAL
1	B	463	ARG
1	B	469	GLN
1	B	490	ASP
1	B	496	LYS
1	B	502	ASN
1	B	510	VAL
1	B	516	THR
1	B	523	ASN
1	B	529	LYS
1	B	541	ASP
1	B	548	LYS
1	B	549	VAL
1	B	587	VAL
1	C	81	GLU
1	C	89	ILE
1	C	90	ASP
1	C	91	LYS
1	C	92	LYS
1	C	96	ASN
1	C	97	SER
1	C	101	ARG
1	C	104	VAL
1	C	108	GLU
1	C	111	LYS
1	C	113	LEU
1	C	116	VAL
1	C	117	ILE
1	C	120	LYS
1	C	123	GLU
1	C	131	LYS
1	C	136	ILE
1	C	137	GLU
1	C	140	ARG
1	C	148	GLN
1	C	158	LEU
1	C	161	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	162	SER
1	C	164	LEU
1	C	166	GLU
1	C	167	THR
1	C	173	ASN
1	C	179	HIS
1	C	189	ASP
1	C	194	LYS
1	C	217	ILE
1	C	219	ASP
1	C	227	ASN
1	C	229	LYS
1	C	235	LYS
1	C	281	LEU
1	C	288	THR
1	C	341	ARG
1	C	353	ARG
1	C	368	SER
1	C	373	MET
1	C	409	GLN
1	C	449	LYS
1	C	453	VAL
1	C	457	GLU
1	C	463	ARG
1	C	469	GLN
1	C	490	ASP
1	C	496	LYS
1	C	497	LYS
1	C	502	ASN
1	C	510	VAL
1	C	516	THR
1	C	523	ASN
1	C	529	LYS
1	C	541	ASP
1	C	545	LYS
1	C	548	LYS
1	C	549	VAL
1	C	589	LYS
1	D	81	GLU
1	D	111	LYS
1	D	112	LYS
1	D	113	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	119	MET
1	D	120	LYS
1	D	123	GLU
1	D	125	GLU
1	D	126	LYS
1	D	127	ARG
1	D	130	GLN
1	D	137	GLU
1	D	158	LEU
1	D	161	ILE
1	D	166	GLU
1	D	167	THR
1	D	173	ASN
1	D	179	HIS
1	D	194	LYS
1	D	197	LEU
1	D	217	ILE
1	D	219	ASP
1	D	220	ILE
1	D	224	ILE
1	D	229	LYS
1	D	235	LYS
1	D	236	ARG
1	D	240	VAL
1	D	261	GLU
1	D	288	THR
1	D	337	LYS
1	D	341	ARG
1	D	368	SER
1	D	384	LYS
1	D	449	LYS
1	D	453	VAL
1	D	457	GLU
1	D	469	GLN
1	D	490	ASP
1	D	496	LYS
1	D	502	ASN
1	D	510	VAL
1	D	516	THR
1	D	529	LYS
1	D	541	ASP
1	D	545	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	549	VAL
1	E	98	LYS
1	E	103	VAL
1	E	107	LYS
1	E	114	SER
1	E	119	MET
1	E	120	LYS
1	E	122	GLU
1	E	125	GLU
1	E	132	LYS
1	E	137	GLU
1	E	140	ARG
1	E	158	LEU
1	E	161	ILE
1	E	162	SER
1	E	164	LEU
1	E	166	GLU
1	E	167	THR
1	E	173	ASN
1	E	179	HIS
1	E	189	ASP
1	E	194	LYS
1	E	214	LEU
1	E	218	HIS
1	E	219	ASP
1	E	220	ILE
1	E	224	ILE
1	E	229	LYS
1	E	261	GLU
1	E	343	ILE
1	E	344	MET
1	E	346	SER
1	E	368	SER
1	E	373	MET
1	E	449	LYS
1	E	453	VAL
1	E	469	GLN
1	E	487	LYS
1	E	490	ASP
1	E	496	LYS
1	E	502	ASN
1	E	510	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	541	ASP
1	E	545	LYS
1	E	548	LYS
1	E	549	VAL
1	E	578	MET
1	E	587	VAL
1	E	591	LYS
1	F	97	SER
1	F	98	LYS
1	F	99	LYS
1	F	105	ASP
1	F	106	LYS
1	F	107	LYS
1	F	116	VAL
1	F	117	ILE
1	F	119	MET
1	F	120	LYS
1	F	122	GLU
1	F	123	GLU
1	F	125	GLU
1	F	131	LYS
1	F	137	GLU
1	F	158	LEU
1	F	161	ILE
1	F	162	SER
1	F	164	LEU
1	F	166	GLU
1	F	167	THR
1	F	173	ASN
1	F	179	HIS
1	F	189	ASP
1	F	211	LYS
1	F	214	LEU
1	F	219	ASP
1	F	220	ILE
1	F	229	LYS
1	F	235	LYS
1	F	260	VAL
1	F	261	GLU
1	F	288	THR
1	F	343	ILE
1	F	368	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	373	MET
1	F	448	LEU
1	F	449	LYS
1	F	453	VAL
1	F	457	GLU
1	F	469	GLN
1	F	490	ASP
1	F	496	LYS
1	F	502	ASN
1	F	510	VAL
1	F	516	THR
1	F	541	ASP
1	F	545	LYS
1	F	549	VAL
1	F	591	LYS
1	G	81	GLU
1	G	84	LYS
1	G	97	SER
1	G	98	LYS
1	G	108	GLU
1	G	114	SER
1	G	119	MET
1	G	122	GLU
1	G	123	GLU
1	G	125	GLU
1	G	137	GLU
1	G	158	LEU
1	G	161	ILE
1	G	162	SER
1	G	164	LEU
1	G	166	GLU
1	G	167	THR
1	G	173	ASN
1	G	179	HIS
1	G	189	ASP
1	G	194	LYS
1	G	214	LEU
1	G	215	ARG
1	G	217	ILE
1	G	219	ASP
1	G	224	ILE
1	G	235	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	261	GLU
1	G	288	THR
1	G	341	ARG
1	G	343	ILE
1	G	344	MET
1	G	358	GLU
1	G	373	MET
1	G	449	LYS
1	G	453	VAL
1	G	457	GLU
1	G	469	GLN
1	G	490	ASP
1	G	496	LYS
1	G	502	ASN
1	G	510	VAL
1	G	516	THR
1	G	541	ASP
1	G	545	LYS
1	G	549	VAL
1	G	585	LEU
1	H	140	ARG
1	H	141	LYS
1	H	143	THR
1	H	148	GLN
1	H	152	LYS
1	H	154	GLU
1	H	155	LYS
1	H	164	LEU
1	H	166	GLU
1	H	167	THR
1	H	173	ASN
1	H	179	HIS
1	H	189	ASP
1	H	197	LEU
1	H	214	LEU
1	H	217	ILE
1	H	218	HIS
1	H	227	ASN
1	H	235	LYS
1	H	281	LEU
1	H	288	THR
1	H	341	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	353	ARG
1	H	368	SER
1	H	373	MET
1	H	396	LYS
1	H	449	LYS
1	H	453	VAL
1	H	457	GLU
1	H	469	GLN
1	H	490	ASP
1	H	496	LYS
1	H	502	ASN
1	H	510	VAL
1	H	516	THR
1	H	529	LYS
1	H	541	ASP
1	H	545	LYS
1	H	549	VAL
1	H	589	LYS
1	I	96	ASN
1	I	97	SER
1	I	98	LYS
1	I	114	SER
1	I	118	ASN
1	I	119	MET
1	I	122	GLU
1	I	137	GLU
1	I	140	ARG
1	I	148	GLN
1	I	158	LEU
1	I	161	ILE
1	I	162	SER
1	I	164	LEU
1	I	166	GLU
1	I	167	THR
1	I	173	ASN
1	I	179	HIS
1	I	189	ASP
1	I	194	LYS
1	I	211	LYS
1	I	217	ILE
1	I	219	ASP
1	I	224	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	235	LYS
1	I	236	ARG
1	I	261	GLU
1	I	262	ARG
1	I	288	THR
1	I	295	LYS
1	I	321	LEU
1	I	337	LYS
1	I	341	ARG
1	I	449	LYS
1	I	453	VAL
1	I	469	GLN
1	I	487	LYS
1	I	490	ASP
1	I	496	LYS
1	I	502	ASN
1	I	510	VAL
1	I	529	LYS
1	I	541	ASP
1	I	545	LYS
1	I	548	LYS
1	I	549	VAL
1	I	578	MET
1	I	587	VAL
1	J	64	MET
1	J	65	ARG
1	J	91	LYS
1	J	96	ASN
1	J	98	LYS
1	J	99	LYS
1	J	114	SER
1	J	118	ASN
1	J	119	MET
1	J	123	GLU
1	J	140	ARG
1	J	141	LYS
1	J	150	LYS
1	J	152	LYS
1	J	158	LEU
1	J	161	ILE
1	J	162	SER
1	J	164	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	167	THR
1	J	173	ASN
1	J	179	HIS
1	J	186	LYS
1	J	194	LYS
1	J	214	LEU
1	J	256	LEU
1	J	288	THR
1	J	337	LYS
1	J	341	ARG
1	J	343	ILE
1	J	373	MET
1	J	379	LEU
1	J	449	LYS
1	J	453	VAL
1	J	457	GLU
1	J	469	GLN
1	J	479	LYS
1	J	487	LYS
1	J	490	ASP
1	J	496	LYS
1	J	497	LYS
1	J	502	ASN
1	J	509	GLU
1	J	510	VAL
1	J	518	GLN
1	J	529	LYS
1	J	541	ASP
1	J	545	LYS
1	J	548	LYS
1	J	549	VAL
1	J	590	SER
1	K	84	LYS
1	K	86	VAL
1	K	137	GLU
1	K	140	ARG
1	K	166	GLU
1	K	167	THR
1	K	173	ASN
1	K	179	HIS
1	K	194	LYS
1	K	200	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	216	TYR
1	K	217	ILE
1	K	219	ASP
1	K	220	ILE
1	K	224	ILE
1	K	229	LYS
1	K	231	GLU
1	K	236	ARG
1	K	256	LEU
1	K	261	GLU
1	K	288	THR
1	K	334	LYS
1	K	335	LYS
1	K	341	ARG
1	K	344	MET
1	K	348	ILE
1	K	358	GLU
1	K	363	LEU
1	K	373	MET
1	K	396	LYS
1	K	409	GLN
1	K	449	LYS
1	K	453	VAL
1	K	457	GLU
1	K	469	GLN
1	K	487	LYS
1	K	490	ASP
1	K	502	ASN
1	K	510	VAL
1	K	516	THR
1	K	541	ASP
1	K	545	LYS
1	K	546	ASN
1	K	549	VAL
1	K	587	VAL
1	L	84	LYS
1	L	138	PHE
1	L	140	ARG
1	L	141	LYS
1	L	143	THR
1	L	154	GLU
1	L	163	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	164	LEU
1	L	166	GLU
1	L	173	ASN
1	L	179	HIS
1	L	189	ASP
1	L	194	LYS
1	L	211	LYS
1	L	215	ARG
1	L	217	ILE
1	L	218	HIS
1	L	220	ILE
1	L	224	ILE
1	L	235	LYS
1	L	288	THR
1	L	299	LYS
1	L	343	ILE
1	L	344	MET
1	L	347	ARG
1	L	353	ARG
1	L	373	MET
1	L	376	LEU
1	L	396	LYS
1	L	449	LYS
1	L	453	VAL
1	L	457	GLU
1	L	469	GLN
1	L	487	LYS
1	L	490	ASP
1	L	502	ASN
1	L	510	VAL
1	L	516	THR
1	L	529	LYS
1	L	539	MET
1	L	541	ASP
1	L	544	LYS
1	L	545	LYS
1	L	546	ASN
1	L	548	LYS
1	L	549	VAL
1	L	578	MET
1	L	583	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	130	GLN
1	A	144	ASN
1	A	436	GLN
1	A	469	GLN
1	A	499	HIS
1	A	523	ASN
1	A	559	GLN
1	B	102	HIS
1	B	118	ASN
1	B	144	ASN
1	B	471	GLN
1	B	499	HIS
1	C	102	HIS
1	C	135	GLN
1	C	377	GLN
1	C	409	GLN
1	C	436	GLN
1	C	499	HIS
1	D	130	GLN
1	D	144	ASN
1	D	227	ASN
1	D	377	GLN
1	D	471	GLN
1	D	494	ASN
1	D	546	ASN
1	D	559	GLN
1	E	102	HIS
1	E	499	HIS
1	E	546	ASN
1	E	559	GLN
1	F	227	ASN
1	F	436	GLN
1	F	446	ASN
1	F	494	ASN
1	F	499	HIS
1	F	523	ASN
1	G	561	ASN
1	H	218	HIS
1	H	340	HIS
1	H	436	GLN
1	H	499	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	523	ASN
1	I	118	ASN
1	I	144	ASN
1	I	436	GLN
1	I	469	GLN
1	I	499	HIS
1	J	102	HIS
1	J	135	GLN
1	J	144	ASN
1	J	436	GLN
1	J	464	GLN
1	J	469	GLN
1	J	471	GLN
1	J	518	GLN
1	J	523	ASN
1	J	559	GLN
1	J	561	ASN
1	K	144	ASN
1	K	436	GLN
1	K	494	ASN
1	K	523	ASN
1	K	546	ASN
1	K	559	GLN
1	K	580	ASN
1	L	144	ASN
1	L	218	HIS
1	L	340	HIS
1	L	377	GLN
1	L	499	HIS
1	L	580	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	522/650 (80%)	-0.07	5 (0%)	79 66	38, 80, 156, 226	0
1	B	525/650 (80%)	-0.17	9 (1%)	69 53	39, 84, 139, 184	1 (0%)
1	C	522/650 (80%)	0.06	12 (2%)	61 45	50, 93, 183, 243	0
1	D	496/650 (76%)	0.11	23 (4%)	37 27	44, 89, 212, 320	0
1	E	524/650 (80%)	0.03	13 (2%)	58 43	45, 97, 141, 192	1 (0%)
1	F	523/650 (80%)	0.08	23 (4%)	39 28	56, 101, 172, 236	1 (0%)
1	G	520/650 (80%)	-0.03	6 (1%)	76 63	43, 87, 134, 195	0
1	H	465/650 (71%)	-0.08	10 (2%)	62 46	46, 85, 148, 206	0
1	I	519/650 (79%)	-0.10	12 (2%)	61 45	48, 96, 137, 173	0
1	J	518/650 (79%)	0.08	10 (1%)	66 49	46, 102, 197, 236	0
1	K	462/650 (71%)	0.41	28 (6%)	27 20	65, 119, 175, 229	0
1	L	462/650 (71%)	0.30	18 (3%)	43 30	69, 131, 181, 236	0
2	P	5/5 (100%)	0.42	0	100 100	103, 103, 120, 131	0
2	Q	5/5 (100%)	0.37	1 (20%)	3 4	90, 107, 144, 158	0
2	R	5/5 (100%)	1.08	1 (20%)	3 4	96, 100, 134, 135	0
2	S	5/5 (100%)	0.60	0	100 100	84, 86, 122, 128	0
2	T	5/5 (100%)	1.24	1 (20%)	3 4	96, 98, 129, 132	0
2	U	5/5 (100%)	0.91	1 (20%)	3 4	103, 106, 129, 133	0
2	V	5/5 (100%)	0.57	0	100 100	90, 106, 134, 135	0
2	W	4/5 (80%)	0.72	1 (25%)	2 3	84, 87, 108, 122	0
2	X	4/5 (80%)	0.29	0	100 100	97, 111, 115, 116	0
2	Y	4/5 (80%)	0.49	0	100 100	80, 93, 97, 105	0
All	All	6105/7850 (77%)	0.05	174 (2%)	53 39	38, 97, 169, 320	3 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	221	TRP	7.9
1	L	221	TRP	7.6
1	C	221	TRP	6.4
1	D	153	ILE	5.8
1	I	219	ASP	5.5
1	K	161	ILE	5.4
1	D	113	LEU	5.4
1	H	86	VAL	5.1
1	L	153	ILE	4.9
1	D	85	LEU	4.8
1	F	216	TYR	4.8
1	F	221	TRP	4.8
1	K	342	ASP	4.6
1	J	224	ILE	4.6
1	F	227	ASN	4.6
1	K	227	ASN	4.4
1	L	138	PHE	4.3
1	D	216	TYR	4.2
1	L	213	SER	4.2
1	D	161	ILE	4.1
1	E	228	THR	4.0
1	I	218	HIS	4.0
1	H	221	TRP	4.0
2	T	1	GLY	3.9
1	D	160	GLY	3.9
1	H	523	ASN	3.9
1	L	223	TYR	3.9
2	W	1	GLY	3.9
1	D	219	ASP	3.8
1	K	223	TYR	3.8
1	D	225	ALA	3.8
1	D	221	TRP	3.8
1	B	219	ASP	3.7
1	F	222	GLY	3.7
1	I	221	TRP	3.7
1	E	216	TYR	3.6
1	F	100	PRO	3.6
1	E	215	ARG	3.5
1	K	230	LYS	3.5
1	F	104	VAL	3.5
1	H	85	LEU	3.5
1	G	221	TRP	3.5
1	H	218	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	329	ALA	3.4
1	K	85	LEU	3.4
1	D	150	LYS	3.3
1	K	160	GLY	3.3
1	H	164	LEU	3.3
1	E	222	GLY	3.3
1	G	218	HIS	3.2
1	L	220	ILE	3.2
1	F	110	ALA	3.2
1	D	222	GLY	3.2
1	G	224	ILE	3.2
1	K	225	ALA	3.1
1	A	221	TRP	3.1
1	D	116	VAL	3.1
1	C	219	ASP	3.1
1	K	220	ILE	3.1
1	K	211	LYS	3.1
1	K	88	VAL	3.1
1	H	219	ASP	3.1
1	C	218	HIS	3.0
1	K	514	THR	3.0
1	F	213	SER	3.0
1	K	219	ASP	2.9
1	K	138	PHE	2.9
1	L	214	LEU	2.9
1	J	221	TRP	2.8
1	F	223	TYR	2.8
1	D	111	LYS	2.8
1	E	401	MET	2.8
1	B	228	THR	2.8
1	F	514	THR	2.7
1	F	219	ASP	2.7
1	C	214	LEU	2.7
1	F	121	PRO	2.7
1	I	224	ILE	2.7
1	K	228	THR	2.7
1	F	211	LYS	2.7
1	A	104	VAL	2.7
1	C	220	ILE	2.7
1	I	222	GLY	2.7
1	J	524	GLY	2.7
1	I	223	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	224	ILE	2.6
1	I	261	GLU	2.6
1	K	449	LYS	2.6
1	L	224	ILE	2.6
1	L	342	ASP	2.6
1	F	96	ASN	2.6
1	C	116	VAL	2.6
1	L	340	HIS	2.6
1	B	211	LYS	2.6
1	E	223	TYR	2.5
1	J	449	LYS	2.5
1	I	275	ALA	2.5
1	D	228	THR	2.5
1	D	159	PRO	2.5
2	R	5	GLY	2.5
1	F	124	ILE	2.5
1	F	218	HIS	2.5
1	I	214	LEU	2.5
1	I	225	ALA	2.5
1	E	219	ASP	2.5
1	K	329	ALA	2.4
1	E	211	LYS	2.4
1	E	229	LYS	2.4
1	K	214	LEU	2.4
1	G	219	ASP	2.4
1	K	226	PRO	2.4
1	K	86	VAL	2.4
1	C	353	ARG	2.4
1	K	320	GLY	2.4
1	K	216	TYR	2.4
1	F	98	LYS	2.3
1	A	218	HIS	2.3
1	K	340	HIS	2.3
1	D	158	LEU	2.3
1	E	227	ASN	2.3
1	F	108	GLU	2.3
1	H	225	ALA	2.3
1	L	216	TYR	2.3
1	D	223	TYR	2.2
1	K	347	ARG	2.2
1	C	196	ALA	2.2
1	C	222	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	210	SER	2.2
1	G	227	ASN	2.2
1	F	215	ARG	2.2
1	H	499	HIS	2.2
1	F	132	LYS	2.2
1	B	221	TRP	2.2
1	D	124	ILE	2.2
1	I	211	LYS	2.2
1	J	211	LYS	2.2
1	J	499	HIS	2.2
1	C	224	ILE	2.1
1	B	401	MET	2.1
1	F	225	ALA	2.1
1	L	225	ALA	2.1
1	B	230	LYS	2.1
1	F	111	LYS	2.1
1	D	135	GLN	2.1
1	C	234	PRO	2.1
1	D	226	PRO	2.1
2	Q	1	GLY	2.1
1	J	219	ASP	2.1
1	B	529	LYS	2.1
1	D	229	LYS	2.1
1	L	151	LEU	2.1
1	K	401	MET	2.1
1	A	212	GLY	2.1
1	H	524	GLY	2.1
1	L	152	LYS	2.1
1	A	133	ALA	2.1
1	D	415	GLU	2.1
1	B	215	ARG	2.1
1	K	373	MET	2.1
1	L	541	ASP	2.1
1	E	225	ALA	2.1
1	G	225	ALA	2.1
1	B	168	GLU	2.1
1	L	574	PHE	2.1
1	K	260	VAL	2.0
1	J	218	HIS	2.0
2	U	1	GLY	2.0
1	J	214	LEU	2.0
1	E	224	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	385	MET	2.0
1	C	211	LYS	2.0
1	L	545	LYS	2.0
1	D	137	GLU	2.0
1	J	570	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CD	F	801	1/1	0.78	0.11	184,184,184,184	0
3	CD	A	801	1/1	0.83	0.09	139,139,139,139	0
3	CD	E	801	1/1	0.85	0.09	181,181,181,181	0
3	CD	B	801	1/1	0.85	0.11	243,243,243,243	0
3	CD	C	801	1/1	0.87	0.08	72,72,72,72	0
3	CD	G	801	1/1	0.87	0.08	150,150,150,150	0
3	CD	I	801	1/1	0.90	0.12	171,171,171,171	0
3	CD	D	801	1/1	0.91	0.06	120,120,120,120	0
4	CL	D	802	1/1	0.91	0.06	77,77,77,77	0
4	CL	F	802	1/1	0.92	0.05	80,80,80,80	0
3	CD	J	801	1/1	0.95	0.05	104,104,104,104	0
3	CD	H	801	1/1	0.97	0.04	76,76,76,76	0
4	CL	H	802	1/1	0.97	0.04	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.