Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 10:55 PM EDT

PDB ID	:	1WQS
Title	:	Crystal structure of Norovirus 3C-like protease
Authors	:	Nakamura, K.; Someya, Y.; Kumasaka, T.; Tanaka, N.
Deposited on	:	2004-10-01
Resolution	:	2.80 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:

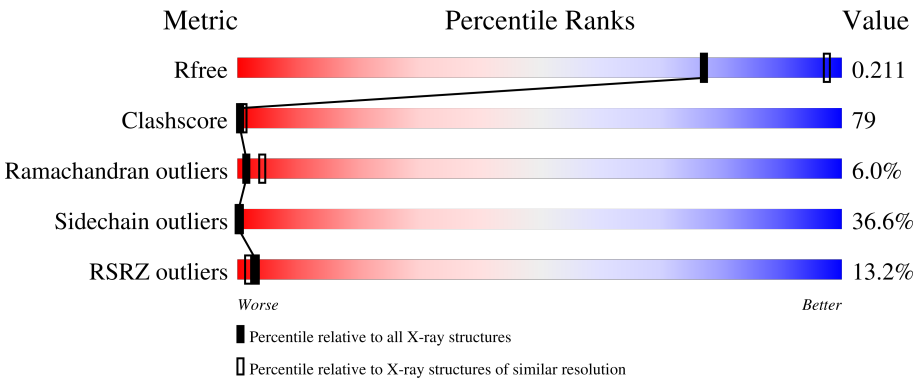
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	173	6%; 23%, 39%, 23%, 14%
1	B	173	18%; 17%, 31%, 32%, 20%
1	C	173	5%; 29%, 28%, 28%, 14%
1	D	173	23%; 18%, 33%, 30%, 18%

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	TLA	A	301	-	-	X	X
4	TAR	A	300	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5367 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.

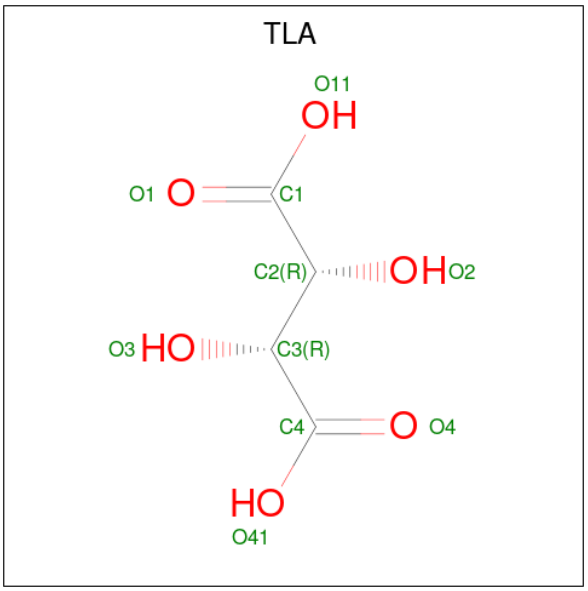
- Molecule 1 is a protein called 3C-like protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1303	829	232	232	10	0	0	0
1	B	173	1303	829	232	232	10	0	0	0
1	C	173	1303	829	232	232	10	0	0	0
1	D	173	1303	829	232	232	10	0	0	0

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

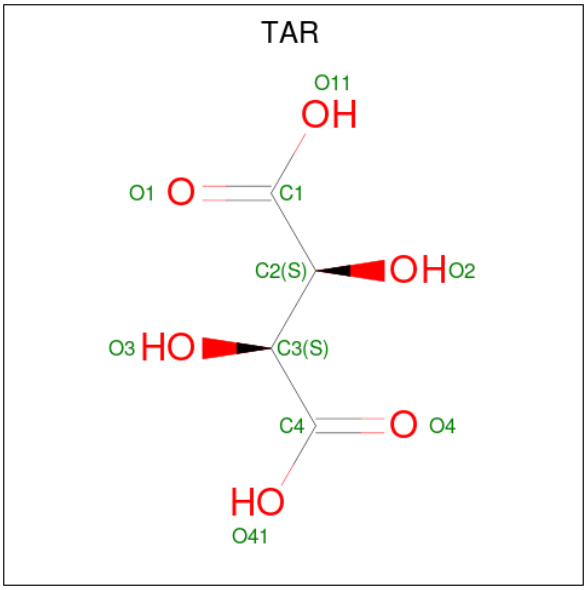
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	10	4	6	0	0

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	4	6	0	0

- Molecule 5 is water.

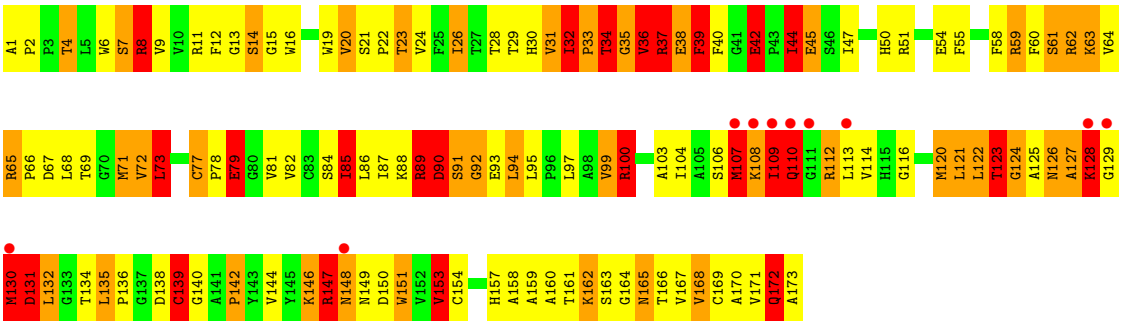
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	33	33	33	0	0
			Total	O		
5	B	22	22	22	0	0
			Total	O		
5	C	41	41	41	0	0
			Total	O		
5	D	31	31	31	0	0

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.

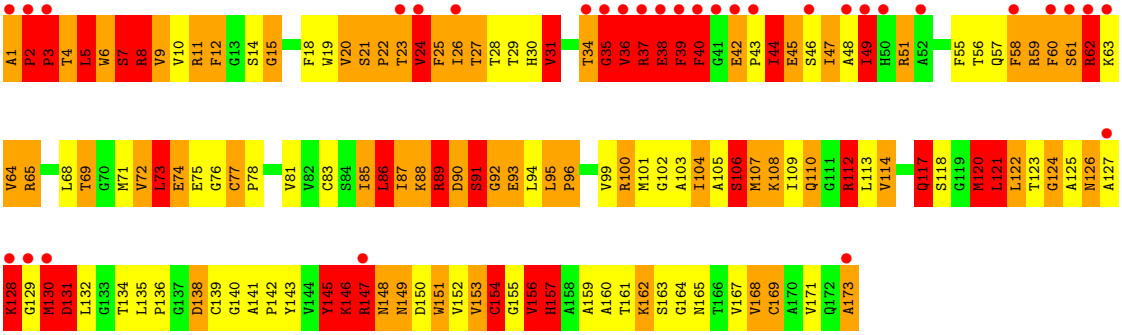
• Molecule 1: 3C-like protease

Chain A:



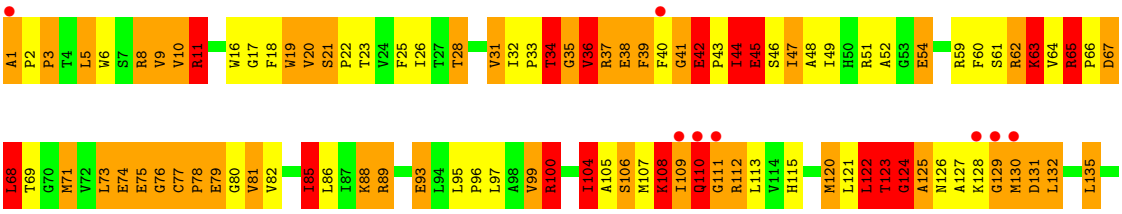
• Molecule 1: 3C-like protease

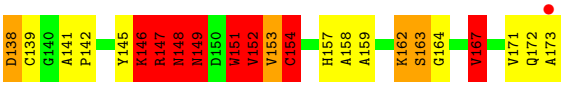
Chain B:



• Molecule 1: 3C-like protease

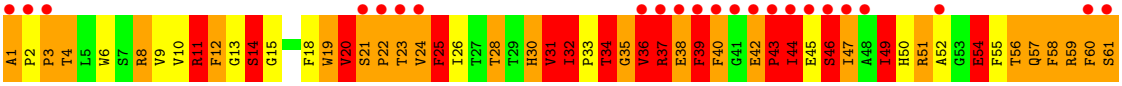
Chain C:

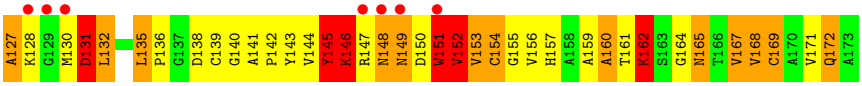




- Molecule 1: 3C-like protease

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	128.89Å 128.89Å 118.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 39.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (8.00-2.80) 99.9 (39.73-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.240 0.212 , 0.211	Depositor DCC
R_{free} test set	2740 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 121.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5367	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TAR, TLA, HG

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	2.29	60/1334 (4.5%)	2.49	93/1810 (5.1%)
1	B	2.47	74/1334 (5.5%)	2.61	114/1810 (6.3%)
1	C	1.98	36/1334 (2.7%)	2.23	68/1810 (3.8%)
1	D	2.23	57/1334 (4.3%)	2.48	95/1810 (5.2%)
All	All	2.25	227/5336 (4.3%)	2.46	370/7240 (5.1%)

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	4
1	B	0	4
1	D	0	4
All	All	0	12

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	VAL	CB-CG2	16.14	1.86	1.52
1	B	173	ALA	CA-CB	15.02	1.83	1.52
1	D	131	ASP	CB-CG	14.10	1.81	1.51
1	A	172	GLN	CB-CG	13.38	1.88	1.52
1	A	172	GLN	CG-CD	12.71	1.80	1.51
1	A	130	MET	CG-SD	12.67	2.14	1.81
1	D	36	VAL	CA-CB	12.56	1.81	1.54
1	B	2	PRO	C-N	12.53	1.58	1.34
1	A	100	ARG	CG-CD	12.22	1.82	1.51
1	B	130	MET	CA-C	11.62	1.83	1.52
1	A	45	GLU	CG-CD	11.14	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	PRO	CA-C	11.04	1.75	1.52
1	B	24	VAL	CA-CB	10.85	1.77	1.54
1	B	75	GLU	CB-CG	10.79	1.72	1.52
1	A	85	ILE	CA-CB	10.67	1.79	1.54
1	D	154	CYS	CB-SG	10.54	2.00	1.82
1	C	45	GLU	CG-CD	10.53	1.67	1.51
1	D	2	PRO	CA-C	10.51	1.73	1.52
1	D	4	THR	CA-CB	10.32	1.80	1.53
1	A	100	ARG	CB-CG	10.18	1.80	1.52
1	B	75	GLU	CG-CD	10.07	1.67	1.51
1	A	131	ASP	N-CA	9.93	1.66	1.46
1	D	90	ASP	CB-CG	9.93	1.72	1.51
1	A	130	MET	CB-CG	9.88	1.82	1.51
1	B	131	ASP	CB-CG	9.88	1.72	1.51
1	B	125	ALA	CA-CB	9.84	1.73	1.52
1	B	62	ARG	CB-CG	9.82	1.79	1.52
1	A	45	GLU	CB-CG	9.70	1.70	1.52
1	D	151	TRP	CB-CG	9.52	1.67	1.50
1	B	127	ALA	CA-CB	9.52	1.72	1.52
1	A	77	CYS	CB-SG	9.48	1.98	1.82
1	B	110	GLN	CB-CG	9.22	1.77	1.52
1	A	124	GLY	N-CA	9.18	1.59	1.46
1	A	151	TRP	CB-CG	-9.08	1.33	1.50
1	D	141	ALA	CA-CB	-9.07	1.33	1.52
1	A	32	ILE	CA-CB	8.80	1.75	1.54
1	C	85	ILE	CA-CB	8.80	1.75	1.54
1	D	148	ASN	CB-CG	8.79	1.71	1.51
1	C	173	ALA	CA-CB	8.72	1.70	1.52
1	C	48	ALA	CA-CB	-8.63	1.34	1.52
1	A	128	LYS	CA-C	8.55	1.75	1.52
1	B	146	LYS	CB-CG	8.51	1.75	1.52
1	B	130	MET	N-CA	8.42	1.63	1.46
1	C	36	VAL	CA-CB	8.38	1.72	1.54
1	C	45	GLU	CB-CG	8.31	1.68	1.52
1	A	34	THR	CA-C	8.25	1.74	1.52
1	D	154	CYS	CA-CB	8.23	1.72	1.53
1	B	36	VAL	N-CA	8.22	1.62	1.46
1	B	153	VAL	CA-CB	-8.20	1.37	1.54
1	A	20	VAL	CB-CG1	-8.12	1.35	1.52
1	B	7	SER	CA-CB	8.08	1.65	1.52
1	D	88	LYS	CE-NZ	8.05	1.69	1.49
1	D	152	VAL	CA-CB	8.02	1.71	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	20	VAL	CB-CG2	7.95	1.69	1.52
1	B	128	LYS	CB-CG	7.93	1.74	1.52
1	B	62	ARG	CA-CB	7.93	1.71	1.53
1	A	110	GLN	N-CA	7.91	1.62	1.46
1	A	34	THR	CA-CB	7.88	1.73	1.53
1	D	36	VAL	CB-CG2	7.86	1.69	1.52
1	A	130	MET	CA-CB	7.82	1.71	1.53
1	C	123	THR	CA-CB	-7.79	1.33	1.53
1	D	50	HIS	CA-CB	7.78	1.71	1.53
1	B	3	PRO	N-CA	7.77	1.60	1.47
1	D	88	LYS	CD-CE	7.76	1.70	1.51
1	A	31	VAL	CB-CG2	-7.76	1.36	1.52
1	C	112	ARG	CB-CG	7.70	1.73	1.52
1	B	62	ARG	CG-CD	7.69	1.71	1.51
1	C	112	ARG	CG-CD	7.67	1.71	1.51
1	D	51	ARG	CB-CG	7.67	1.73	1.52
1	C	152	VAL	CB-CG2	-7.66	1.36	1.52
1	D	23	THR	CA-CB	7.62	1.73	1.53
1	A	35	GLY	CA-C	-7.60	1.39	1.51
1	D	162	LYS	CD-CE	7.51	1.70	1.51
1	B	110	GLN	CG-CD	7.51	1.68	1.51
1	D	61	SER	CA-CB	7.47	1.64	1.52
1	D	83	CYS	CB-SG	7.36	1.94	1.82
1	B	60	PHE	CD2-CE2	7.32	1.53	1.39
1	D	51	ARG	CG-CD	7.31	1.70	1.51
1	B	83	CYS	CB-SG	7.28	1.94	1.82
1	A	168	VAL	CB-CG2	-7.26	1.37	1.52
1	D	44	ILE	CA-CB	-7.23	1.38	1.54
1	B	167	VAL	CB-CG2	-7.21	1.37	1.52
1	D	66	PRO	CB-CG	7.13	1.85	1.50
1	B	1	ALA	CA-CB	7.08	1.67	1.52
1	B	2	PRO	C-O	7.05	1.37	1.23
1	D	32	ILE	CA-CB	7.05	1.71	1.54
1	D	51	ARG	N-CA	7.03	1.60	1.46
1	C	28	THR	CA-CB	-7.03	1.35	1.53
1	A	36	VAL	C-N	-7.01	1.18	1.34
1	C	131	ASP	CA-C	6.97	1.71	1.52
1	A	127	ALA	CA-CB	6.95	1.67	1.52
1	D	131	ASP	CA-CB	6.95	1.69	1.53
1	B	60	PHE	CE1-CZ	6.89	1.50	1.37
1	A	128	LYS	N-CA	6.87	1.60	1.46
1	C	173	ALA	CA-C	6.85	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	19	TRP	CB-CG	6.82	1.62	1.50
1	B	149	ASN	CB-CG	6.78	1.66	1.51
1	B	60	PHE	CA-C	6.76	1.70	1.52
1	B	60	PHE	CB-CG	6.76	1.62	1.51
1	B	60	PHE	CD1-CE1	6.64	1.52	1.39
1	D	167	VAL	CB-CG2	-6.64	1.39	1.52
1	C	123	THR	CB-CG2	-6.62	1.30	1.52
1	D	37	ARG	N-CA	-6.59	1.33	1.46
1	D	88	LYS	CB-CG	6.57	1.70	1.52
1	A	168	VAL	CB-CG1	-6.54	1.39	1.52
1	C	151	TRP	CB-CG	6.50	1.61	1.50
1	A	42	GLU	CB-CG	-6.50	1.39	1.52
1	B	120	MET	SD-CE	-6.45	1.41	1.77
1	A	129	GLY	CA-C	6.41	1.62	1.51
1	B	24	VAL	CB-CG2	6.37	1.66	1.52
1	D	2	PRO	C-N	6.37	1.46	1.34
1	A	108	LYS	CB-CG	6.34	1.69	1.52
1	A	125	ALA	N-CA	6.34	1.59	1.46
1	A	173	ALA	CA-CB	6.33	1.65	1.52
1	B	34	THR	CA-CB	6.33	1.69	1.53
1	B	36	VAL	CB-CG1	6.31	1.66	1.52
1	C	141	ALA	CA-CB	-6.29	1.39	1.52
1	A	58	PHE	CB-CG	-6.26	1.40	1.51
1	D	54	GLU	CB-CG	-6.25	1.40	1.52
1	A	123	THR	CA-C	6.20	1.69	1.52
1	B	87	ILE	CA-CB	6.20	1.69	1.54
1	A	72	VAL	CA-CB	-6.19	1.41	1.54
1	B	22	PRO	CA-C	6.17	1.65	1.52
1	C	54	GLU	CG-CD	6.17	1.61	1.51
1	B	6	TRP	CE3-CZ3	-6.14	1.28	1.38
1	B	24	VAL	CA-C	6.14	1.69	1.52
1	C	110	GLN	CG-CD	6.12	1.65	1.51
1	C	167	VAL	CB-CG2	-6.12	1.40	1.52
1	D	47	ILE	CA-C	-6.11	1.37	1.52
1	B	106	SER	CA-CB	-6.09	1.43	1.52
1	D	149	ASN	CB-CG	6.08	1.65	1.51
1	A	35	GLY	C-O	6.06	1.33	1.23
1	B	112	ARG	CB-CG	6.05	1.68	1.52
1	B	61	SER	N-CA	6.04	1.58	1.46
1	B	156	VAL	CB-CG2	6.03	1.65	1.52
1	A	131	ASP	CB-CG	6.02	1.64	1.51
1	B	65	ARG	C-N	6.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	GLN	CA-CB	6.00	1.67	1.53
1	A	135	LEU	CG-CD2	5.96	1.74	1.51
1	C	34	THR	CB-CG2	5.95	1.72	1.52
1	B	112	ARG	CG-CD	5.94	1.66	1.51
1	C	146	LYS	CG-CD	5.94	1.72	1.52
1	A	37	ARG	N-CA	-5.92	1.34	1.46
1	B	108	LYS	CB-CG	5.89	1.68	1.52
1	C	1	ALA	CA-CB	5.89	1.64	1.52
1	B	65	ARG	CG-CD	5.87	1.66	1.51
1	D	146	LYS	CB-CG	5.87	1.68	1.52
1	C	131	ASP	CB-CG	5.87	1.64	1.51
1	B	83	CYS	CA-CB	5.84	1.66	1.53
1	A	124	GLY	CA-C	5.78	1.61	1.51
1	D	69	THR	CB-CG2	5.78	1.71	1.52
1	B	62	ARG	CA-C	5.75	1.67	1.52
1	D	168	VAL	CB-CG1	5.75	1.65	1.52
1	A	162	LYS	CD-CE	5.73	1.65	1.51
1	B	49	ILE	CA-CB	5.71	1.68	1.54
1	D	86	LEU	CA-CB	5.71	1.66	1.53
1	A	35	GLY	C-N	5.69	1.47	1.34
1	A	63	LYS	CD-CE	5.68	1.65	1.51
1	A	108	LYS	CD-CE	5.68	1.65	1.51
1	B	127	ALA	CA-C	5.67	1.67	1.52
1	B	27	THR	CB-CG2	-5.64	1.33	1.52
1	A	160	ALA	CA-CB	-5.64	1.40	1.52
1	B	31	VAL	CB-CG1	5.64	1.64	1.52
1	B	36	VAL	CA-C	5.62	1.67	1.52
1	D	83	CYS	CA-CB	5.59	1.66	1.53
1	B	31	VAL	CA-CB	5.57	1.66	1.54
1	B	2	PRO	N-CA	5.56	1.56	1.47
1	A	161	THR	CA-CB	-5.55	1.39	1.53
1	B	2	PRO	N-CD	5.51	1.55	1.47
1	D	36	VAL	CA-C	5.51	1.67	1.52
1	B	147	ARG	CG-CD	5.48	1.65	1.51
1	A	153	VAL	CB-CG1	-5.47	1.41	1.52
1	D	4	THR	N-CA	5.44	1.57	1.46
1	D	50	HIS	CA-C	5.44	1.67	1.52
1	A	123	THR	C-N	5.43	1.42	1.33
1	C	131	ASP	C-O	5.42	1.33	1.23
1	A	33	PRO	CB-CG	5.40	1.76	1.50
1	D	130	MET	CA-CB	5.40	1.65	1.53
1	C	112	ARG	CA-CB	5.39	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	PHE	CA-CB	5.39	1.65	1.53
1	D	160	ALA	CA-CB	-5.39	1.41	1.52
1	A	126	ASN	CB-CG	5.38	1.63	1.51
1	B	1	ALA	C-N	5.36	1.44	1.34
1	B	127	ALA	N-CA	5.36	1.57	1.46
1	B	44	ILE	CA-C	5.35	1.66	1.52
1	C	127	ALA	N-CA	5.33	1.57	1.46
1	C	8	ARG	CA-C	-5.33	1.39	1.52
1	D	112	ARG	CB-CG	5.33	1.67	1.52
1	A	151	TRP	CE3-CZ3	-5.30	1.29	1.38
1	B	145	TYR	CD2-CE2	5.30	1.47	1.39
1	A	128	LYS	CB-CG	5.30	1.66	1.52
1	D	1	ALA	CA-CB	5.29	1.63	1.52
1	D	31	VAL	CB-CG1	5.28	1.64	1.52
1	D	111	GLY	CA-C	5.28	1.60	1.51
1	C	104	ILE	CA-CB	-5.26	1.42	1.54
1	B	74	GLU	CG-CD	5.26	1.59	1.51
1	C	63	LYS	CB-CG	5.26	1.66	1.52
1	C	77	CYS	CB-SG	-5.25	1.73	1.81
1	A	35	GLY	N-CA	5.25	1.53	1.46
1	D	85	ILE	C-O	-5.25	1.13	1.23
1	B	35	GLY	CA-C	5.25	1.60	1.51
1	B	47	ILE	CA-CB	5.24	1.66	1.54
1	A	79	GLU	CB-CG	5.23	1.62	1.52
1	B	76	GLY	CA-C	5.23	1.60	1.51
1	C	9	VAL	CB-CG1	5.21	1.63	1.52
1	D	46	SER	CA-CB	5.21	1.60	1.52
1	A	39	PHE	CE1-CZ	5.20	1.47	1.37
1	A	36	VAL	C-O	-5.15	1.13	1.23
1	B	37	ARG	CA-C	5.15	1.66	1.52
1	C	120	MET	SD-CE	5.13	2.06	1.77
1	B	38	GLU	CG-CD	5.12	1.59	1.51
1	C	44	ILE	CB-CG2	-5.12	1.36	1.52
1	C	109	ILE	CA-CB	5.11	1.66	1.54
1	A	44	ILE	CB-CG2	-5.11	1.37	1.52
1	B	61	SER	CA-C	5.10	1.66	1.52
1	C	81	VAL	CB-CG1	-5.09	1.42	1.52
1	D	44	ILE	CB-CG2	5.08	1.68	1.52
1	C	19	TRP	CB-CG	5.07	1.59	1.50
1	D	80	GLY	CA-C	-5.07	1.43	1.51
1	A	36	VAL	CA-CB	5.05	1.65	1.54
1	A	32	ILE	CA-C	-5.04	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLN	CB-CG	5.04	1.66	1.52
1	D	148	ASN	CA-CB	5.03	1.66	1.53
1	D	40	PHE	CD1-CE1	-5.02	1.29	1.39
1	B	63	LYS	CD-CE	5.02	1.63	1.51
1	D	88	LYS	CG-CD	5.01	1.69	1.52
1	D	153	VAL	CB-CG2	-5.01	1.42	1.52

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	65	ARG	NE-CZ-NH2	16.00	128.30	120.30
1	A	130	MET	CG-SD-CE	15.01	124.22	100.20
1	A	34	THR	N-CA-CB	-14.57	82.62	110.30
1	C	65	ARG	NE-CZ-NH2	14.41	127.50	120.30
1	B	36	VAL	N-CA-C	13.71	148.02	111.00
1	D	35	GLY	N-CA-C	13.67	147.27	113.10
1	A	37	ARG	N-CA-CB	-13.61	86.10	110.60
1	A	135	LEU	CA-CB-CG	13.15	145.56	115.30
1	B	3	PRO	N-CA-C	12.80	145.38	112.10
1	D	65	ARG	NE-CZ-NH2	12.43	126.52	120.30
1	D	4	THR	N-CA-CB	11.75	132.63	110.30
1	A	147	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	A	37	ARG	NE-CZ-NH1	-11.67	114.46	120.30
1	B	72	VAL	CB-CA-C	-11.64	89.29	111.40
1	D	83	CYS	CA-CB-SG	11.57	134.82	114.00
1	D	85	ILE	CG1-CB-CG2	-11.40	86.31	111.40
1	C	147	ARG	NE-CZ-NH1	-11.27	114.67	120.30
1	B	112	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	B	34	THR	N-CA-CB	11.19	131.55	110.30
1	D	51	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	D	109	ILE	N-CA-CB	-11.17	85.11	110.80
1	A	39	PHE	CB-CG-CD1	-11.05	113.07	120.80
1	D	154	CYS	CA-CB-SG	10.93	133.68	114.00
1	D	50	HIS	CB-CA-C	10.79	131.98	110.40
1	B	34	THR	CA-C-N	-10.78	94.63	116.20
1	A	8	ARG	NE-CZ-NH1	-10.65	114.97	120.30
1	C	51	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	168	VAL	CB-CA-C	-10.42	91.59	111.40
1	A	36	VAL	N-CA-C	10.39	139.04	111.00
1	B	5	LEU	CB-CG-CD2	-10.35	93.41	111.00
1	D	108	LYS	CD-CE-NZ	10.30	135.39	111.70
1	A	37	ARG	CA-CB-CG	10.27	136.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ASP	CB-CG-OD2	-10.27	109.06	118.30
1	D	65	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	B	39	PHE	C-N-CA	10.12	147.00	121.70
1	C	42	GLU	CB-CA-C	9.79	129.97	110.40
1	B	91	SER	N-CA-CB	9.76	125.14	110.50
1	A	168	VAL	CG1-CB-CG2	-9.67	95.43	110.90
1	D	37	ARG	N-CA-CB	-9.62	93.29	110.60
1	A	34	THR	N-CA-C	9.59	136.90	111.00
1	B	126	ASN	N-CA-C	9.54	136.77	111.00
1	A	147	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	C	89	ARG	CG-CD-NE	-9.45	91.96	111.80
1	D	37	ARG	N-CA-C	9.38	136.34	111.00
1	A	85	ILE	CG1-CB-CG2	-9.33	90.88	111.40
1	B	90	ASP	C-N-CA	-9.11	98.92	121.70
1	D	37	ARG	NE-CZ-NH1	-8.99	115.81	120.30
1	C	11	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	B	92	GLY	CA-C-N	-8.91	97.60	117.20
1	C	127	ALA	N-CA-CB	8.90	122.57	110.10
1	B	112	ARG	CA-CB-CG	8.89	132.97	113.40
1	B	130	MET	N-CA-C	8.87	134.94	111.00
1	B	154	CYS	CA-CB-SG	8.82	129.88	114.00
1	D	51	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	A	131	ASP	CB-CG-OD2	8.75	126.17	118.30
1	B	77	CYS	N-CA-CB	8.69	126.25	110.60
1	B	3	PRO	CA-N-CD	-8.67	99.36	111.50
1	D	47	ILE	CB-CA-C	-8.65	94.30	111.60
1	A	130	MET	CA-CB-CG	8.64	127.99	113.30
1	D	130	MET	CA-CB-CG	8.64	127.98	113.30
1	A	125	ALA	N-CA-CB	8.56	122.09	110.10
1	C	77	CYS	CA-CB-SG	-8.56	98.60	114.00
1	B	58	PHE	CB-CG-CD2	-8.45	114.88	120.80
1	C	95	LEU	CB-CG-CD2	-8.45	96.63	111.00
1	C	44	ILE	CG1-CB-CG2	-8.44	92.83	111.40
1	D	90	ASP	CB-CG-OD2	8.42	125.88	118.30
1	A	44	ILE	CG1-CB-CG2	-8.40	92.93	111.40
1	C	131	ASP	C-N-CA	8.39	142.67	121.70
1	D	24	VAL	N-CA-C	8.34	133.51	111.00
1	D	124	GLY	N-CA-C	8.33	133.93	113.10
1	C	67	ASP	CB-CG-OD1	8.29	125.76	118.30
1	A	135	LEU	CB-CG-CD2	8.27	125.06	111.00
1	A	132	LEU	CA-CB-CG	8.26	134.30	115.30
1	B	63	LYS	CB-CA-C	-8.25	93.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	122	LEU	CB-CG-CD1	-8.23	97.01	111.00
1	A	94	LEU	CB-CG-CD1	-8.17	97.11	111.00
1	A	135	LEU	CB-CG-CD1	-8.15	97.15	111.00
1	D	146	LYS	CD-CE-NZ	8.13	130.40	111.70
1	A	123	THR	CA-CB-CG2	-8.07	101.10	112.40
1	A	123	THR	N-CA-C	8.06	132.75	111.00
1	D	44	ILE	N-CA-C	8.03	132.69	111.00
1	B	36	VAL	CG1-CB-CG2	8.02	123.73	110.90
1	D	36	VAL	N-CA-C	7.97	132.52	111.00
1	B	47	ILE	CB-CA-C	-7.95	95.69	111.60
1	B	62	ARG	CA-CB-CG	7.90	130.78	113.40
1	D	72	VAL	CB-CA-C	-7.86	96.47	111.40
1	B	65	ARG	CD-NE-CZ	7.83	134.56	123.60
1	B	24	VAL	CB-CA-C	-7.77	96.64	111.40
1	A	37	ARG	CB-CA-C	-7.76	94.88	110.40
1	C	147	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	B	148	ASN	C-N-CA	7.76	141.09	121.70
1	A	36	VAL	CB-CA-C	-7.75	96.67	111.40
1	C	47	ILE	CB-CA-C	-7.69	96.21	111.60
1	A	36	VAL	CA-C-N	7.69	134.12	117.20
1	D	36	VAL	CA-C-N	7.68	134.10	117.20
1	C	154	CYS	N-CA-CB	-7.67	96.80	110.60
1	B	8	ARG	N-CA-CB	7.66	124.39	110.60
1	D	168	VAL	CB-CA-C	-7.63	96.91	111.40
1	C	51	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	C	138	ASP	CB-CG-OD1	7.58	125.13	118.30
1	D	36	VAL	CB-CA-C	-7.58	96.99	111.40
1	B	131	ASP	CB-CG-OD2	7.57	125.11	118.30
1	A	151	TRP	CA-CB-CG	-7.54	99.38	113.70
1	B	74	GLU	CB-CA-C	7.52	125.43	110.40
1	B	146	LYS	CB-CG-CD	7.51	131.12	111.60
1	C	41	GLY	C-N-CA	-7.50	102.94	121.70
1	B	39	PHE	CA-C-N	-7.49	100.72	117.20
1	B	146	LYS	N-CA-CB	-7.49	97.12	110.60
1	B	63	LYS	CA-CB-CG	7.48	129.85	113.40
1	A	39	PHE	N-CA-CB	7.47	124.05	110.60
1	D	24	VAL	CB-CA-C	-7.46	97.22	111.40
1	A	172	GLN	CB-CG-CD	7.44	130.95	111.60
1	D	135	LEU	CB-CG-CD2	-7.44	98.35	111.00
1	B	65	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	D	162	LYS	CD-CE-NZ	7.42	128.76	111.70
1	A	107	MET	CA-CB-CG	7.41	125.90	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	MET	CA-CB-CG	7.40	125.89	113.30
1	A	33	PRO	C-N-CA	-7.35	103.33	121.70
1	C	123	THR	CA-CB-CG2	-7.35	102.11	112.40
1	B	35	GLY	CA-C-O	-7.34	107.38	120.60
1	A	147	ARG	N-CA-C	-7.33	91.22	111.00
1	A	32	ILE	CB-CA-C	-7.31	96.97	111.60
1	C	112	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	C	131	ASP	N-CA-C	7.24	130.55	111.00
1	A	112	ARG	CG-CD-NE	7.23	126.99	111.80
1	D	44	ILE	CG1-CB-CG2	7.21	127.25	111.40
1	D	4	THR	N-CA-C	-7.18	91.60	111.00
1	A	31	VAL	C-N-CA	-7.15	103.83	121.70
1	C	34	THR	N-CA-C	7.12	130.22	111.00
1	D	2	PRO	N-CA-C	-7.11	93.61	112.10
1	A	33	PRO	N-CA-C	7.09	130.55	112.10
1	B	64	VAL	CA-C-N	-7.07	101.65	117.20
1	C	8	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	135	LEU	CB-CA-C	-7.00	96.90	110.20
1	C	124	GLY	C-N-CA	-6.99	104.23	121.70
1	A	131	ASP	OD1-CG-OD2	-6.97	110.05	123.30
1	D	131	ASP	CB-CG-OD2	6.97	124.57	118.30
1	B	90	ASP	CA-C-N	6.92	132.41	117.20
1	B	2	PRO	N-CA-C	-6.90	94.15	112.10
1	B	95	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	A	112	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	B	7	SER	CB-CA-C	6.88	123.17	110.10
1	A	123	THR	CA-C-N	6.85	129.90	116.20
1	B	122	LEU	CB-CG-CD2	6.85	122.64	111.00
1	C	131	ASP	CB-CG-OD2	6.84	124.46	118.30
1	D	113	LEU	CB-CG-CD2	6.83	122.61	111.00
1	B	131	ASP	OD1-CG-OD2	-6.80	110.38	123.30
1	C	122	LEU	N-CA-C	6.78	129.30	111.00
1	B	127	ALA	N-CA-CB	6.77	119.58	110.10
1	D	1	ALA	N-CA-C	6.77	129.27	111.00
1	B	138	ASP	C-N-CA	-6.76	104.79	121.70
1	B	131	ASP	CB-CG-OD1	6.75	124.37	118.30
1	D	25	PHE	CB-CG-CD2	-6.75	116.08	120.80
1	C	100	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	160	ALA	N-CA-C	6.73	129.16	111.00
1	B	34	THR	O-C-N	6.72	134.63	123.20
1	A	39	PHE	CB-CG-CD2	6.71	125.49	120.80
1	B	37	ARG	NE-CZ-NH1	-6.71	116.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	37	ARG	CB-CA-C	-6.71	96.99	110.40
1	B	93	GLU	N-CA-C	-6.70	92.92	111.00
1	A	61	SER	N-CA-CB	-6.68	100.47	110.50
1	D	88	LYS	CD-CE-NZ	6.68	127.06	111.70
1	A	85	ILE	CA-CB-CG2	6.66	124.22	110.90
1	D	131	ASP	N-CA-C	-6.66	93.03	111.00
1	B	61	SER	N-CA-CB	6.63	120.45	110.50
1	B	27	THR	OG1-CB-CG2	-6.61	94.79	110.00
1	B	27	THR	N-CA-CB	6.60	122.84	110.30
1	A	38	GLU	OE1-CD-OE2	6.59	131.21	123.30
1	D	106	SER	N-CA-C	-6.59	93.21	111.00
1	C	148	ASN	CB-CA-C	6.58	123.57	110.40
1	D	109	ILE	N-CA-C	6.58	128.78	111.00
1	D	94	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	A	169	CYS	CA-CB-SG	6.57	125.83	114.00
1	A	164	GLY	N-CA-C	6.55	129.49	113.10
1	B	74	GLU	CA-CB-CG	6.54	127.79	113.40
1	D	50	HIS	CA-C-N	-6.54	102.82	117.20
1	B	37	ARG	CD-NE-CZ	6.50	132.70	123.60
1	D	8	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	112	ARG	CD-NE-CZ	6.46	132.65	123.60
1	D	131	ASP	C-N-CA	6.46	137.85	121.70
1	D	11	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	B	36	VAL	CB-CA-C	-6.41	99.23	111.40
1	D	113	LEU	CB-CG-CD1	-6.40	100.11	111.00
1	C	65	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	100	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	B	110	GLN	CB-CA-C	6.38	123.16	110.40
1	D	85	ILE	CA-C-N	6.36	131.19	117.20
1	B	40	PHE	CB-CA-C	6.36	123.11	110.40
1	C	154	CYS	CA-CB-SG	6.33	125.39	114.00
1	D	39	PHE	C-N-CA	6.32	137.49	121.70
1	C	95	LEU	CB-CA-C	-6.31	98.22	110.20
1	D	3	PRO	CA-C-N	6.30	131.07	117.20
1	B	9	VAL	CG1-CB-CG2	6.29	120.96	110.90
1	A	90	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	134	THR	C-N-CA	-6.26	106.04	121.70
1	C	146	LYS	CB-CG-CD	6.26	127.87	111.60
1	A	100	ARG	N-CA-C	-6.25	94.11	111.00
1	C	171	VAL	CG1-CB-CG2	-6.25	100.90	110.90
1	A	14	SER	N-CA-CB	-6.23	101.15	110.50
1	A	100	ARG	NE-CZ-NH2	6.23	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ARG	CA-CB-CG	6.21	127.06	113.40
1	C	42	GLU	N-CA-C	-6.20	94.27	111.00
1	C	112	ARG	CA-CB-CG	6.19	127.02	113.40
1	B	147	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	D	113	LEU	CA-CB-CG	-6.17	101.10	115.30
1	A	34	THR	C-N-CA	6.17	135.25	122.30
1	C	36	VAL	CB-CA-C	-6.17	99.68	111.40
1	D	131	ASP	CB-CA-C	6.15	122.70	110.40
1	B	89	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	D	56	THR	CA-CB-CG2	-6.15	103.79	112.40
1	A	108	LYS	N-CA-CB	-6.15	99.54	110.60
1	A	153	VAL	CB-CA-C	-6.14	99.73	111.40
1	B	8	ARG	CB-CA-C	-6.13	98.14	110.40
1	D	104	ILE	CB-CA-C	-6.12	99.36	111.60
1	C	35	GLY	CA-C-O	-6.10	109.61	120.60
1	D	46	SER	O-C-N	6.10	132.46	122.70
1	D	107	MET	CB-CA-C	-6.09	98.22	110.40
1	B	9	VAL	N-CA-C	-6.08	94.60	111.00
1	A	65	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	92	GLY	CA-C-O	6.07	131.52	120.60
1	C	42	GLU	CG-CD-OE2	-6.06	106.17	118.30
1	D	153	VAL	CB-CA-C	-6.04	99.92	111.40
1	D	108	LYS	CA-CB-CG	6.03	126.66	113.40
1	D	39	PHE	CA-C-N	-6.02	103.96	117.20
1	B	75	GLU	CB-CA-C	6.01	122.41	110.40
1	C	68	LEU	CB-CG-CD1	-6.00	100.79	111.00
1	A	7	SER	C-N-CA	-6.00	106.70	121.70
1	A	37	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	C	148	ASN	N-CA-CB	-5.99	99.82	110.60
1	A	42	GLU	CB-CA-C	5.98	122.36	110.40
1	C	77	CYS	CB-CA-C	-5.98	98.43	110.40
1	D	40	PHE	N-CA-C	-5.97	94.88	111.00
1	A	40	PHE	CB-CA-C	5.96	122.33	110.40
1	A	128	LYS	N-CA-C	5.95	127.08	111.00
1	A	165	ASN	CB-CA-C	5.95	122.31	110.40
1	D	36	VAL	O-C-N	-5.95	113.18	122.70
1	D	112	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	108	LYS	CB-CA-C	5.94	122.28	110.40
1	A	62	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	63	LYS	CB-CG-CD	5.91	126.95	111.60
1	B	86	LEU	CB-CG-CD1	-5.91	100.96	111.00
1	D	112	ARG	NE-CZ-NH1	5.91	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	ALA	N-CA-CB	5.90	118.36	110.10
1	B	77	CYS	N-CA-C	-5.90	95.07	111.00
1	C	76	GLY	CA-C-O	-5.90	109.99	120.60
1	D	36	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	A	35	GLY	CA-C-O	-5.85	110.07	120.60
1	B	114	VAL	CB-CA-C	-5.85	100.29	111.40
1	A	129	GLY	N-CA-C	-5.85	98.48	113.10
1	B	73	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	D	67	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	72	VAL	CB-CA-C	-5.84	100.31	111.40
1	B	43	PRO	CA-N-CD	-5.82	103.35	111.50
1	D	100	ARG	N-CA-C	-5.82	95.30	111.00
1	A	147	ARG	CD-NE-CZ	5.78	131.69	123.60
1	B	110	GLN	N-CA-C	-5.78	95.39	111.00
1	B	38	GLU	N-CA-C	5.77	126.57	111.00
1	C	108	LYS	CB-CG-CD	5.76	126.58	111.60
1	B	26	ILE	N-CA-CB	-5.76	97.56	110.80
1	D	57	GLN	CB-CA-C	-5.76	98.88	110.40
1	B	63	LYS	N-CA-C	-5.75	95.48	111.00
1	C	5	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	128	LYS	CB-CG-CD	5.74	126.52	111.60
1	B	77	CYS	CA-CB-SG	5.73	124.31	114.00
1	B	5	LEU	CB-CG-CD1	5.72	120.73	111.00
1	B	121	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	C	76	GLY	CA-C-N	5.72	129.80	117.20
1	D	86	LEU	CA-CB-CG	5.71	128.44	115.30
1	C	54	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	B	130	MET	CG-SD-CE	5.70	109.32	100.20
1	B	130	MET	O-C-N	-5.69	113.60	122.70
1	A	100	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	120	MET	N-CA-CB	5.69	120.83	110.60
1	A	89	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	148	ASN	N-CA-C	-5.68	95.66	111.00
1	B	112	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	90	ASP	N-CA-CB	5.67	120.81	110.60
1	C	81	VAL	CB-CA-C	-5.67	100.63	111.40
1	D	65	ARG	CD-NE-CZ	5.65	131.51	123.60
1	C	11	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	A	139	CYS	CA-CB-SG	5.64	124.15	114.00
1	A	171	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	D	46	SER	CA-C-N	-5.64	104.79	117.20
1	B	8	ARG	C-N-CA	-5.64	107.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	123	THR	C-N-CA	5.62	134.11	122.30
1	C	11	ARG	CG-CD-NE	5.59	123.54	111.80
1	C	122	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	79	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	B	128	LYS	CA-CB-CG	5.55	125.62	113.40
1	D	14	SER	CB-CA-C	-5.55	99.56	110.10
1	A	123	THR	CA-C-O	-5.53	108.49	120.10
1	C	89	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	D	40	PHE	N-CA-CB	5.53	120.55	110.60
1	C	76	GLY	N-CA-C	-5.51	99.32	113.10
1	D	43	PRO	CA-N-CD	-5.51	103.79	111.50
1	A	58	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	A	71	MET	CG-SD-CE	5.49	108.99	100.20
1	B	4	THR	CB-CA-C	-5.49	96.78	111.60
1	A	35	GLY	O-C-N	5.49	131.48	122.70
1	A	89	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	58	PHE	N-CA-C	-5.47	96.22	111.00
1	B	8	ARG	N-CA-C	-5.47	96.24	111.00
1	B	46	SER	C-N-CA	5.45	135.32	121.70
1	D	86	LEU	CB-CG-CD1	5.45	120.26	111.00
1	B	75	GLU	N-CA-CB	-5.44	100.80	110.60
1	B	153	VAL	CG1-CB-CG2	5.44	119.61	110.90
1	C	112	ARG	C-N-CA	5.44	135.30	121.70
1	B	168	VAL	N-CA-CB	5.43	123.45	111.50
1	B	38	GLU	CA-CB-CG	5.43	125.34	113.40
1	C	131	ASP	CA-C-N	-5.42	105.27	117.20
1	D	165	ASN	CB-CA-C	-5.42	99.56	110.40
1	B	58	PHE	CB-CG-CD1	5.42	124.59	120.80
1	C	111	GLY	N-CA-C	-5.42	99.56	113.10
1	D	94	LEU	N-CA-C	-5.41	96.39	111.00
1	D	37	ARG	CA-C-O	5.41	131.46	120.10
1	A	63	LYS	CD-CE-NZ	5.41	124.14	111.70
1	A	14	SER	N-CA-C	-5.39	96.45	111.00
1	B	88	LYS	CD-CE-NZ	5.38	124.06	111.70
1	B	74	GLU	N-CA-CB	-5.37	100.93	110.60
1	C	104	ILE	N-CA-C	-5.37	96.50	111.00
1	D	37	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	24	VAL	N-CA-C	5.34	125.43	111.00
1	C	93	GLU	N-CA-CB	-5.33	101.00	110.60
1	A	91	SER	N-CA-C	-5.33	96.61	111.00
1	D	37	ARG	CD-NE-CZ	5.32	131.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	37	ARG	CA-CB-CG	5.32	125.11	113.40
1	B	138	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	96	PRO	N-CA-C	-5.30	98.31	112.10
1	B	88	LYS	N-CA-C	-5.28	96.74	111.00
1	B	117	GLN	CA-CB-CG	5.27	125.00	113.40
1	B	149	ASN	N-CA-C	5.26	125.19	111.00
1	C	39	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	B	139	CYS	C-N-CA	-5.24	111.30	122.30
1	D	89	ARG	N-CA-CB	-5.22	101.19	110.60
1	B	15	GLY	N-CA-C	5.19	126.08	113.10
1	C	11	ARG	CD-NE-CZ	5.19	130.87	123.60
1	B	1	ALA	N-CA-C	-5.18	97.01	111.00
1	C	149	ASN	N-CA-CB	-5.18	101.27	110.60
1	D	68	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	A	108	LYS	CD-CE-NZ	5.16	123.58	111.70
1	A	36	VAL	CA-C-O	-5.15	109.28	120.10
1	A	73	LEU	CB-CA-C	-5.15	100.42	110.20
1	B	127	ALA	C-N-CA	5.15	134.57	121.70
1	D	2	PRO	C-N-CD	5.14	139.20	128.40
1	D	86	LEU	CA-C-N	-5.14	105.88	117.20
1	B	100	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	71	MET	O-C-N	5.13	130.91	122.70
1	D	13	GLY	N-CA-C	-5.11	100.33	113.10
1	A	95	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	D	25	PHE	N-CA-C	5.11	124.79	111.00
1	B	129	GLY	CA-C-O	-5.10	111.42	120.60
1	D	51	ARG	CD-NE-CZ	5.09	130.72	123.60
1	D	130	MET	CA-C-O	5.09	130.78	120.10
1	A	107	MET	N-CA-CB	5.08	119.75	110.60
1	B	30	HIS	C-N-CA	-5.08	109.00	121.70
1	C	35	GLY	N-CA-C	-5.08	100.41	113.10
1	C	173	ALA	CA-C-O	-5.07	109.45	120.10
1	B	110	GLN	CA-CB-CG	5.07	124.54	113.40
1	C	89	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	146	LYS	CB-CA-C	5.06	120.51	110.40
1	B	63	LYS	CA-C-N	5.03	128.27	117.20
1	C	147	ARG	C-N-CA	-5.03	109.12	121.70
1	D	108	LYS	N-CA-CB	5.03	119.65	110.60
1	A	32	ILE	CA-C-N	-5.02	103.03	117.10
1	C	88	LYS	CD-CE-NZ	5.02	123.25	111.70
1	B	69	THR	N-CA-C	-5.02	97.44	111.00
1	D	127	ALA	N-CA-CB	5.02	117.12	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	131	ASP	OD1-CG-OD2	-5.02	113.77	123.30
1	D	114	VAL	CG1-CB-CG2	5.01	118.92	110.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ILE	Peptide
1	A	128	LYS	Mainchain
1	A	130	MET	Peptide
1	A	32	ILE	Mainchain
1	B	145	TYR	Sidechain
1	B	157	HIS	Sidechain
1	B	2	PRO	Mainchain
1	B	35	GLY	Mainchain
1	D	145	TYR	Sidechain
1	D	25	PHE	Sidechain
1	D	36	VAL	Peptide
1	D	37	ARG	Mainchain

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	1303	0	1312	197	4
1	B	1303	0	1310	243	0
1	C	1303	0	1312	164	0
1	D	1303	0	1310	247	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	4	6	0
4	A	10	0	3	3	0
5	A	33	0	0	40	2
5	B	22	0	0	25	0
5	C	41	0	0	27	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	31	0	0	40	0
All	All	5367	0	5251	822	6

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 79.

All (822) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:CA	1:A:32:ILE:CB	1.75	1.62
1:C:85:ILE:CA	1:C:85:ILE:CB	1.75	1.59
1:B:62:ARG:CG	1:B:62:ARG:CB	1.79	1.59
1:D:4:THR:CB	1:D:4:THR:CA	1.80	1.59
1:A:100:ARG:CG	1:A:100:ARG:CB	1.80	1.57
3:A:301:TLA:C2	3:A:301:TLA:C3	1.82	1.57
1:B:24:VAL:CB	1:B:24:VAL:CA	1.77	1.57
1:B:110:GLN:CG	1:B:110:GLN:CB	1.77	1.57
1:B:146:LYS:CG	1:B:146:LYS:CB	1.75	1.55
1:D:36:VAL:CB	1:D:36:VAL:CA	1.81	1.54
1:A:85:ILE:CB	1:A:85:ILE:CA	1.79	1.53
1:A:128:LYS:C	1:A:128:LYS:CA	1.75	1.53
1:B:2:PRO:C	1:B:2:PRO:CA	1.74	1.53
1:A:100:ARG:CG	1:A:100:ARG:CD	1.82	1.53
1:A:130:MET:CG	1:A:130:MET:CB	1.83	1.53
1:D:88:LYS:CE	1:D:88:LYS:NZ	1.69	1.52
1:A:33:PRO:CB	1:A:33:PRO:CG	1.77	1.51
1:A:172:GLN:CG	1:A:172:GLN:CB	1.88	1.50
1:B:173:ALA:CA	1:B:173:ALA:CB	1.84	1.50
1:B:36:VAL:CB	1:B:36:VAL:CG2	1.86	1.49
1:D:131:ASP:CB	1:D:131:ASP:CG	1.81	1.49
1:A:172:GLN:CG	1:A:172:GLN:CD	1.80	1.48
1:B:130:MET:CA	1:B:130:MET:C	1.83	1.46
1:D:108:LYS:HE3	1:D:108:LYS:CA	1.42	1.44
1:C:120:MET:SD	1:C:120:MET:CE	2.06	1.43
1:B:71:MET:SD	1:B:71:MET:CE	2.05	1.42
1:D:108:LYS:HE3	1:D:108:LYS:N	1.31	1.42
1:D:66:PRO:CB	1:D:66:PRO:CG	1.85	1.39
1:A:130:MET:CG	1:A:130:MET:SD	2.14	1.36
1:A:88:LYS:HD2	5:A:1030:HOH:O	1.28	1.32
1:D:22:PRO:HB3	1:D:65:ARG:O	1.16	1.29
1:A:9:VAL:HB	5:A:1030:HOH:O	1.14	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:HG13	5:B:1019:HOH:O	1.16	1.28
1:C:77:CYS:HB2	1:C:78:PRO:CD	1.58	1.27
1:D:108:LYS:CE	1:D:108:LYS:H	1.45	1.26
1:C:164:GLY:HA2	5:C:1043:HOH:O	1.37	1.21
1:D:43:PRO:HD2	1:D:46:SER:OG	1.39	1.20
1:D:108:LYS:N	1:D:108:LYS:CE	2.03	1.20
1:B:20:VAL:HG11	1:B:26:ILE:HD13	1.20	1.19
1:D:37:ARG:O	5:D:1026:HOH:O	1.56	1.18
1:A:31:VAL:HG13	5:A:1004:HOH:O	1.46	1.15
1:B:7:SER:HA	1:B:88:LYS:HZ1	1.13	1.12
1:C:77:CYS:HB2	1:C:78:PRO:HD2	1.23	1.11
1:A:28:THR:HB	5:A:1006:HOH:O	1.52	1.09
1:B:22:PRO:HB3	1:B:65:ARG:O	1.50	1.08
1:C:2:PRO:HB2	5:C:1032:HOH:O	1.54	1.07
1:A:32:ILE:H	1:A:33:PRO:HD3	1.08	1.07
1:D:100:ARG:O	5:D:1030:HOH:O	1.72	1.07
1:D:157:HIS:HE1	5:D:1019:HOH:O	1.35	1.05
1:D:168:VAL:HG13	5:D:1038:HOH:O	1.57	1.05
1:B:72:VAL:HG12	1:B:73:LEU:N	1.64	1.05
1:B:2:PRO:HB2	1:C:130:MET:HG2	1.37	1.04
1:A:77:CYS:SG	1:A:78:PRO:HD2	1.96	1.04
1:B:113:LEU:HG	5:B:1014:HOH:O	1.59	1.03
1:B:73:LEU:C	1:B:73:LEU:HD12	1.76	1.03
1:D:119:GLY:HA2	5:D:1030:HOH:O	1.59	1.02
1:D:86:LEU:HD11	1:D:144:VAL:HG21	1.42	1.01
1:C:38:GLU:CD	1:C:41:GLY:HA2	1.80	1.01
1:A:31:VAL:O	1:A:31:VAL:HG22	1.60	1.00
1:D:119:GLY:CA	5:D:1030:HOH:O	2.09	1.00
1:C:35:GLY:O	1:C:36:VAL:HG13	1.62	1.00
1:B:5:LEU:HD23	1:B:5:LEU:C	1.79	0.99
1:C:139:CYS:SG	5:C:1030:HOH:O	2.20	0.98
1:A:139:CYS:SG	4:A:300:TAR:O4	2.22	0.97
1:C:149:ASN:ND2	1:C:149:ASN:H	1.53	0.97
1:D:22:PRO:CB	1:D:65:ARG:O	2.11	0.97
1:B:85:ILE:HD11	1:B:87:ILE:HD11	1.44	0.97
1:C:115:HIS:HB2	5:C:1042:HOH:O	1.64	0.97
1:C:78:PRO:HG2	1:C:81:VAL:CG2	1.94	0.96
1:A:128:LYS:HB2	1:A:131:ASP:OD1	1.67	0.94
1:B:19:TRP:CZ2	1:B:40:PHE:CD2	2.55	0.94
1:D:22:PRO:HB3	1:D:65:ARG:C	1.88	0.94
1:D:90:ASP:HA	5:D:1029:HOH:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:OE2	1:C:41:GLY:HA2	1.67	0.93
1:D:73:LEU:HD12	1:D:73:LEU:O	1.67	0.93
1:A:32:ILE:H	1:A:33:PRO:CD	1.81	0.93
1:D:144:VAL:O	1:D:145:TYR:HB3	1.65	0.93
1:A:154:CYS:N	5:A:1026:HOH:O	2.01	0.93
1:B:23:THR:O	1:B:60:PHE:HB2	1.67	0.93
1:C:100:ARG:HD2	5:C:1039:HOH:O	1.66	0.93
1:A:139:CYS:SG	4:A:300:TAR:C4	2.57	0.92
1:A:32:ILE:CB	1:A:32:ILE:C	2.36	0.92
1:D:108:LYS:CA	1:D:108:LYS:CE	2.37	0.92
1:C:146:LYS:H	1:C:146:LYS:HD2	1.33	0.91
1:B:72:VAL:CG1	1:B:73:LEU:N	2.33	0.91
1:B:105:ALA:HB3	1:B:107:MET:CE	2.01	0.91
1:C:77:CYS:CB	1:C:78:PRO:CD	2.43	0.91
1:C:153:VAL:HG12	5:C:1027:HOH:O	1.70	0.91
1:D:85:ILE:HD11	1:D:99:VAL:HG21	1.52	0.91
1:B:38:GLU:HB2	5:B:1009:HOH:O	1.71	0.90
1:B:7:SER:HA	1:B:88:LYS:NZ	1.86	0.90
1:C:38:GLU:OE1	1:C:41:GLY:HA2	1.71	0.90
1:B:37:ARG:O	1:B:44:ILE:HG22	1.72	0.90
1:C:149:ASN:H	1:C:149:ASN:HD22	1.02	0.90
1:D:168:VAL:HA	5:D:1038:HOH:O	1.69	0.90
1:A:126:ASN:O	1:A:131:ASP:HB3	1.73	0.89
1:D:23:THR:HB	1:D:59:ARG:HD2	1.55	0.89
1:A:32:ILE:N	1:A:33:PRO:HD3	1.86	0.88
1:B:162:LYS:HD2	1:B:162:LYS:H	1.38	0.88
1:A:93:GLU:OE2	1:D:3:PRO:HD3	1.73	0.88
1:B:77:CYS:HB3	1:B:81:VAL:HG11	1.56	0.88
1:B:9:VAL:O	1:B:88:LYS:HE3	1.71	0.88
1:A:77:CYS:SG	1:A:81:VAL:HG22	2.13	0.88
1:A:1:ALA:HB1	1:A:2:PRO:HD2	1.55	0.87
1:A:50:HIS:HB3	1:A:172:GLN:HE22	1.38	0.87
1:B:85:ILE:CG2	1:B:99:VAL:HG21	2.05	0.87
1:B:130:MET:C	1:B:130:MET:HA	1.93	0.87
1:B:2:PRO:HB2	1:C:130:MET:CG	2.04	0.87
1:C:75:GLU:HG3	1:C:172:GLN:HE21	1.40	0.87
1:A:123:THR:HG21	1:D:96:PRO:HB2	1.55	0.86
1:B:141:ALA:N	5:B:1025:HOH:O	2.08	0.86
1:B:57:GLN:C	1:B:58:PHE:HD2	1.79	0.86
1:A:168:VAL:HB	5:A:1020:HOH:O	1.76	0.86
5:B:1017:HOH:O	1:C:124:GLY:HA3	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TRP:HB2	5:A:1005:HOH:O	1.74	0.86
1:B:19:TRP:HZ2	1:B:40:PHE:CD2	1.94	0.86
1:D:108:LYS:H	1:D:108:LYS:HE2	1.38	0.86
1:A:36:VAL:HB	1:A:37:ARG:HB2	1.56	0.86
1:B:7:SER:CA	1:B:88:LYS:HZ1	1.88	0.86
1:C:74:GLU:OE2	1:C:145:TYR:OH	1.92	0.86
1:B:37:ARG:O	1:B:44:ILE:CG2	2.23	0.86
1:B:64:VAL:HG23	1:B:65:ARG:N	1.90	0.85
1:C:125:ALA:HB2	1:D:100:ARG:HH22	1.40	0.85
1:A:33:PRO:O	1:A:35:GLY:N	2.09	0.85
1:D:73:LEU:HD12	1:D:73:LEU:C	1.95	0.85
1:B:20:VAL:O	1:B:71:MET:N	2.10	0.85
1:B:42:GLU:O	5:B:1009:HOH:O	1.94	0.85
1:B:65:ARG:HG2	5:B:1023:HOH:O	1.77	0.84
1:C:80:GLY:CA	5:C:1039:HOH:O	2.24	0.84
1:D:44:ILE:HB	5:D:1026:HOH:O	1.78	0.84
1:D:20:VAL:O	1:D:70:GLY:HA2	1.78	0.84
1:D:104:ILE:HD13	1:D:104:ILE:H	1.42	0.84
1:D:37:ARG:HG2	1:D:38:GLU:H	1.40	0.83
1:C:78:PRO:HG2	1:C:81:VAL:HG21	1.60	0.83
1:B:5:LEU:HD23	1:B:6:TRP:N	1.94	0.83
1:B:135:LEU:HB3	1:B:136:PRO:HD2	1.58	0.83
1:C:79:GLU:OE1	1:D:165:ASN:HB3	1.79	0.83
1:B:106:SER:C	1:B:107:MET:HG2	1.99	0.83
1:B:135:LEU:HB3	1:B:136:PRO:CD	2.09	0.83
1:A:123:THR:O	1:A:123:THR:HG22	1.79	0.82
1:C:85:ILE:CA	1:C:85:ILE:CG2	2.57	0.82
1:B:24:VAL:HG12	1:B:25:PHE:H	1.45	0.82
1:D:19:TRP:CZ2	1:D:40:PHE:CD2	2.67	0.82
1:D:6:TRP:CH2	1:D:94:LEU:HB3	2.13	0.82
1:D:14:SER:HB2	1:D:31:VAL:HG22	1.61	0.82
1:D:37:ARG:CG	1:D:38:GLU:H	1.70	0.82
1:B:6:TRP:CG	1:B:94:LEU:HD23	2.14	0.82
1:A:32:ILE:N	1:A:33:PRO:CD	2.38	0.81
1:B:20:VAL:CG1	1:B:26:ILE:HD13	2.09	0.81
1:C:146:LYS:H	1:C:146:LYS:CD	1.89	0.81
1:A:6:TRP:O	1:A:88:LYS:NZ	2.14	0.81
1:D:109:ILE:HG21	1:D:159:ALA:HB1	1.62	0.81
1:A:32:ILE:HG13	1:A:33:PRO:N	1.96	0.81
1:B:6:TRP:CD2	1:B:94:LEU:HD23	2.16	0.81
1:B:38:GLU:CB	5:B:1009:HOH:O	2.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLN:O	1:D:58:PHE:HD1	1.63	0.81
1:A:13:GLY:C	1:A:15:GLY:H	1.83	0.80
1:A:79:GLU:CD	1:B:161:THR:HG21	2.02	0.80
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.45	0.80
1:A:146:LYS:NZ	1:A:149:ASN:O	2.14	0.80
1:D:14:SER:CB	1:D:31:VAL:HG22	2.12	0.80
1:D:85:ILE:CD1	1:D:99:VAL:HG21	2.11	0.80
1:C:16:TRP:CH2	1:C:88:LYS:HB3	2.16	0.80
1:B:109:ILE:O	1:B:162:LYS:CE	2.30	0.80
1:D:52:ALA:N	5:D:1027:HOH:O	2.14	0.80
1:A:31:VAL:HG12	5:A:1006:HOH:O	1.80	0.79
1:A:64:VAL:O	5:A:1013:HOH:O	1.99	0.79
1:C:2:PRO:HD3	1:C:151:TRP:CH2	2.16	0.79
1:C:125:ALA:O	1:C:126:ASN:OD1	1.99	0.79
1:A:77:CYS:SG	1:A:78:PRO:CD	2.70	0.79
1:C:78:PRO:HG2	1:C:81:VAL:HG23	1.64	0.79
1:A:139:CYS:O	5:A:1005:HOH:O	1.99	0.79
1:A:42:GLU:HB2	5:A:1009:HOH:O	1.82	0.79
1:A:32:ILE:CG1	1:A:33:PRO:N	2.46	0.79
1:D:55:PHE:CE2	1:D:172:GLN:HB2	2.19	0.78
1:A:31:VAL:O	1:A:31:VAL:CG2	2.29	0.78
1:A:159:ALA:N	5:A:1035:HOH:O	2.16	0.78
1:C:149:ASN:HD22	1:C:149:ASN:N	1.79	0.78
1:B:3:PRO:O	1:B:5:LEU:N	2.16	0.78
1:D:94:LEU:N	1:D:94:LEU:HD12	1.99	0.78
1:A:85:ILE:CB	1:A:85:ILE:HA	2.08	0.78
1:B:40:PHE:CD1	5:B:1008:HOH:O	2.37	0.78
1:B:102:GLY:O	1:B:117:GLN:NE2	2.17	0.77
1:C:128:LYS:CG	1:C:129:GLY:N	2.48	0.77
1:A:1:ALA:HB1	1:A:2:PRO:CD	2.15	0.77
1:C:125:ALA:N	5:C:1031:HOH:O	2.18	0.77
1:D:66:PRO:HD2	1:D:67:ASP:OD1	1.84	0.77
1:A:148:ASN:HB3	1:A:149:ASN:OD1	1.84	0.77
1:B:64:VAL:CG2	1:B:65:ARG:N	2.48	0.77
1:A:128:LYS:HD2	1:D:146:LYS:HE2	1.67	0.76
1:C:18:PHE:CD2	1:C:142:PRO:HG3	2.21	0.76
1:B:140:GLY:O	1:B:156:VAL:HG12	1.84	0.76
1:C:38:GLU:OE2	1:C:41:GLY:CA	2.33	0.76
1:C:131:ASP:HB2	5:C:1044:HOH:O	1.87	0.75
1:B:38:GLU:CA	5:B:1009:HOH:O	2.33	0.75
1:A:32:ILE:C	1:A:32:ILE:HG13	2.07	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:CD2	4:A:300:TAR:O4	2.39	0.75
1:D:47:ILE:HG13	1:D:60:PHE:CD2	2.21	0.75
1:D:4:THR:CB	1:D:4:THR:HA	2.14	0.74
1:C:81:VAL:HG12	1:C:82:VAL:N	2.02	0.74
1:C:100:ARG:HG2	1:C:100:ARG:HH21	1.52	0.74
1:C:19:TRP:HZ2	1:C:40:PHE:CD2	2.06	0.74
1:D:101:MET:HA	5:D:1030:HOH:O	1.86	0.74
1:A:128:LYS:CB	1:A:131:ASP:OD1	2.35	0.73
1:C:148:ASN:HB2	1:C:149:ASN:HD22	1.53	0.73
1:B:146:LYS:HG2	1:B:146:LYS:N	2.03	0.73
1:A:78:PRO:O	1:A:81:VAL:HG13	1.89	0.73
1:C:19:TRP:CZ2	1:C:40:PHE:CD2	2.76	0.73
1:C:154:CYS:N	5:C:1027:HOH:O	2.20	0.73
1:B:2:PRO:C	1:B:2:PRO:N	2.43	0.73
1:B:64:VAL:CG2	1:B:65:ARG:H	2.02	0.73
1:C:3:PRO:HD2	5:C:1032:HOH:O	1.89	0.73
1:B:153:VAL:HG12	1:B:154:CYS:N	2.04	0.72
1:C:75:GLU:HG3	1:C:172:GLN:NE2	2.03	0.72
1:C:147:ARG:O	1:C:148:ASN:O	2.07	0.72
1:B:15:GLY:HA3	1:B:31:VAL:HG21	1.69	0.72
1:B:85:ILE:CG2	1:B:99:VAL:CG2	2.67	0.72
1:C:80:GLY:HA2	5:C:1039:HOH:O	1.88	0.72
1:C:148:ASN:HA	5:C:1046:HOH:O	1.89	0.72
1:A:60:PHE:HA	5:A:1031:HOH:O	1.87	0.72
1:A:85:ILE:CA	1:A:85:ILE:HB	2.12	0.72
1:B:78:PRO:O	1:B:81:VAL:HG12	1.89	0.72
1:B:24:VAL:CB	1:B:24:VAL:C	2.58	0.72
1:D:132:LEU:HA	5:D:1036:HOH:O	1.90	0.72
1:B:55:PHE:CD1	1:B:56:THR:N	2.58	0.72
1:D:73:LEU:C	1:D:73:LEU:CD1	2.57	0.72
1:A:127:ALA:O	1:A:128:LYS:HG2	1.89	0.72
1:A:158:ALA:C	5:A:1035:HOH:O	2.28	0.72
1:C:66:PRO:CD	5:C:1038:HOH:O	2.37	0.72
1:D:4:THR:CB	1:D:4:THR:C	2.57	0.71
1:C:66:PRO:HD2	5:C:1038:HOH:O	1.88	0.71
1:D:107:MET:HG3	1:D:109:ILE:HD11	1.72	0.71
1:A:32:ILE:C	1:A:32:ILE:CG1	2.59	0.71
1:B:141:ALA:HB2	5:B:1025:HOH:O	1.89	0.71
1:C:125:ALA:CB	1:D:100:ARG:HH22	2.02	0.71
1:B:140:GLY:C	1:B:156:VAL:HG12	2.11	0.71
1:C:80:GLY:O	1:C:100:ARG:HD3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:VAL:HG11	1:B:147:ARG:NH2	2.06	0.71
1:C:38:GLU:OE2	1:C:41:GLY:C	2.29	0.71
1:B:105:ALA:HB3	1:B:107:MET:HE2	1.71	0.70
1:D:168:VAL:CA	5:D:1038:HOH:O	2.33	0.70
1:A:66:PRO:HD2	1:A:67:ASP:H	1.56	0.70
1:D:43:PRO:HD2	1:D:46:SER:HG	1.54	0.70
1:A:85:ILE:CA	1:A:85:ILE:CG1	2.67	0.70
5:C:1043:HOH:O	1:D:79:GLU:HB2	1.91	0.70
1:D:1:ALA:HB3	1:D:6:TRP:HE1	1.55	0.70
1:D:6:TRP:CD2	1:D:94:LEU:HD23	2.27	0.69
1:D:148:ASN:C	1:D:150:ASP:H	1.94	0.69
1:A:28:THR:CB	5:A:1006:HOH:O	2.24	0.69
1:D:21:SER:CB	1:D:24:VAL:HG23	2.22	0.69
1:D:36:VAL:CB	1:D:36:VAL:C	2.60	0.69
1:D:102:GLY:O	1:D:117:GLN:OE1	2.11	0.69
1:A:47:ILE:HD12	1:A:60:PHE:CD2	2.28	0.69
1:D:59:ARG:HH21	1:D:59:ARG:HB2	1.58	0.69
3:A:301:TLA:C2	3:A:301:TLA:C4	2.71	0.69
1:B:24:VAL:HG12	1:B:25:PHE:N	2.07	0.68
1:C:23:THR:O	1:C:60:PHE:HD1	1.76	0.68
1:B:146:LYS:CG	1:B:146:LYS:N	2.55	0.68
1:A:123:THR:HA	1:D:98:ALA:HB2	1.74	0.68
1:B:24:VAL:CA	1:B:24:VAL:CG1	2.70	0.68
1:A:153:VAL:HG12	5:A:1026:HOH:O	1.93	0.68
1:B:109:ILE:O	1:B:162:LYS:HE2	1.93	0.68
1:B:140:GLY:O	1:B:156:VAL:CG1	2.41	0.68
1:C:8:ARG:HD3	1:C:19:TRP:O	1.93	0.68
1:C:77:CYS:HB2	1:C:78:PRO:HD3	1.69	0.68
1:C:100:ARG:HH21	1:C:100:ARG:CG	2.07	0.68
1:B:22:PRO:O	1:B:64:VAL:CG2	2.41	0.67
1:C:123:THR:O	1:C:124:GLY:O	2.12	0.67
1:D:97:LEU:HD22	1:D:123:THR:HG21	1.77	0.67
1:C:147:ARG:O	1:C:148:ASN:C	2.31	0.67
1:B:58:PHE:HD2	1:B:58:PHE:N	1.90	0.67
1:A:50:HIS:CB	1:A:172:GLN:HE22	2.06	0.67
3:A:301:TLA:C2	3:A:301:TLA:H3	2.18	0.67
1:D:26:ILE:HD11	1:D:73:LEU:CD2	2.25	0.67
1:D:57:GLN:O	1:D:58:PHE:CD1	2.46	0.67
1:C:46:SER:O	1:C:61:SER:OG	2.11	0.67
1:A:73:LEU:HA	1:A:153:VAL:HG23	1.77	0.67
1:B:1:ALA:HB1	5:C:1045:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PHE:CE2	1:B:40:PHE:HE2	2.13	0.67
5:C:1043:HOH:O	1:D:79:GLU:CB	2.43	0.66
1:C:17:GLY:HA3	1:C:25:PHE:CZ	2.30	0.66
1:D:21:SER:HB2	1:D:24:VAL:HG23	1.76	0.66
1:A:42:GLU:OE1	5:A:1031:HOH:O	2.13	0.66
1:C:2:PRO:O	1:C:6:TRP:HD1	1.78	0.66
1:C:38:GLU:HB2	1:C:42:GLU:O	1.96	0.66
1:C:78:PRO:CG	1:C:81:VAL:HG21	2.24	0.66
1:D:37:ARG:CG	1:D:38:GLU:N	2.47	0.66
1:B:90:ASP:C	1:B:92:GLY:N	2.49	0.66
1:B:123:THR:HG22	1:C:122:LEU:HD23	1.78	0.66
1:A:146:LYS:NZ	1:A:149:ASN:C	2.48	0.66
1:B:87:ILE:HD12	1:B:138:ASP:HB3	1.76	0.66
1:D:168:VAL:CG1	5:D:1038:HOH:O	2.25	0.66
1:B:143:TYR:HE2	1:B:157:HIS:HB2	1.61	0.65
1:D:6:TRP:CE2	1:D:94:LEU:HD23	2.31	0.65
1:D:162:LYS:CD	5:D:1023:HOH:O	2.44	0.65
1:B:85:ILE:CD1	1:B:87:ILE:HD11	2.22	0.65
1:C:128:LYS:HG2	1:C:129:GLY:N	2.11	0.65
1:D:47:ILE:HG13	1:D:60:PHE:HD2	1.61	0.65
1:D:51:ARG:C	5:D:1027:HOH:O	2.33	0.65
1:A:88:LYS:CD	5:A:1030:HOH:O	2.07	0.65
1:C:128:LYS:CG	1:C:129:GLY:H	2.09	0.65
1:B:22:PRO:CB	1:B:65:ARG:O	2.38	0.65
1:A:79:GLU:OE1	1:B:161:THR:HG21	1.97	0.65
1:A:32:ILE:CA	1:A:32:ILE:HB	2.15	0.65
1:A:165:ASN:HD21	1:B:100:ARG:NH1	1.95	0.64
1:B:105:ALA:HB3	1:B:107:MET:HE3	1.78	0.64
1:A:38:GLU:HB2	1:A:42:GLU:O	1.98	0.64
1:A:148:ASN:HA	5:A:1027:HOH:O	1.97	0.64
1:B:95:LEU:HD11	1:B:131:ASP:O	1.97	0.64
1:B:112:ARG:NH2	1:B:159:ALA:HB2	2.13	0.64
1:D:127:ALA:HB2	5:D:1033:HOH:O	1.97	0.64
5:B:1017:HOH:O	1:C:124:GLY:CA	2.38	0.63
1:B:65:ARG:HB3	1:B:68:LEU:CD1	2.27	0.63
1:B:90:ASP:C	1:B:92:GLY:H	2.02	0.63
1:C:109:ILE:HD12	1:C:110:GLN:N	2.13	0.63
1:A:13:GLY:C	1:A:15:GLY:N	2.48	0.63
3:A:301:TLA:C3	3:A:301:TLA:O2	2.46	0.63
1:C:125:ALA:O	1:C:126:ASN:CG	2.36	0.63
1:B:162:LYS:H	1:B:162:LYS:CD	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HG3	1:A:131:ASP:OD1	1.98	0.63
1:A:36:VAL:HG12	1:A:37:ARG:CZ	2.29	0.63
1:A:126:ASN:O	1:A:131:ASP:CB	2.46	0.63
1:A:42:GLU:CB	5:A:1009:HOH:O	2.43	0.62
1:A:54:GLU:O	1:A:54:GLU:HG3	1.99	0.62
1:B:22:PRO:O	1:B:64:VAL:HG22	1.98	0.62
1:C:128:LYS:HG3	1:C:129:GLY:H	1.64	0.62
1:A:50:HIS:CB	1:A:172:GLN:NE2	2.62	0.62
1:D:117:GLN:C	5:D:1038:HOH:O	2.37	0.62
1:B:55:PHE:HD1	1:B:56:THR:H	1.48	0.62
1:D:71:MET:HE3	1:D:151:TRP:HB3	1.82	0.62
1:A:28:THR:CG2	5:A:1006:HOH:O	2.46	0.62
1:D:108:LYS:H	1:D:108:LYS:NZ	1.96	0.62
1:B:94:LEU:N	1:B:94:LEU:HD12	2.15	0.62
1:B:57:GLN:O	1:B:58:PHE:HD2	1.82	0.62
1:A:33:PRO:O	1:A:34:THR:C	2.36	0.62
1:A:128:LYS:N	1:A:131:ASP:HB2	2.14	0.62
1:A:50:HIS:HB3	1:A:172:GLN:NE2	2.12	0.61
1:B:35:GLY:C	1:B:36:VAL:CG1	2.68	0.61
1:B:123:THR:O	1:B:124:GLY:C	2.39	0.61
1:D:52:ALA:CA	5:D:1027:HOH:O	2.47	0.61
1:D:21:SER:CB	1:D:22:PRO:CD	2.78	0.61
1:D:66:PRO:HD2	1:D:67:ASP:H	1.66	0.61
1:D:104:ILE:HA	1:D:117:GLN:HA	1.82	0.61
1:A:131:ASP:O	1:D:1:ALA:HB2	2.01	0.61
1:C:66:PRO:N	5:C:1038:HOH:O	2.30	0.61
1:C:77:CYS:CB	1:C:78:PRO:HD2	2.15	0.61
1:C:100:ARG:CD	5:C:1039:HOH:O	2.34	0.61
1:D:1:ALA:HB3	1:D:6:TRP:NE1	2.14	0.61
1:B:90:ASP:O	1:B:92:GLY:N	2.34	0.61
1:D:47:ILE:HG22	1:D:49:ILE:HG12	1.81	0.61
1:A:114:VAL:HG11	1:A:168:VAL:HG21	1.83	0.61
1:B:48:ALA:HB3	1:B:59:ARG:HB3	1.81	0.61
1:A:8:ARG:HB2	1:A:19:TRP:HB2	1.83	0.60
1:B:19:TRP:NE1	1:B:65:ARG:HD3	2.15	0.60
1:B:145:TYR:O	1:B:151:TRP:HD1	1.84	0.60
1:D:39:PHE:N	1:D:42:GLU:O	2.34	0.60
1:C:16:TRP:CZ2	1:C:88:LYS:HB3	2.36	0.60
1:D:12:PHE:CD2	1:D:25:PHE:HZ	2.19	0.60
1:B:89:ARG:NH2	1:B:138:ASP:OD2	2.35	0.60
1:D:66:PRO:CD	1:D:67:ASP:OD1	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HD22	1:D:136:PRO:HD2	1.82	0.60
1:A:128:LYS:C	1:A:128:LYS:CB	2.69	0.60
1:B:72:VAL:HG11	1:B:147:ARG:HH21	1.67	0.60
1:D:51:ARG:HA	1:D:56:THR:HA	1.83	0.60
1:D:19:TRP:CH2	1:D:40:PHE:CD2	2.90	0.60
1:D:94:LEU:N	1:D:94:LEU:CD1	2.64	0.60
1:A:23:THR:OG1	1:A:59:ARG:HD2	2.02	0.59
1:A:85:ILE:HG13	1:A:87:ILE:CD1	2.32	0.59
1:B:44:ILE:HG23	1:B:45:GLU:OE2	2.01	0.59
1:D:51:ARG:HG2	5:D:1027:HOH:O	2.02	0.59
1:C:2:PRO:O	1:C:6:TRP:CD1	2.54	0.59
1:C:10:VAL:HG23	1:C:11:ARG:O	2.02	0.59
1:C:44:ILE:HG22	1:C:45:GLU:N	2.16	0.59
1:A:42:GLU:OE2	5:A:1009:HOH:O	2.17	0.59
1:B:42:GLU:HG2	1:B:62:ARG:HD3	1.84	0.59
1:D:6:TRP:CZ2	1:D:94:LEU:HB3	2.38	0.59
1:D:65:ARG:HB3	1:D:68:LEU:CD1	2.33	0.59
1:D:108:LYS:HE3	1:D:108:LYS:C	2.20	0.59
1:B:25:PHE:C	1:B:26:ILE:HD12	2.23	0.59
1:B:36:VAL:HG23	1:B:36:VAL:O	2.03	0.59
1:B:146:LYS:CG	1:B:146:LYS:CA	2.77	0.59
1:A:24:VAL:HG22	1:A:59:ARG:HD3	1.85	0.59
1:B:121:LEU:HD22	1:B:164:GLY:O	2.02	0.59
1:D:14:SER:HB3	1:D:31:VAL:CG2	2.33	0.59
1:A:32:ILE:HG13	1:A:33:PRO:CA	2.33	0.58
1:C:123:THR:O	1:C:124:GLY:C	2.41	0.58
1:B:6:TRP:C	1:B:88:LYS:HZ1	2.06	0.58
1:C:85:ILE:CB	1:C:85:ILE:C	2.69	0.58
1:C:97:LEU:HA	5:C:1041:HOH:O	2.02	0.58
1:D:165:ASN:ND2	5:D:1012:HOH:O	2.31	0.58
1:A:31:VAL:CG1	5:A:1006:HOH:O	2.46	0.58
1:D:131:ASP:HA	5:D:1035:HOH:O	2.03	0.58
1:C:21:SER:CB	1:C:22:PRO:CD	2.82	0.58
1:D:95:LEU:HD11	5:D:1036:HOH:O	2.03	0.58
1:A:86:LEU:HB2	1:A:142:PRO:HG2	1.85	0.58
1:B:36:VAL:CG2	1:B:36:VAL:CA	2.76	0.58
1:D:14:SER:CB	1:D:31:VAL:CG2	2.81	0.58
1:B:20:VAL:HG11	1:B:26:ILE:CD1	2.13	0.58
1:C:104:ILE:CG2	1:C:105:ALA:N	2.65	0.58
1:D:91:SER:HB3	1:D:93:GLU:HG3	1.85	0.58
1:B:141:ALA:CA	5:B:1025:HOH:O	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:VAL:CA	1:D:36:VAL:CG1	2.78	0.58
1:D:46:SER:CB	1:D:47:ILE:HD12	2.34	0.58
1:A:36:VAL:HG12	1:A:37:ARG:NH2	2.20	0.57
1:D:36:VAL:CB	1:D:36:VAL:N	2.65	0.57
1:D:57:GLN:C	1:D:58:PHE:HD1	2.08	0.57
1:A:128:LYS:HB2	1:A:131:ASP:CG	2.23	0.57
1:A:150:ASP:HB2	5:A:1028:HOH:O	2.04	0.57
1:B:58:PHE:N	1:B:58:PHE:CD2	2.69	0.57
1:C:6:TRP:C	1:C:8:ARG:H	2.06	0.57
1:A:32:ILE:CB	1:A:32:ILE:N	2.61	0.57
1:B:6:TRP:CZ2	1:B:86:LEU:HD12	2.38	0.57
1:B:73:LEU:HD12	1:B:74:GLU:N	2.17	0.57
1:D:44:ILE:HG23	1:D:45:GLU:N	2.17	0.57
1:A:36:VAL:HG23	1:A:37:ARG:H	1.70	0.57
1:B:148:ASN:HB3	1:B:149:ASN:HD22	1.69	0.57
1:C:1:ALA:HB1	1:C:5:LEU:HD23	1.85	0.57
1:B:42:GLU:CD	1:B:62:ARG:HD2	2.24	0.57
1:D:21:SER:HB2	1:D:24:VAL:CG2	2.35	0.57
1:D:55:PHE:CD2	1:D:172:GLN:HB2	2.39	0.57
1:B:96:PRO:HB2	1:C:123:THR:CG2	2.34	0.57
1:D:9:VAL:O	1:D:88:LYS:HD3	2.03	0.57
1:D:86:LEU:HD11	1:D:144:VAL:CG2	2.28	0.57
1:A:32:ILE:CA	1:A:32:ILE:CG1	2.75	0.57
1:B:12:PHE:CD2	1:B:25:PHE:HZ	2.23	0.57
1:A:104:ILE:N	5:A:1034:HOH:O	2.37	0.57
1:B:19:TRP:CD1	1:B:65:ARG:HD3	2.40	0.57
1:B:44:ILE:HD13	1:B:44:ILE:C	2.25	0.57
1:B:24:VAL:O	1:B:25:PHE:HB2	2.05	0.56
1:B:35:GLY:C	1:B:36:VAL:HG13	2.24	0.56
1:B:64:VAL:HG23	1:B:65:ARG:HB2	1.86	0.56
1:A:66:PRO:CD	1:A:67:ASP:H	2.14	0.56
1:B:68:LEU:HD21	5:B:1023:HOH:O	2.05	0.56
1:B:146:LYS:HG2	1:B:146:LYS:H	1.69	0.56
1:B:153:VAL:HG12	1:B:155:GLY:H	1.69	0.56
1:C:89:ARG:NH2	1:C:138:ASP:OD2	2.38	0.56
1:C:148:ASN:HB2	1:C:149:ASN:ND2	2.20	0.56
1:D:127:ALA:CB	5:D:1034:HOH:O	2.54	0.56
1:D:153:VAL:HG12	1:D:154:CYS:N	2.20	0.56
1:A:72:VAL:HG12	1:A:73:LEU:N	2.20	0.56
1:B:85:ILE:HG23	1:B:99:VAL:CG2	2.35	0.56
1:D:6:TRP:CG	1:D:94:LEU:HD23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:CYS:SG	1:A:81:VAL:CG2	2.92	0.56
1:B:44:ILE:HD13	1:B:44:ILE:O	2.05	0.56
1:C:81:VAL:CG1	1:C:82:VAL:N	2.66	0.56
1:C:85:ILE:HD11	1:C:99:VAL:CG1	2.36	0.56
1:D:108:LYS:NZ	1:D:109:ILE:N	2.54	0.56
1:B:85:ILE:HG22	1:B:99:VAL:HG21	1.86	0.56
1:B:141:ALA:CB	5:B:1025:HOH:O	2.51	0.56
1:D:14:SER:HB3	1:D:31:VAL:HG22	1.88	0.56
1:A:82:VAL:HG23	1:A:99:VAL:O	2.06	0.56
1:A:12:PHE:HD1	5:A:1004:HOH:O	1.89	0.55
1:D:127:ALA:HA	1:D:131:ASP:HB3	1.88	0.55
1:B:112:ARG:HH22	1:B:159:ALA:HB2	1.70	0.55
1:B:113:LEU:C	1:B:113:LEU:HD23	2.27	0.55
1:A:128:LYS:C	1:A:128:LYS:HA	2.11	0.55
1:B:57:GLN:O	1:B:58:PHE:CD2	2.60	0.55
1:C:18:PHE:HD2	1:C:142:PRO:HG3	1.72	0.55
1:A:60:PHE:CA	5:A:1031:HOH:O	2.49	0.55
1:B:107:MET:O	1:B:109:ILE:HD12	2.07	0.55
1:B:29:THR:C	1:B:31:VAL:H	2.10	0.55
1:B:36:VAL:CG2	1:B:36:VAL:HB	2.22	0.55
1:C:109:ILE:HG12	1:C:159:ALA:HB1	1.89	0.55
1:D:26:ILE:HD11	1:D:73:LEU:HD22	1.89	0.55
1:A:99:VAL:HG13	1:A:121:LEU:HD12	1.87	0.55
1:A:128:LYS:CG	1:A:131:ASP:OD1	2.54	0.55
1:B:96:PRO:HB2	1:C:123:THR:HG21	1.88	0.54
1:A:103:ALA:HB1	5:A:1034:HOH:O	2.06	0.54
1:D:104:ILE:HG22	1:D:117:GLN:HB2	1.90	0.54
1:B:107:MET:C	1:B:109:ILE:HD12	2.28	0.54
1:B:9:VAL:HB	1:B:88:LYS:HE3	1.90	0.54
1:B:87:ILE:HD13	1:B:141:ALA:CB	2.38	0.54
1:B:93:GLU:C	1:B:94:LEU:HD12	2.28	0.54
1:B:105:ALA:CB	1:B:107:MET:HE2	2.37	0.54
1:D:51:ARG:HG3	1:D:56:THR:OG1	2.07	0.54
1:A:6:TRP:CE3	1:A:94:LEU:HD23	2.43	0.54
1:C:148:ASN:CB	1:C:149:ASN:HD22	2.20	0.54
1:B:3:PRO:C	1:B:5:LEU:N	2.57	0.54
1:B:148:ASN:N	5:B:1026:HOH:O	2.41	0.54
1:D:21:SER:HB3	1:D:22:PRO:CD	2.38	0.54
1:A:78:PRO:HG2	1:A:81:VAL:HG11	1.90	0.54
1:A:85:ILE:HG13	1:A:87:ILE:HD12	1.90	0.54
1:C:52:ALA:HA	5:C:1017:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PHE:CE1	1:B:153:VAL:HG21	2.43	0.53
1:C:158:ALA:O	1:C:159:ALA:HB2	2.08	0.53
1:D:148:ASN:C	1:D:150:ASP:N	2.60	0.53
1:D:86:LEU:CD1	1:D:144:VAL:HG21	2.28	0.53
1:B:3:PRO:C	1:B:5:LEU:H	2.10	0.53
1:A:28:THR:HG22	1:A:30:HIS:H	1.73	0.53
1:C:99:VAL:HG12	1:C:121:LEU:HA	1.91	0.53
1:B:104:ILE:HD11	5:B:1012:HOH:O	2.09	0.53
1:A:79:GLU:CG	1:B:161:THR:HG21	2.37	0.53
1:A:107:MET:CG	1:A:109:ILE:HD11	2.39	0.53
1:A:66:PRO:CD	1:A:67:ASP:N	2.71	0.53
1:D:59:ARG:HH21	1:D:59:ARG:CB	2.21	0.53
1:D:144:VAL:O	1:D:145:TYR:CB	2.43	0.53
1:A:77:CYS:SG	1:A:78:PRO:N	2.80	0.53
1:C:85:ILE:HD11	1:C:99:VAL:HG11	1.91	0.53
1:D:37:ARG:HG2	1:D:38:GLU:HG3	1.91	0.53
1:A:140:GLY:HA3	5:A:1005:HOH:O	2.09	0.53
1:C:33:PRO:HA	5:C:1013:HOH:O	2.09	0.52
1:C:76:GLY:HA2	1:C:154:CYS:O	2.09	0.52
1:D:162:LYS:CD	1:D:162:LYS:H	2.21	0.52
1:B:9:VAL:HB	1:B:88:LYS:CE	2.40	0.52
1:B:37:ARG:HD3	1:B:38:GLU:HB3	1.91	0.52
1:B:109:ILE:HG22	1:B:110:GLN:HG2	1.91	0.52
1:C:65:ARG:HG2	1:C:65:ARG:HH21	1.74	0.52
1:B:19:TRP:CE2	1:B:65:ARG:HD3	2.45	0.52
1:B:96:PRO:HG2	1:C:123:THR:HG21	1.91	0.52
1:B:77:CYS:CB	1:B:81:VAL:HG11	2.34	0.52
1:C:78:PRO:HD2	1:C:81:VAL:HG21	1.90	0.52
1:D:19:TRP:HZ2	1:D:40:PHE:CD2	2.26	0.52
1:D:46:SER:HB2	1:D:47:ILE:HD12	1.90	0.52
1:A:4:THR:O	1:A:7:SER:HB3	2.09	0.52
1:B:149:ASN:N	5:B:1026:HOH:O	2.42	0.52
1:B:55:PHE:HD2	1:B:171:VAL:O	1.93	0.52
1:D:26:ILE:HG22	1:D:156:VAL:HG11	1.92	0.52
1:A:90:ASP:OD1	3:A:301:TLA:C2	2.58	0.52
1:D:146:LYS:NZ	1:D:149:ASN:HA	2.25	0.52
1:D:1:ALA:CB	1:D:6:TRP:HE1	2.21	0.51
1:D:108:LYS:HZ1	1:D:109:ILE:N	2.08	0.51
1:B:77:CYS:HB3	1:B:78:PRO:HD2	1.91	0.51
1:D:52:ALA:HA	5:D:1027:HOH:O	2.10	0.51
1:B:22:PRO:O	1:B:64:VAL:HG21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:HG12	1:C:64:VAL:O	2.10	0.51
1:C:62:ARG:O	1:C:64:VAL:HG23	2.09	0.51
1:C:31:VAL:HG21	1:C:139:CYS:HB2	1.91	0.51
1:C:129:GLY:O	1:C:130:MET:HE2	2.10	0.51
1:D:54:GLU:O	1:D:54:GLU:HG3	2.10	0.51
1:D:162:LYS:H	1:D:162:LYS:HD2	1.74	0.51
1:B:8:ARG:HG3	1:B:18:PHE:CE2	2.45	0.51
1:B:90:ASP:O	1:B:91:SER:C	2.39	0.51
1:D:42:GLU:CA	1:D:42:GLU:OE1	2.59	0.51
1:D:28:THR:HG21	1:D:139:CYS:HB3	1.93	0.51
1:A:90:ASP:OD1	3:A:301:TLA:C1	2.58	0.51
1:B:6:TRP:O	1:B:88:LYS:NZ	2.42	0.51
1:B:21:SER:HB2	1:B:24:VAL:HG23	1.92	0.51
1:B:26:ILE:HG23	1:B:156:VAL:HG22	1.91	0.51
1:D:28:THR:HG22	1:D:140:GLY:HA2	1.92	0.51
1:B:29:THR:C	1:B:31:VAL:N	2.64	0.50
1:C:1:ALA:CB	1:C:5:LEU:HD23	2.40	0.50
1:C:35:GLY:O	1:C:36:VAL:CG1	2.48	0.50
1:A:35:GLY:N	5:A:1008:HOH:O	2.43	0.50
1:A:66:PRO:HD2	1:A:67:ASP:N	2.23	0.50
1:A:146:LYS:C	1:A:147:ARG:O	2.44	0.50
1:D:12:PHE:CD2	1:D:25:PHE:CZ	2.99	0.50
1:D:44:ILE:CG2	1:D:45:GLU:N	2.74	0.50
1:B:39:PHE:N	5:B:1009:HOH:O	2.44	0.50
1:D:4:THR:CA	1:D:4:THR:CG2	2.86	0.50
1:D:47:ILE:HG22	1:D:49:ILE:H	1.76	0.50
1:A:159:ALA:HB3	1:A:168:VAL:CG2	2.42	0.50
1:B:25:PHE:C	1:B:25:PHE:CD1	2.85	0.50
1:C:20:VAL:HG11	1:C:26:ILE:HD12	1.94	0.50
1:B:27:THR:OG1	1:B:28:THR:N	2.45	0.50
1:C:78:PRO:CD	1:C:81:VAL:HG21	2.42	0.49
1:C:125:ALA:HB2	1:D:100:ARG:NH2	2.17	0.49
1:A:50:HIS:HB2	1:A:172:GLN:NE2	2.26	0.49
1:A:123:THR:HB	1:A:126:ASN:OD1	2.12	0.49
1:B:153:VAL:CG1	1:B:154:CYS:N	2.73	0.49
1:B:65:ARG:CG	5:B:1023:HOH:O	2.48	0.49
1:D:12:PHE:HD1	1:D:12:PHE:O	1.96	0.49
1:D:145:TYR:CE2	1:D:152:VAL:HG22	2.47	0.49
1:B:29:THR:O	1:B:31:VAL:N	2.46	0.49
1:B:55:PHE:CD2	1:B:171:VAL:O	2.66	0.49
1:D:44:ILE:O	1:D:44:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HG2	1:A:147:ARG:NH1	2.15	0.49
1:B:57:GLN:C	1:B:58:PHE:CD2	2.71	0.49
1:C:107:MET:HB3	1:D:105:ALA:HB2	1.95	0.49
1:C:146:LYS:HD2	1:C:146:LYS:N	2.15	0.49
1:B:11:ARG:HG3	1:B:12:PHE:N	2.27	0.49
1:D:51:ARG:CZ	5:D:1027:HOH:O	2.61	0.49
1:D:88:LYS:HE3	5:D:1028:HOH:O	2.13	0.49
1:A:77:CYS:SG	1:A:78:PRO:O	2.57	0.49
1:C:2:PRO:HB2	1:C:3:PRO:HD2	1.95	0.49
1:C:162:LYS:O	1:C:163:SER:O	2.31	0.49
1:A:107:MET:HG3	1:A:109:ILE:HD11	1.94	0.48
1:B:40:PHE:HA	5:B:1008:HOH:O	2.13	0.48
1:C:80:GLY:C	1:C:100:ARG:HD3	2.34	0.48
1:D:146:LYS:HZ1	1:D:149:ASN:HA	1.77	0.48
1:A:116:GLY:HA3	5:A:1020:HOH:O	2.12	0.48
1:D:102:GLY:N	1:D:118:SER:O	2.34	0.48
1:D:104:ILE:HD13	1:D:104:ILE:N	2.21	0.48
1:B:25:PHE:O	1:B:26:ILE:HD12	2.12	0.48
1:C:1:ALA:HB1	1:C:5:LEU:CD2	2.43	0.48
1:C:6:TRP:C	1:C:8:ARG:N	2.66	0.48
1:C:49:ILE:N	1:C:49:ILE:HD12	2.28	0.48
1:D:108:LYS:N	1:D:108:LYS:NZ	2.58	0.48
1:A:140:GLY:CA	5:A:1005:HOH:O	2.61	0.48
1:B:102:GLY:N	1:B:118:SER:O	2.38	0.48
1:A:16:TRP:CB	5:A:1005:HOH:O	2.47	0.48
1:B:51:ARG:HB2	1:B:56:THR:HG23	1.95	0.48
1:A:157:HIS:CD2	5:A:1035:HOH:O	2.67	0.48
1:B:36:VAL:CG2	1:B:36:VAL:C	2.82	0.48
1:D:33:PRO:O	1:D:34:THR:C	2.51	0.48
1:D:47:ILE:HG22	1:D:49:ILE:N	2.29	0.48
1:D:120:MET:N	5:D:1030:HOH:O	2.43	0.48
1:D:126:ASN:OD1	1:D:131:ASP:OD1	2.31	0.48
1:A:79:GLU:HG2	1:B:161:THR:HG21	1.96	0.48
1:A:99:VAL:HG13	1:A:121:LEU:CD1	2.43	0.48
1:B:19:TRP:CZ2	1:B:40:PHE:HD2	2.24	0.48
1:D:26:ILE:HG23	1:D:55:PHE:CE1	2.48	0.48
1:D:51:ARG:HB2	1:D:56:THR:HG23	1.96	0.48
1:B:24:VAL:O	1:B:25:PHE:CB	2.62	0.47
1:B:65:ARG:HB3	1:B:68:LEU:HD12	1.95	0.47
1:C:104:ILE:HG23	1:C:105:ALA:N	2.29	0.47
1:D:1:ALA:N	1:D:6:TRP:HE1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:GLY:HA2	5:D:1024:HOH:O	2.14	0.47
1:A:89:ARG:HB3	1:A:93:GLU:HG2	1.96	0.47
1:C:109:ILE:HD12	1:C:110:GLN:H	1.79	0.47
1:D:32:ILE:HG22	1:D:33:PRO:HD2	1.96	0.47
1:B:6:TRP:O	1:B:88:LYS:CE	2.62	0.47
1:B:37:ARG:C	1:B:44:ILE:HG21	2.35	0.47
1:B:93:GLU:OE2	1:C:1:ALA:N	2.46	0.47
1:C:44:ILE:O	1:C:47:ILE:HG12	2.14	0.47
1:D:12:PHE:O	1:D:12:PHE:CD1	2.66	0.47
1:A:32:ILE:CA	1:A:32:ILE:CG2	2.80	0.47
1:A:87:ILE:HD11	1:A:97:LEU:HD12	1.96	0.47
1:B:7:SER:CA	1:B:88:LYS:NZ	2.63	0.47
1:B:85:ILE:HG23	1:B:99:VAL:HG23	1.96	0.47
1:B:109:ILE:HD13	1:B:114:VAL:HG23	1.97	0.47
1:C:28:THR:HG21	1:C:157:HIS:O	2.15	0.47
1:D:19:TRP:CH2	1:D:40:PHE:HD2	2.33	0.47
1:D:43:PRO:CD	1:D:46:SER:OG	2.34	0.47
1:A:122:LEU:HB3	5:D:1011:HOH:O	2.15	0.47
1:B:135:LEU:CB	1:B:136:PRO:CD	2.75	0.47
1:D:37:ARG:C	5:D:1026:HOH:O	2.29	0.47
1:D:85:ILE:CD1	1:D:99:VAL:CG2	2.89	0.47
1:D:162:LYS:HD2	5:D:1023:HOH:O	2.13	0.47
1:A:16:TRP:CH2	1:A:88:LYS:HB3	2.51	0.46
1:A:166:THR:HG22	1:A:167:VAL:N	2.28	0.46
1:D:107:MET:H	1:D:107:MET:HG2	1.60	0.46
1:A:79:GLU:HG2	1:B:163:SER:OG	2.15	0.46
1:B:14:SER:OG	1:B:31:VAL:HG22	2.16	0.46
1:C:86:LEU:HB2	1:C:142:PRO:HG2	1.98	0.46
1:D:65:ARG:HB3	1:D:68:LEU:CG	2.45	0.46
1:B:2:PRO:C	1:B:2:PRO:CB	2.77	0.46
1:B:6:TRP:O	1:B:9:VAL:HB	2.15	0.46
1:B:109:ILE:O	1:B:162:LYS:HE3	2.14	0.46
1:C:44:ILE:HA	1:C:47:ILE:HG12	1.97	0.46
1:D:123:THR:HB	1:D:132:LEU:HB3	1.97	0.46
1:B:12:PHE:CE2	1:B:25:PHE:CZ	3.04	0.46
1:B:122:LEU:HA	1:B:122:LEU:HD12	1.77	0.46
1:C:44:ILE:CG2	1:C:45:GLU:N	2.78	0.46
1:A:39:PHE:CZ	1:A:44:ILE:HD11	2.51	0.46
1:C:109:ILE:HG12	1:C:159:ALA:CB	2.45	0.46
1:D:132:LEU:HD13	5:D:1036:HOH:O	2.15	0.46
1:B:96:PRO:CG	1:C:123:THR:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:CG1	1:C:88:LYS:HD2	2.46	0.46
1:C:107:MET:CG	1:C:109:ILE:HG23	2.46	0.46
1:B:145:TYR:O	1:B:151:TRP:CD1	2.67	0.46
1:C:96:PRO:O	1:C:96:PRO:HG2	2.16	0.46
1:D:99:VAL:HG22	1:D:121:LEU:HD12	1.97	0.46
1:A:19:TRP:CD2	1:A:65:ARG:HG3	2.50	0.46
1:D:135:LEU:CD2	1:D:136:PRO:HD2	2.45	0.46
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.53	0.46
1:D:100:ARG:C	5:D:1030:HOH:O	2.36	0.45
1:D:162:LYS:HG3	5:D:1023:HOH:O	2.15	0.45
1:A:88:LYS:CE	5:A:1030:HOH:O	2.49	0.45
1:D:44:ILE:HA	1:D:47:ILE:HD13	1.98	0.45
1:D:65:ARG:HB3	1:D:68:LEU:HG	1.97	0.45
1:A:26:ILE:HG13	1:A:55:PHE:CZ	2.51	0.45
1:A:85:ILE:HG13	1:A:87:ILE:HD11	1.99	0.45
1:B:36:VAL:CG2	1:B:36:VAL:O	2.64	0.45
1:C:108:LYS:NZ	1:D:104:ILE:HD11	2.31	0.45
1:A:29:THR:O	1:A:33:PRO:HD3	2.16	0.45
1:A:30:HIS:CD2	1:A:30:HIS:C	2.90	0.45
1:A:144:VAL:HG12	1:A:153:VAL:HG13	1.97	0.45
1:B:37:ARG:C	1:B:44:ILE:CG2	2.85	0.45
5:C:1043:HOH:O	1:D:79:GLU:HB3	2.12	0.45
1:D:36:VAL:HB	1:D:37:ARG:HB2	1.99	0.45
1:D:45:GLU:C	1:D:47:ILE:N	2.64	0.45
1:D:55:PHE:CE2	1:D:172:GLN:HG3	2.51	0.45
1:D:26:ILE:HD11	1:D:73:LEU:HD23	1.97	0.45
1:C:73:LEU:HD23	1:C:153:VAL:O	2.17	0.45
1:C:149:ASN:ND2	1:C:149:ASN:N	2.34	0.45
1:C:157:HIS:HE1	1:C:167:VAL:HG22	1.82	0.45
1:D:62:ARG:O	1:D:64:VAL:N	2.50	0.45
1:B:38:GLU:HA	5:B:1009:HOH:O	2.08	0.45
1:B:150:ASP:N	5:B:1026:HOH:O	2.32	0.45
1:D:85:ILE:N	1:D:85:ILE:HD13	2.31	0.45
1:C:67:ASP:N	5:C:1038:HOH:O	2.08	0.45
1:C:5:LEU:O	1:C:8:ARG:HB2	2.17	0.45
1:D:104:ILE:HG12	1:D:104:ILE:O	2.16	0.45
1:B:57:GLN:CG	1:B:58:PHE:N	2.79	0.45
1:B:85:ILE:HG21	1:B:99:VAL:HG21	1.91	0.45
1:A:36:VAL:HG23	1:A:37:ARG:N	2.31	0.44
1:A:85:ILE:N	1:A:97:LEU:O	2.45	0.44
1:B:121:LEU:HA	1:B:121:LEU:HD12	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HG3	1:A:131:ASP:CG	2.38	0.44
1:B:19:TRP:CH2	1:B:40:PHE:CD2	3.05	0.44
1:C:68:LEU:C	1:C:68:LEU:HD12	2.36	0.44
1:D:99:VAL:HA	1:D:120:MET:O	2.16	0.44
1:A:116:GLY:CA	5:A:1020:HOH:O	2.65	0.44
1:B:72:VAL:HG23	1:B:150:ASP:OD1	2.18	0.44
1:B:130:MET:HA	1:B:131:ASP:N	2.32	0.44
1:C:131:ASP:HB3	1:C:132:LEU:H	1.30	0.44
1:A:30:HIS:HE2	1:A:139:CYS:HG	1.66	0.44
1:B:19:TRP:CH2	1:B:40:PHE:HD2	2.36	0.44
1:C:106:SER:O	1:D:105:ALA:HB1	2.18	0.44
1:D:46:SER:HG	1:D:46:SER:H	1.64	0.44
1:D:65:ARG:HA	1:D:66:PRO:HD3	1.33	0.44
1:A:123:THR:O	1:A:123:THR:CG2	2.55	0.44
1:B:48:ALA:O	1:B:49:ILE:C	2.56	0.44
1:D:18:PHE:CD2	1:D:142:PRO:HG3	2.52	0.44
1:D:26:ILE:HG23	1:D:55:PHE:HE1	1.82	0.44
1:D:139:CYS:HB3	1:D:157:HIS:O	2.18	0.44
1:A:87:ILE:CD1	1:A:97:LEU:HD12	2.47	0.44
1:A:92:GLY:N	5:A:1018:HOH:O	2.50	0.44
1:A:121:LEU:C	1:A:122:LEU:HD13	2.39	0.44
1:A:147:ARG:HG3	1:A:148:ASN:N	2.33	0.44
1:B:51:ARG:HA	1:B:56:THR:HA	1.99	0.44
1:D:114:VAL:HG11	1:D:168:VAL:HG21	2.00	0.44
1:D:160:ALA:HB2	1:D:167:VAL:HG12	1.99	0.44
1:B:120:MET:HA	1:B:165:ASN:O	2.18	0.43
1:C:65:ARG:HG3	1:C:67:ASP:OD1	2.18	0.43
1:D:65:ARG:NH2	1:D:68:LEU:HD21	2.33	0.43
1:A:100:ARG:CG	1:A:100:ARG:NE	2.73	0.43
1:A:165:ASN:ND2	1:B:100:ARG:NH1	2.62	0.43
1:B:2:PRO:CA	1:B:3:PRO:N	2.77	0.43
1:C:130:MET:O	1:C:131:ASP:OD1	2.36	0.43
1:A:87:ILE:HD13	1:A:97:LEU:HG	2.01	0.43
1:A:116:GLY:C	5:A:1020:HOH:O	2.57	0.43
1:D:21:SER:HB3	1:D:22:PRO:HD2	1.99	0.43
1:A:114:VAL:CG1	1:A:168:VAL:HG21	2.47	0.43
1:B:96:PRO:CB	1:C:123:THR:HG21	2.48	0.43
1:D:15:GLY:HA3	1:D:31:VAL:HG21	2.00	0.43
1:D:59:ARG:HH21	1:D:59:ARG:CG	2.31	0.43
1:B:9:VAL:CB	1:B:88:LYS:HE3	2.49	0.43
1:B:153:VAL:HG12	1:B:154:CYS:H	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:HIS:C	1:D:30:HIS:CD2	2.91	0.43
1:D:37:ARG:HG2	1:D:38:GLU:CG	2.48	0.43
1:B:109:ILE:HD13	1:B:114:VAL:CG2	2.48	0.43
1:C:47:ILE:HD12	1:C:60:PHE:CD2	2.53	0.43
1:C:80:GLY:HA3	5:C:1039:HOH:O	2.05	0.43
1:D:43:PRO:HD2	1:D:43:PRO:O	2.18	0.43
1:A:55:PHE:CE2	1:A:172:GLN:HG2	2.53	0.43
1:C:31:VAL:O	1:C:32:ILE:C	2.57	0.43
1:C:19:TRP:CZ2	1:C:40:PHE:HD2	2.33	0.43
1:D:6:TRP:CD1	1:D:94:LEU:HD23	2.54	0.43
1:D:12:PHE:CE2	1:D:25:PHE:CZ	3.06	0.43
1:D:114:VAL:CG1	1:D:168:VAL:HG21	2.48	0.43
1:B:146:LYS:CG	1:B:146:LYS:H	2.26	0.43
1:B:168:VAL:HG12	1:B:169:CYS:N	2.33	0.43
1:D:21:SER:HB3	1:D:24:VAL:H	1.84	0.43
1:D:51:ARG:NE	5:D:1027:HOH:O	2.51	0.43
1:D:153:VAL:HG12	1:D:155:GLY:H	1.83	0.43
1:B:12:PHE:CE2	1:B:25:PHE:HZ	2.37	0.43
1:B:28:THR:O	1:B:29:THR:C	2.56	0.43
1:C:10:VAL:CG1	1:C:19:TRP:HD1	2.32	0.43
1:D:6:TRP:CZ3	1:D:94:LEU:HB3	2.53	0.43
1:D:49:ILE:HG12	1:D:49:ILE:H	1.10	0.43
1:D:107:MET:HG3	1:D:109:ILE:CD1	2.45	0.43
1:D:108:LYS:CE	1:D:108:LYS:C	2.83	0.43
1:A:20:VAL:HG23	1:A:71:MET:HB2	2.01	0.42
1:B:56:THR:HG22	1:B:58:PHE:HE2	1.84	0.42
1:D:127:ALA:HB3	5:D:1034:HOH:O	2.19	0.42
1:B:25:PHE:C	1:B:26:ILE:CD1	2.88	0.42
1:A:61:SER:N	5:A:1031:HOH:O	2.41	0.42
1:D:12:PHE:HE2	1:D:40:PHE:CE2	2.37	0.42
1:A:26:ILE:CG1	1:A:55:PHE:CZ	3.02	0.42
1:C:32:ILE:CG2	1:C:33:PRO:CD	2.98	0.42
1:A:47:ILE:HD12	1:A:60:PHE:HD2	1.82	0.42
1:A:99:VAL:HG12	1:A:120:MET:O	2.19	0.42
1:A:166:THR:OG1	1:B:103:ALA:HB2	2.20	0.42
1:D:47:ILE:HG21	1:D:49:ILE:CD1	2.50	0.42
1:B:22:PRO:HA	1:B:64:VAL:CG2	2.49	0.42
1:B:40:PHE:CA	5:B:1008:HOH:O	2.66	0.42
1:D:55:PHE:HB2	1:D:171:VAL:O	2.19	0.42
1:A:149:ASN:OD1	1:A:149:ASN:N	2.46	0.42
1:C:32:ILE:HG22	1:C:33:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:PHE:CD2	1:D:40:PHE:CZ	3.08	0.42
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.68	0.42
1:D:8:ARG:HH11	1:D:8:ARG:HD2	1.53	0.42
1:A:55:PHE:HE2	1:A:172:GLN:HG2	1.85	0.42
1:B:18:PHE:CD2	1:B:142:PRO:HG3	2.55	0.42
1:A:120:MET:HG3	1:B:120:MET:HE2	2.02	0.41
1:A:139:CYS:C	5:A:1005:HOH:O	2.51	0.41
1:B:146:LYS:NZ	1:C:132:LEU:HD23	2.35	0.41
1:C:145:TYR:CE2	1:C:152:VAL:CG2	3.03	0.41
1:D:37:ARG:HG2	1:D:38:GLU:N	2.21	0.41
1:D:82:VAL:O	1:D:82:VAL:CG2	2.68	0.41
1:A:107:MET:HG2	1:A:109:ILE:HD11	2.01	0.41
1:D:89:ARG:NH2	1:D:138:ASP:OD2	2.54	0.41
1:C:71:MET:HE2	1:C:153:VAL:CG2	2.50	0.41
1:A:38:GLU:HB2	1:A:42:GLU:C	2.41	0.41
1:A:146:LYS:HZ3	1:A:149:ASN:C	2.24	0.41
1:C:126:ASN:ND2	5:C:1043:HOH:O	2.54	0.41
1:D:85:ILE:HD11	1:D:143:TYR:CE1	2.55	0.41
1:D:162:LYS:CE	5:D:1023:HOH:O	2.69	0.41
1:A:148:ASN:HB3	1:A:149:ASN:H	1.60	0.41
1:C:138:ASP:O	1:C:139:CYS:C	2.59	0.41
1:D:80:GLY:O	1:D:81:VAL:C	2.56	0.41
1:B:37:ARG:HD3	1:B:37:ARG:C	2.40	0.41
1:C:44:ILE:O	1:C:46:SER:N	2.54	0.41
1:D:147:ARG:HB2	1:D:152:VAL:HG11	2.02	0.41
1:A:73:LEU:HA	1:A:153:VAL:O	2.21	0.41
1:B:86:LEU:HB2	1:B:142:PRO:HG2	2.03	0.41
1:D:11:ARG:O	1:D:12:PHE:HB2	2.19	0.41
1:A:124:GLY:HA2	1:D:82:VAL:CG2	2.50	0.41
1:D:38:GLU:HA	1:D:42:GLU:O	2.20	0.41
1:D:85:ILE:HG23	1:D:143:TYR:CE2	2.56	0.41
1:D:162:LYS:CG	5:D:1023:HOH:O	2.69	0.41
1:D:168:VAL:HG12	1:D:169:CYS:N	2.35	0.41
1:A:1:ALA:CB	1:A:2:PRO:CD	2.84	0.41
1:A:55:PHE:HB2	1:A:170:ALA:HB1	2.02	0.41
1:B:65:ARG:HG2	1:B:68:LEU:HD11	2.03	0.41
1:C:100:ARG:CG	1:C:100:ARG:NH2	2.75	0.41
1:A:120:MET:HE3	5:B:1005:HOH:O	2.21	0.40
1:B:126:ASN:O	1:B:128:LYS:NZ	2.54	0.40
1:D:36:VAL:CG1	1:D:36:VAL:N	2.84	0.40
1:D:51:ARG:CG	5:D:1027:HOH:O	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LYS:NZ	1:D:108:LYS:C	2.74	0.40
1:D:147:ARG:HB2	1:D:152:VAL:CG1	2.51	0.40
1:A:32:ILE:CB	1:A:33:PRO:N	2.77	0.40
1:B:37:ARG:O	1:B:44:ILE:HG21	2.13	0.40
1:A:19:TRP:HB3	1:A:68:LEU:CD1	2.51	0.40
1:C:62:ARG:O	1:C:63:LYS:C	2.60	0.40
1:D:34:THR:O	1:D:34:THR:OG1	2.37	0.40
1:B:2:PRO:CB	1:C:130:MET:HG2	2.28	0.40
1:B:94:LEU:N	1:B:94:LEU:CD1	2.83	0.40
1:D:65:ARG:HH21	1:D:68:LEU:HD21	1.86	0.40
1:D:95:LEU:HG	1:D:95:LEU:O	2.22	0.40

All (6) 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)
5:A:1011:HOH:O	5:C:1016:HOH:O[6_655]	1.64	0.56
5:A:1010:HOH:O	5:C:1017:HOH:O[6_655]	1.88	0.32
1:A:47:ILE:O	5:C:1017:HOH:O[6_655]	2.04	0.16
1:A:62:ARG:NH1	5:C:1033:HOH:O[5_554]	2.08	0.12
1:A:37:ARG:CD	5:C:1040:HOH:O[5_554]	2.10	0.10
1:A:37:ARG:CG	5:C:1040:HOH:O[5_554]	2.15	0.05

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	171/173 (99%)	143 (84%)	17 (10%)	11 (6%)	1 3
1	B	171/173 (99%)	133 (78%)	29 (17%)	9 (5%)	2 6
1	C	171/173 (99%)	142 (83%)	20 (12%)	9 (5%)	2 6
1	D	171/173 (99%)	131 (77%)	28 (16%)	12 (7%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	684/692 (99%)	549 (80%)	94 (14%)	41 (6%)	1 4

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	109	ILE
1	C	36	VAL
1	C	124	GLY
1	C	148	ASN
1	D	35	GLY
1	D	109	ILE
1	A	36	VAL
1	A	37	ARG
1	A	91	SER
1	A	131	ASP
1	A	148	ASN
1	B	4	THR
1	B	40	PHE
1	B	62	ARG
1	B	112	ARG
1	B	124	GLY
1	C	129	GLY
1	D	34	THR
1	D	63	LYS
1	D	145	TYR
1	A	92	GLY
1	A	110	GLN
1	B	147	ARG
1	C	163	SER
1	D	12	PHE
1	D	22	PRO
1	D	105	ALA
1	B	3	PRO
1	B	91	SER
1	C	34	THR
1	C	45	GLU
1	A	147	ARG
1	D	36	VAL
1	B	49	ILE
1	C	111	GLY
1	D	49	ILE

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Mol	Chain	Res	Type
1	C	21	SER
1	D	43	PRO
1	D	44	ILE
1	A	32	ILE

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	138/138 (100%)	90 (65%)	48 (35%)	0	0
1	B	138/138 (100%)	85 (62%)	53 (38%)	0	0
1	C	138/138 (100%)	88 (64%)	50 (36%)	0	0
1	D	138/138 (100%)	87 (63%)	51 (37%)	0	0
All	All	552/552 (100%)	350 (63%)	202 (37%)	0	0

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ARG
1	A	11	ARG
1	A	14	SER
1	A	21	SER
1	A	22	PRO
1	A	23	THR
1	A	26	ILE
1	A	32	ILE
1	A	39	PHE
1	A	42	GLU
1	A	44	ILE
1	A	45	GLU
1	A	51	ARG
1	A	59	ARG
1	A	63	LYS
1	A	69	THR

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Mol	Chain	Res	Type
1	A	73	LEU
1	A	79	GLU
1	A	84	SER
1	A	85	ILE
1	A	89	ARG
1	A	90	ASP
1	A	99	VAL
1	A	100	ARG
1	A	106	SER
1	A	107	MET
1	A	108	LYS
1	A	110	GLN
1	A	112	ARG
1	A	113	LEU
1	A	121	LEU
1	A	122	LEU
1	A	123	THR
1	A	130	MET
1	A	131	ASP
1	A	132	LEU
1	A	135	LEU
1	A	136	PRO
1	A	139	CYS
1	A	142	PRO
1	A	146	LYS
1	A	147	ARG
1	A	151	TRP
1	A	153	VAL
1	A	162	LYS
1	A	163	SER
1	A	172	GLN
1	B	5	LEU
1	B	7	SER
1	B	8	ARG
1	B	10	VAL
1	B	11	ARG
1	B	12	PHE
1	B	20	VAL
1	B	21	SER
1	B	23	THR
1	B	24	VAL
1	B	25	PHE

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Mol	Chain	Res	Type
1	B	31	VAL
1	B	34	THR
1	B	36	VAL
1	B	37	ARG
1	B	38	GLU
1	B	39	PHE
1	B	42	GLU
1	B	44	ILE
1	B	45	GLU
1	B	47	ILE
1	B	51	ARG
1	B	59	ARG
1	B	61	SER
1	B	69	THR
1	B	73	LEU
1	B	85	ILE
1	B	86	LEU
1	B	89	ARG
1	B	91	SER
1	B	101	MET
1	B	104	ILE
1	B	106	SER
1	B	107	MET
1	B	108	LYS
1	B	112	ARG
1	B	117	GLN
1	B	120	MET
1	B	121	LEU
1	B	128	LYS
1	B	130	MET
1	B	131	ASP
1	B	132	LEU
1	B	134	THR
1	B	146	LYS
1	B	147	ARG
1	B	151	TRP
1	B	152	VAL
1	B	154	CYS
1	B	156	VAL
1	B	157	HIS
1	B	162	LYS
1	B	169	CYS

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Mol	Chain	Res	Type
1	C	3	PRO
1	C	10	VAL
1	C	11	ARG
1	C	20	VAL
1	C	31	VAL
1	C	34	THR
1	C	37	ARG
1	C	38	GLU
1	C	39	PHE
1	C	42	GLU
1	C	43	PRO
1	C	44	ILE
1	C	54	GLU
1	C	59	ARG
1	C	62	ARG
1	C	63	LYS
1	C	65	ARG
1	C	68	LEU
1	C	69	THR
1	C	71	MET
1	C	73	LEU
1	C	74	GLU
1	C	75	GLU
1	C	78	PRO
1	C	79	GLU
1	C	85	ILE
1	C	93	GLU
1	C	99	VAL
1	C	100	ARG
1	C	104	ILE
1	C	106	SER
1	C	108	LYS
1	C	110	GLN
1	C	112	ARG
1	C	113	LEU
1	C	122	LEU
1	C	123	THR
1	C	130	MET
1	C	132	LEU
1	C	135	LEU
1	C	146	LYS
1	C	147	ARG

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Mol	Chain	Res	Type
1	C	148	ASN
1	C	149	ASN
1	C	151	TRP
1	C	152	VAL
1	C	153	VAL
1	C	154	CYS
1	C	162	LYS
1	C	167	VAL
1	D	10	VAL
1	D	11	ARG
1	D	14	SER
1	D	20	VAL
1	D	21	SER
1	D	28	THR
1	D	30	HIS
1	D	31	VAL
1	D	32	ILE
1	D	34	THR
1	D	36	VAL
1	D	37	ARG
1	D	38	GLU
1	D	39	PHE
1	D	42	GLU
1	D	43	PRO
1	D	44	ILE
1	D	46	SER
1	D	49	ILE
1	D	54	GLU
1	D	59	ARG
1	D	60	PHE
1	D	61	SER
1	D	62	ARG
1	D	65	ARG
1	D	67	ASP
1	D	68	LEU
1	D	73	LEU
1	D	81	VAL
1	D	85	ILE
1	D	86	LEU
1	D	88	LYS
1	D	89	ARG
1	D	99	VAL

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Mol	Chain	Res	Type
1	D	104	ILE
1	D	106	SER
1	D	107	MET
1	D	108	LYS
1	D	117	GLN
1	D	121	LEU
1	D	128	LYS
1	D	131	ASP
1	D	132	LEU
1	D	145	TYR
1	D	146	LYS
1	D	151	TRP
1	D	152	VAL
1	D	161	THR
1	D	162	LYS
1	D	169	CYS
1	D	172	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	B	57	GLN
1	B	149	ASN
1	C	149	ASN
1	C	172	GLN
1	D	30	HIS
1	D	117	GLN
1	D	157	HIS
1	D	172	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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TLA	A	301	1	9,9,9	5.41	5 (55%)	12,12,12	4.71	6 (50%)
4	TAR	A	300	1	9,9,9	3.70	3 (33%)	12,12,12	3.10	8 (66%)

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	TLA	A	301	1	-	2/12/12/12	-
4	TAR	A	300	1	-	3/12/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	TLA	C2-C1	10.64	1.67	1.52
3	A	301	TLA	C3-C2	9.19	1.82	1.53
4	A	300	TAR	O3-C3	7.63	1.57	1.42
3	A	301	TLA	O2-C2	6.91	1.55	1.42
4	A	300	TAR	O2-C2	6.33	1.54	1.42
4	A	300	TAR	O41-C4	-3.49	1.19	1.30
3	A	301	TLA	O41-C4	-3.01	1.21	1.30
3	A	301	TLA	O4-C4	2.03	1.28	1.22

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	TLA	O2-C2-C3	-8.25	93.38	110.17
3	A	301	TLA	O2-C2-C1	-7.54	94.57	110.69
4	A	300	TAR	C2-C3-C4	6.80	124.89	109.82
3	A	301	TLA	O3-C3-C2	6.61	123.63	110.17
3	A	301	TLA	O3-C3-C4	-6.56	96.68	110.69
3	A	301	TLA	C3-C2-C1	5.99	123.10	109.82
4	A	300	TAR	O11-C1-C2	4.47	125.73	113.31
4	A	300	TAR	O3-C3-C4	3.12	117.36	110.69
4	A	300	TAR	O2-C2-C3	3.00	116.27	110.17
3	A	301	TLA	O11-C1-O1	-2.81	117.71	124.08
4	A	300	TAR	O41-C4-C3	2.58	120.48	113.31
4	A	300	TAR	O11-C1-O1	-2.49	118.43	124.08
4	A	300	TAR	O1-C1-C2	-2.39	115.25	121.62
4	A	300	TAR	O2-C2-C1	2.20	115.40	110.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	300	TAR	O2-C2-C3-O3
3	A	301	TLA	O2-C2-C3-O3
4	A	300	TAR	C1-C2-C3-O3
4	A	300	TAR	O2-C2-C3-C4
3	A	301	TLA	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	TLA	6	0
4	A	300	TAR	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:VAL	C	37:ARG	N	1.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	173/173 (100%)	0.14	10 (5%)	23	15	23, 49, 101, 135	0
1	B	173/173 (100%)	0.80	32 (18%)	1	1	33, 75, 129, 147	0
1	C	173/173 (100%)	0.08	9 (5%)	27	18	23, 51, 98, 135	0
1	D	173/173 (100%)	0.84	40 (23%)	0	0	33, 66, 120, 141	0
All	All	692/692 (100%)	0.47	91 (13%)	3	2	23, 60, 117, 147	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	GLY	7.6
1	A	130	MET	7.2
1	B	2	PRO	6.4
1	D	40	PHE	6.0
1	D	1	ALA	5.7
1	A	129	GLY	5.7
1	B	173	ALA	5.7
1	D	41	GLY	5.4
1	D	3	PRO	5.0
1	D	61	SER	4.9
1	A	107	MET	4.9
1	D	148	ASN	4.9
1	B	38	GLU	4.9
1	B	39	PHE	4.7
1	D	66	PRO	4.7
1	C	130	MET	4.6
1	D	2	PRO	4.6
1	D	129	GLY	4.2
1	D	67	ASP	4.1
1	B	63	LYS	4.1
1	B	37	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	4.0
1	B	48	ALA	4.0
1	D	39	PHE	4.0
1	D	68	LEU	3.9
1	D	70	GLY	3.9
1	C	128	LYS	3.8
1	B	130	MET	3.8
1	D	22	PRO	3.6
1	A	110	GLN	3.6
1	D	36	VAL	3.6
1	B	41	GLY	3.5
1	B	50	HIS	3.5
1	B	36	VAL	3.5
1	B	40	PHE	3.4
1	B	26	ILE	3.4
1	D	23	THR	3.4
1	C	109	ILE	3.3
1	C	111	GLY	3.3
1	D	147	ARG	3.2
1	A	148	ASN	3.2
1	C	110	GLN	3.2
1	A	128	LYS	3.1
1	B	49	ILE	3.1
1	D	47	ILE	3.1
1	A	113	LEU	3.1
1	B	23	THR	3.1
1	D	62	ARG	3.1
1	A	109	ILE	3.0
1	D	21	SER	3.0
1	B	3	PRO	3.0
1	C	1	ALA	3.0
1	D	38	GLU	2.9
1	D	63	LYS	2.9
1	B	43	PRO	2.9
1	D	46	SER	2.9
1	B	60	PHE	2.9
1	D	44	ILE	2.9
1	A	108	LYS	2.9
1	B	127	ALA	2.8
1	B	62	ARG	2.8
1	D	128	LYS	2.8
1	D	69	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	149	ASN	2.7
1	D	37	ARG	2.7
1	D	24	VAL	2.7
1	B	42	GLU	2.7
1	B	46	SER	2.7
1	B	52	ALA	2.7
1	C	129	GLY	2.7
1	C	173	ALA	2.6
1	D	43	PRO	2.6
1	D	151	TRP	2.5
1	D	52	ALA	2.5
1	B	24	VAL	2.5
1	B	61	SER	2.5
1	D	60	PHE	2.5
1	D	48	ALA	2.5
1	D	45	GLU	2.5
1	A	111	GLY	2.4
1	B	58	PHE	2.4
1	C	40	PHE	2.4
1	B	147	ARG	2.4
1	D	130	MET	2.4
1	B	128	LYS	2.3
1	B	34	THR	2.2
1	D	64	VAL	2.2
1	D	65	ARG	2.2
1	D	111	GLY	2.1
1	B	35	GLY	2.1
1	D	42	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TLA	A	301	10/10	0.45	0.62	152,162,165,167	0
4	TAR	A	300	10/10	0.91	0.22	68,107,112,113	0
2	HG	A	1002	1/1	0.97	0.15	65,65,65,65	1
2	HG	C	1006	1/1	0.98	0.12	75,75,75,75	1
2	HG	B	1003	1/1	0.98	0.15	69,69,69,69	1
2	HG	B	1004	1/1	0.98	0.14	118,118,118,118	1
2	HG	D	1008	1/1	0.99	0.19	96,96,96,96	1
2	HG	C	1005	1/1	0.99	0.11	60,60,60,60	1
2	HG	A	1001	1/1	0.99	0.15	81,81,81,81	1
2	HG	D	1007	1/1	1.00	0.20	64,64,64,64	1

6.5 Other polymers (i)

There are no such residues in this entry.