



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:41 PM UTC

PDB ID : 4DK1 / pdb_00004dk1
Title : Crystal Structure of MacA-MexA chimeric protein, containing the Pseudomonas aeruginosa MexA alpha-hairpin domain.
Authors : Xu, Y.; Ha, N.C.
Deposited on : 2012-02-03
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

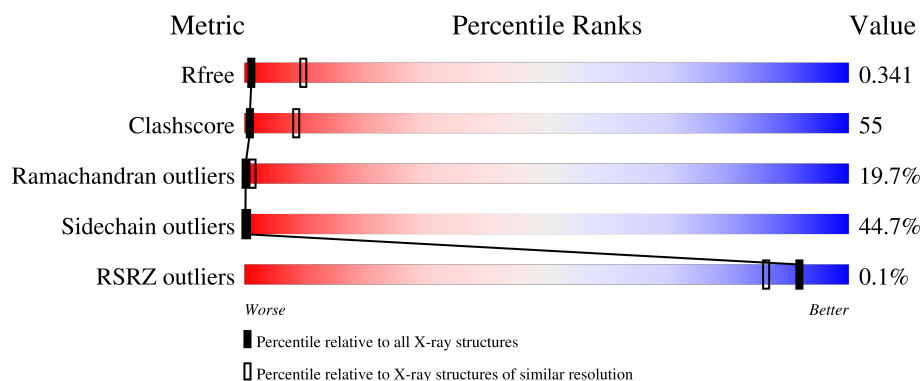
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	341	
1	B	341	
1	C	341	
1	D	341	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8568 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 Putative MacA, Multidrug resistance protein mexA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	Se	4	0	0
			2108	1316	355	435	2			
1	B	285	Total	C	N	O	Se	4	0	0
			2191	1369	369	451	2			
1	C	278	Total	C	N	O	Se	4	0	0
			2135	1336	358	439	2			
1	D	278	Total	C	N	O	Se	4	0	0
			2134	1334	359	439	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP Q2EHL9
A	27	ALA	-	expression tag	UNP Q2EHL9
A	28	MSE	-	expression tag	UNP Q2EHL9
A	29	ASP	-	expression tag	UNP Q2EHL9
A	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
A	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
B	26	GLY	-	expression tag	UNP Q2EHL9
B	27	ALA	-	expression tag	UNP Q2EHL9
B	28	MSE	-	expression tag	UNP Q2EHL9
B	29	ASP	-	expression tag	UNP Q2EHL9
B	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
B	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
C	26	GLY	-	expression tag	UNP Q2EHL9
C	27	ALA	-	expression tag	UNP Q2EHL9
C	28	MSE	-	expression tag	UNP Q2EHL9
C	29	ASP	-	expression tag	UNP Q2EHL9
C	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
C	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
D	26	GLY	-	expression tag	UNP Q2EHL9
D	27	ALA	-	expression tag	UNP Q2EHL9
D	28	MSE	-	expression tag	UNP Q2EHL9

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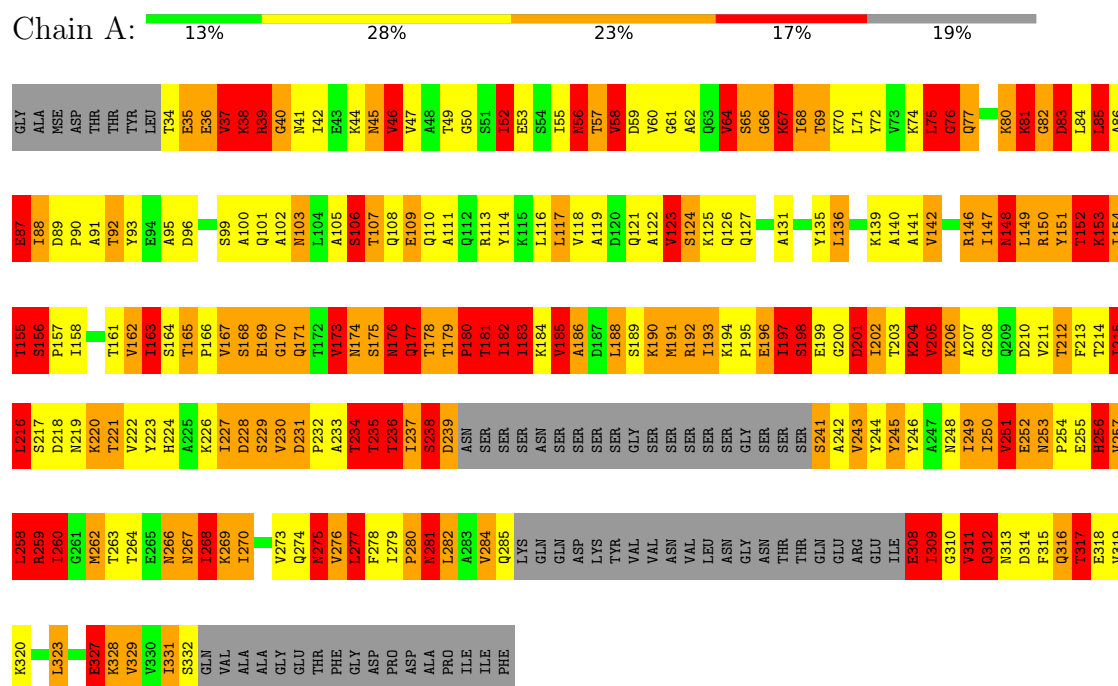
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Chain	Residue	Modelled	Actual	Comment	Reference
D	29	ASP	-	expression tag	UNP Q2EHL9
D	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
D	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9

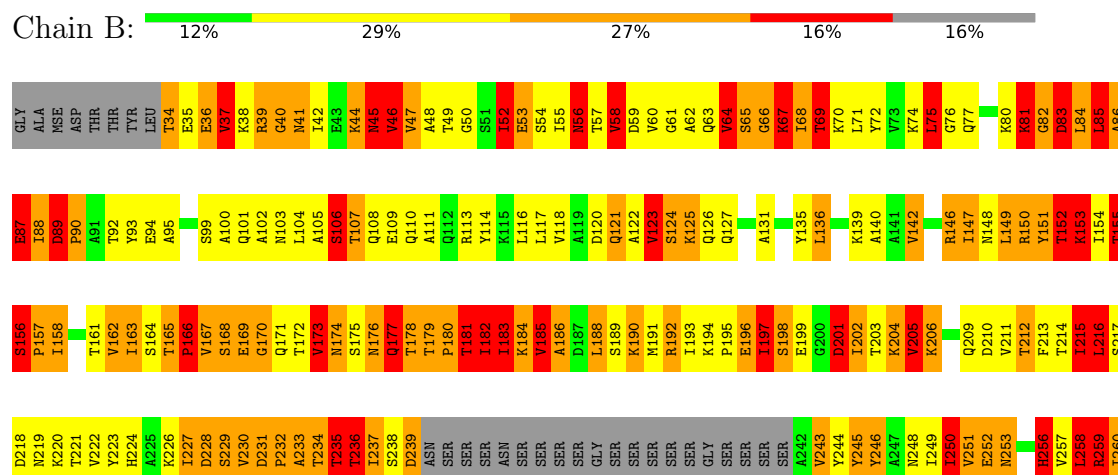
3 Residue-property plots

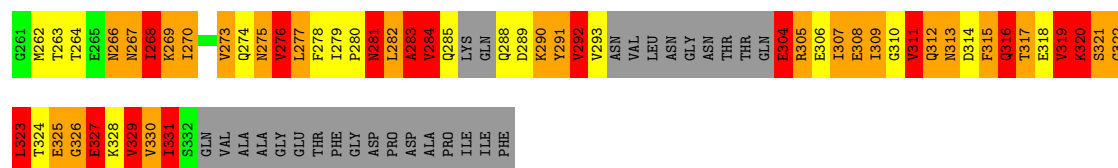
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Putative MacA, Multidrug resistance protein mexA



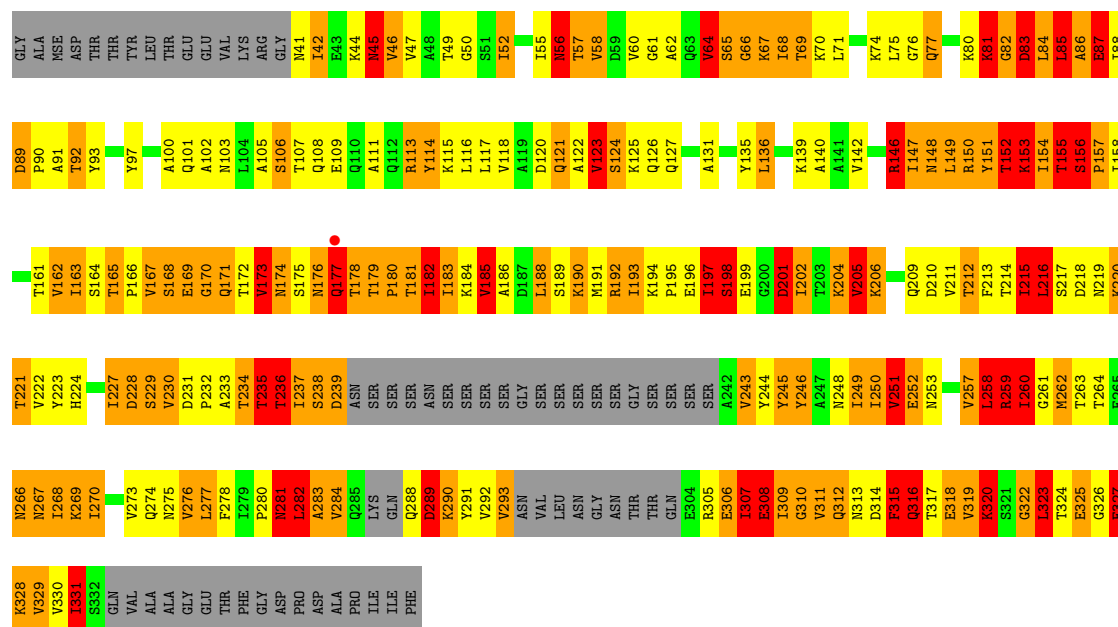
- Molecule 1: Putative MacA, Multidrug resistance protein mexA





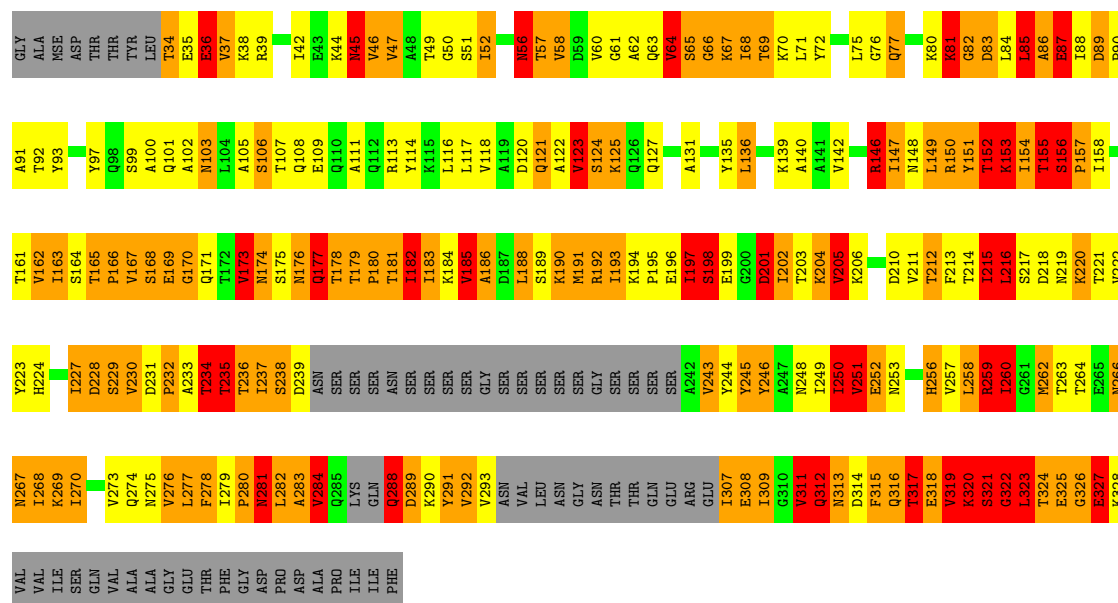
• Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain C: 16% 27% 27% 12% 18%



• Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain D: 16% 26% 27% 12% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.71Å 151.71Å 216.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 3.50 19.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.95-3.50) 91.4 (19.95-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 3.52Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.314 , 0.368 0.287 , 0.341	Depositor DCC
R_{free} test set	1709 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.277 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	8568	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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

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	1.60	29/2127 (1.4%)	2.02	79/2884 (2.7%)
1	B	1.59	30/2210 (1.4%)	1.96	79/2994 (2.6%)
1	C	1.26	7/2154 (0.3%)	1.81	53/2920 (1.8%)
1	D	1.28	11/2153 (0.5%)	1.83	63/2917 (2.2%)
All	All	1.44	77/8644 (0.9%)	1.91	274/11715 (2.3%)

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	23
1	B	0	25
1	C	0	22
1	D	0	24
All	All	0	94

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	VAL	CA-CB	-13.43	1.41	1.55
1	A	179	THR	C-O	-9.52	1.12	1.24
1	B	45	ASN	CG-ND2	-8.33	1.15	1.33
1	B	121	GLN	CD-NE2	-7.99	1.16	1.33
1	A	58	VAL	CA-CB	-7.66	1.47	1.55
1	D	260	ILE	CA-CB	7.58	1.64	1.54
1	B	186	ALA	CA-CB	-7.55	1.41	1.53
1	B	179	THR	C-O	-7.47	1.14	1.24
1	A	309	ILE	CA-CB	7.39	1.64	1.54
1	A	162	VAL	CA-CB	-7.20	1.45	1.53
1	B	231	ASP	CA-C	-7.20	1.43	1.52
1	A	331	ILE	CA-CB	7.16	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	VAL	CA-CB	-6.99	1.48	1.55
1	B	253	ASN	CG-ND2	6.92	1.47	1.33
1	C	179	THR	C-O	-6.80	1.16	1.24
1	A	231	ASP	CA-C	-6.70	1.44	1.52
1	A	260	ILE	CA-CB	6.63	1.63	1.54
1	B	69	THR	CA-CB	-6.63	1.42	1.53
1	B	185	VAL	CA-CB	-6.58	1.45	1.55
1	A	65	SER	CA-C	-6.45	1.44	1.52
1	D	317	THR	CA-CB	6.43	1.64	1.53
1	D	64	VAL	C-O	-6.42	1.16	1.24
1	A	309	ILE	CA-C	6.36	1.60	1.52
1	B	88	ILE	CA-CB	6.30	1.60	1.54
1	A	103	ASN	CA-C	6.25	1.61	1.52
1	B	121	GLN	CD-OE1	-6.25	1.11	1.23
1	A	183	ILE	CA-C	-6.23	1.45	1.52
1	D	186	ALA	CA-CB	-6.15	1.44	1.53
1	B	233	ALA	CA-CB	-6.11	1.43	1.53
1	B	162	VAL	CA-CB	-6.09	1.47	1.53
1	B	331	ILE	CA-CB	6.05	1.62	1.54
1	D	185	VAL	CA-CB	-6.04	1.49	1.55
1	D	103	ASN	CA-C	5.83	1.60	1.52
1	B	235	THR	CA-CB	-5.82	1.43	1.53
1	D	179	THR	C-O	-5.80	1.16	1.24
1	B	165	THR	C-N	-5.76	1.27	1.34
1	B	196	GLU	CG-CD	5.70	1.66	1.52
1	A	46	VAL	CA-C	-5.69	1.46	1.52
1	B	47	VAL	N-CA	-5.62	1.39	1.46
1	A	186	ALA	CA-CB	-5.60	1.44	1.53
1	A	316	GLN	CG-CD	5.58	1.66	1.52
1	D	152	THR	N-CA	5.55	1.53	1.46
1	A	165	THR	C-O	-5.54	1.17	1.24
1	C	307	ILE	CA-CB	5.54	1.61	1.54
1	A	67	LYS	CA-C	-5.51	1.45	1.52
1	A	251	VAL	CA-C	-5.50	1.45	1.52
1	D	152	THR	CA-C	5.50	1.60	1.52
1	B	90	PRO	CA-C	5.48	1.58	1.52
1	C	249	ILE	CA-CB	-5.48	1.47	1.54
1	A	249	ILE	CA-CB	-5.43	1.47	1.54
1	D	278	PHE	CA-C	5.38	1.59	1.52
1	B	258	LEU	CA-C	-5.37	1.45	1.52
1	C	235	THR	CA-CB	-5.36	1.44	1.53
1	A	259	ARG	CA-C	-5.35	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	ILE	CG1-CD1	-5.34	1.30	1.51
1	B	75	LEU	CA-C	-5.33	1.46	1.52
1	B	65	SER	CA-C	-5.32	1.45	1.52
1	B	256	HIS	CG-CD2	5.31	1.41	1.35
1	B	64	VAL	CA-CB	-5.30	1.47	1.54
1	A	243	VAL	N-CA	5.23	1.52	1.46
1	A	185	VAL	CA-CB	-5.21	1.47	1.55
1	A	171	GLN	CA-C	-5.20	1.46	1.52
1	D	235	THR	CA-CB	-5.19	1.44	1.53
1	A	196	GLU	CG-CD	5.17	1.65	1.52
1	A	262	MSE	CA-C	-5.17	1.45	1.52
1	A	207	ALA	CA-C	-5.13	1.46	1.52
1	B	45	ASN	CG-OD1	-5.12	1.13	1.23
1	A	165	THR	CA-C	-5.12	1.46	1.52
1	C	316	GLN	N-CA	5.09	1.52	1.46
1	A	179	THR	CA-CB	-5.08	1.45	1.53
1	A	183	ILE	N-CA	-5.08	1.40	1.46
1	B	46	VAL	CA-C	-5.06	1.47	1.53
1	A	175	SER	CA-C	-5.05	1.46	1.52
1	B	75	LEU	CG-CD1	5.03	1.69	1.52
1	B	48	ALA	CA-CB	5.03	1.61	1.53
1	B	67	LYS	CA-C	-5.03	1.46	1.53
1	C	260	ILE	CA-CB	5.01	1.62	1.54

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	THR	CA-C-N	-18.67	102.02	120.31
1	C	179	THR	C-N-CA	-18.67	102.02	120.31
1	B	179	THR	CA-C-N	-17.13	103.52	120.31
1	B	179	THR	C-N-CA	-17.13	103.52	120.31
1	D	179	THR	CA-C-N	-16.29	102.88	120.14
1	D	179	THR	C-N-CA	-16.29	102.88	120.14
1	B	189	SER	N-CA-C	-15.62	85.91	109.81
1	A	189	SER	N-CA-C	-15.58	87.25	109.69
1	B	253	ASN	CA-C-N	-15.56	105.12	120.52
1	B	253	ASN	C-N-CA	-15.56	105.12	120.52
1	A	253	ASN	CA-C-N	-15.20	105.47	120.52
1	A	253	ASN	C-N-CA	-15.20	105.47	120.52
1	A	179	THR	CA-C-N	-14.95	104.30	120.14
1	A	179	THR	C-N-CA	-14.95	104.30	120.14
1	C	189	SER	N-CA-C	-14.89	87.03	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	SER	N-CA-C	-13.86	88.61	109.81
1	D	253	ASN	CA-C-N	-13.26	107.48	120.21
1	D	253	ASN	C-N-CA	-13.26	107.48	120.21
1	C	253	ASN	CA-C-N	-12.18	108.52	120.21
1	C	253	ASN	C-N-CA	-12.18	108.52	120.21
1	B	198	SER	N-CA-C	11.76	125.45	108.86
1	A	198	SER	N-CA-C	11.74	125.41	108.86
1	A	243	VAL	N-CA-C	11.55	125.43	107.98
1	A	243	VAL	CB-CA-C	-10.91	99.44	111.23
1	C	243	VAL	N-CA-C	10.79	124.28	107.98
1	D	154	ILE	N-CA-C	10.74	121.44	111.45
1	B	243	VAL	N-CA-C	10.72	124.45	107.73
1	A	162	VAL	CB-CA-C	-10.69	99.69	111.23
1	D	309	ILE	N-CA-C	10.64	123.07	108.17
1	B	320	LYS	N-CA-C	-10.50	93.75	109.81
1	A	146	ARG	NE-CZ-NH2	10.35	128.51	119.20
1	C	312	GLN	N-CA-C	10.17	125.65	109.79
1	C	198	SER	N-CA-C	9.80	122.68	108.86
1	D	198	SER	N-CA-C	9.71	122.55	108.86
1	D	243	VAL	N-CA-C	9.58	122.67	107.73
1	B	146	ARG	NE-CZ-NH2	9.44	127.70	119.20
1	D	56	ASN	N-CA-C	9.27	123.24	109.24
1	D	283	ALA	N-CA-C	-9.19	102.64	112.93
1	D	312	GLN	N-CA-C	9.14	124.03	109.86
1	B	168	SER	N-CA-C	9.14	123.94	109.50
1	A	83	ASP	N-CA-C	9.01	123.39	109.60
1	A	309	ILE	N-CA-C	8.97	127.99	109.34
1	D	292	VAL	N-CA-C	8.85	122.38	109.63
1	D	83	ASP	N-CA-C	8.75	122.99	109.60
1	A	56	ASN	N-CA-C	8.73	122.15	109.14
1	C	283	ALA	N-CA-C	-8.72	102.71	112.57
1	C	56	ASN	N-CA-C	8.72	122.13	109.14
1	C	168	SER	N-CA-C	8.65	123.17	109.50
1	D	325	GLU	N-CA-C	8.53	122.28	108.63
1	B	62	ALA	N-CA-C	8.29	122.68	110.17
1	C	162	VAL	CB-CA-C	-8.26	100.75	111.25
1	A	165	THR	CA-C-N	8.25	127.90	119.82
1	A	165	THR	C-N-CA	8.25	127.90	119.82
1	D	168	SER	N-CA-C	8.21	122.47	109.50
1	B	179	THR	CB-CA-C	-8.10	97.38	109.60
1	B	156	SER	CB-CA-C	-8.07	102.18	110.17
1	A	168	SER	N-CA-C	8.06	122.23	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	VAL	CB-CA-C	-8.03	101.05	111.25
1	B	56	ASN	N-CA-C	7.98	121.03	109.14
1	B	243	VAL	CB-CA-C	-7.98	101.12	111.25
1	C	62	ALA	N-CA-C	7.86	122.54	110.36
1	B	282	LEU	N-CA-C	7.83	121.62	109.96
1	A	146	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	D	57	THR	CB-CA-C	-7.75	94.99	110.42
1	B	58	VAL	N-CA-C	7.70	118.50	107.88
1	A	142	VAL	N-CA-C	7.65	118.45	110.72
1	A	100	ALA	N-CA-C	7.58	121.79	112.54
1	C	58	VAL	N-CA-C	7.57	117.75	108.06
1	A	183	ILE	N-CA-C	-7.54	97.64	108.42
1	D	62	ALA	N-CA-C	7.51	122.00	110.36
1	A	331	ILE	N-CA-C	7.48	118.14	108.12
1	A	76	GLY	N-CA-C	-7.47	95.47	113.18
1	A	58	VAL	N-CA-C	7.45	118.16	107.88
1	C	243	VAL	CB-CA-C	-7.44	103.20	111.23
1	A	323	LEU	N-CA-C	-7.37	90.36	111.00
1	D	243	VAL	CB-CA-C	-7.28	102.00	111.25
1	D	313	ASN	N-CA-C	7.26	126.25	110.80
1	B	142	VAL	N-CA-C	7.14	117.94	110.72
1	B	83	ASP	N-CA-C	7.14	126.00	110.80
1	A	62	ALA	N-CA-C	7.13	120.93	110.17
1	B	158	ILE	CB-CA-C	-7.12	105.05	111.74
1	B	162	VAL	CB-CA-C	-7.10	102.24	111.25
1	D	320	LYS	N-CA-C	-7.09	103.10	114.09
1	D	177	GLN	CB-CA-C	7.09	121.46	109.55
1	A	236	THR	N-CA-C	-7.08	103.63	112.90
1	D	91	ALA	N-CA-C	7.02	119.58	111.02
1	C	177	GLN	CB-CA-C	6.98	121.28	109.55
1	A	154	ILE	N-CA-C	6.98	117.94	111.45
1	D	146	ARG	NE-CZ-NH2	-6.97	112.93	119.20
1	D	177	GLN	CA-CB-CG	6.96	128.02	114.10
1	C	292	VAL	N-CA-C	6.95	118.57	107.73
1	B	146	ARG	NE-CZ-NH1	-6.95	114.55	121.50
1	A	177	GLN	CA-CB-CG	6.94	127.97	114.10
1	C	146	ARG	NE-CZ-NH1	6.89	128.40	121.50
1	B	165	THR	CA-C-N	6.89	126.58	119.82
1	B	165	THR	C-N-CA	6.89	126.58	119.82
1	C	146	ARG	NE-CZ-NH2	-6.88	113.00	119.20
1	D	146	ARG	NE-CZ-NH1	6.87	128.37	121.50
1	B	215	ILE	CB-CA-C	-6.82	100.10	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	VAL	N-CA-C	6.82	117.72	108.17
1	D	77	GLN	N-CA-C	-6.81	99.12	109.95
1	A	256	HIS	N-CA-C	-6.80	103.15	113.89
1	B	256	HIS	N-CA-C	-6.77	103.83	111.14
1	C	315	PHE	N-CA-C	-6.77	104.06	112.72
1	B	177	GLN	CA-CB-CG	6.72	127.55	114.10
1	C	177	GLN	CA-CB-CG	6.72	127.54	114.10
1	B	219	ASN	N-CA-C	6.72	118.60	111.28
1	A	156	SER	N-CA-C	6.65	120.37	108.47
1	A	39	ARG	CB-CA-C	-6.63	108.94	116.63
1	C	204	LYS	N-CA-C	-6.63	99.31	109.65
1	B	284	VAL	N-CA-C	6.61	123.10	109.34
1	C	83	ASP	N-CA-C	6.61	124.87	110.80
1	B	283	ALA	N-CA-C	-6.58	100.52	109.54
1	D	87	GLU	CA-C-N	6.58	129.49	120.35
1	D	87	GLU	C-N-CA	6.58	129.49	120.35
1	A	65	SER	N-CA-C	-6.56	96.83	110.80
1	B	125	LYS	N-CA-C	-6.46	104.60	114.16
1	B	201	ASP	N-CA-C	-6.43	105.30	113.02
1	B	309	ILE	N-CA-C	6.43	116.84	108.35
1	B	184	LYS	N-CA-C	-6.43	98.92	109.40
1	C	171	GLN	N-CA-C	6.43	118.76	108.41
1	D	58	VAL	N-CA-C	6.41	116.27	108.06
1	D	245	TYR	CB-CA-C	-6.40	102.14	111.23
1	B	87	GLU	CA-C-N	6.38	129.22	120.35
1	B	87	GLU	C-N-CA	6.38	129.22	120.35
1	D	124	SER	N-CA-C	6.37	124.38	110.80
1	B	327	GLU	N-CA-C	6.37	124.36	110.80
1	B	85	LEU	CA-C-N	6.32	133.07	121.70
1	B	85	LEU	C-N-CA	6.32	133.07	121.70
1	B	100	ALA	N-CA-C	6.29	120.22	112.54
1	C	123	VAL	N-CA-C	6.29	118.94	109.20
1	A	87	GLU	CA-C-N	6.26	129.06	120.35
1	A	87	GLU	C-N-CA	6.26	129.06	120.35
1	B	236	THR	N-CA-C	-6.26	104.69	112.90
1	D	327	GLU	N-CA-C	6.26	124.14	110.80
1	A	312	GLN	N-CA-C	6.26	120.64	113.19
1	C	289	ASP	N-CA-C	6.25	128.49	111.00
1	A	163	ILE	N-CA-C	-6.23	105.07	110.74
1	D	99	SER	N-CA-C	6.23	118.59	111.11
1	C	57	THR	CB-CA-C	-6.23	98.03	110.42
1	B	330	VAL	N-CA-C	6.22	122.29	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	ARG	CD-NE-CZ	6.21	133.10	124.40
1	B	323	LEU	N-CA-C	6.21	128.39	111.00
1	C	124	SER	N-CA-C	6.21	124.02	110.80
1	C	326	GLY	N-CA-C	6.19	123.91	115.30
1	B	124	SER	N-CA-C	6.17	123.94	110.80
1	D	215	ILE	CB-CA-C	-6.17	101.17	111.29
1	D	156	SER	CB-CA-C	-6.16	103.00	110.08
1	B	215	ILE	N-CA-C	6.14	122.12	109.34
1	A	153	LYS	N-CA-C	6.12	118.93	109.07
1	D	204	LYS	N-CA-C	-6.12	100.11	109.65
1	D	281	ASN	N-CA-C	6.12	123.83	110.80
1	C	219	ASN	N-CA-C	6.11	117.94	111.28
1	A	41	ASN	CA-C-N	-6.07	112.61	121.71
1	A	41	ASN	C-N-CA	-6.07	112.61	121.71
1	B	183	ILE	N-CA-C	-6.04	99.79	108.42
1	B	204	LYS	N-CA-C	-6.02	100.25	109.65
1	A	235	THR	N-CA-C	6.02	123.62	110.80
1	D	85	LEU	CA-C-N	6.00	132.49	121.70
1	D	85	LEU	C-N-CA	6.00	132.49	121.70
1	D	153	LYS	N-CA-C	5.98	118.98	109.24
1	A	126	GLN	N-CA-C	-5.96	106.56	113.88
1	D	165	THR	CA-C-N	5.94	125.64	119.82
1	D	165	THR	C-N-CA	5.94	125.64	119.82
1	A	204	LYS	N-CA-C	-5.93	100.39	109.65
1	A	317	THR	N-CA-C	5.93	123.43	110.80
1	C	77	GLN	N-CA-C	-5.92	100.05	109.59
1	B	123	VAL	N-CA-C	5.91	118.27	109.17
1	B	316	GLN	N-CA-C	-5.89	101.64	110.06
1	C	323	LEU	N-CA-C	5.89	127.48	111.00
1	A	124	SER	N-CA-C	5.88	123.33	110.80
1	D	156	SER	N-CA-C	5.87	118.98	108.47
1	C	42	ILE	CB-CA-C	-5.85	102.48	111.31
1	D	219	ASN	N-CA-C	5.85	117.66	111.28
1	A	75	LEU	N-CA-C	5.82	123.19	110.80
1	C	201	ASP	N-CA-C	-5.81	105.77	112.92
1	D	323	LEU	N-CA-C	5.80	127.25	111.00
1	C	126	GLN	N-CA-C	-5.80	106.85	114.04
1	B	41	ASN	N-CA-C	5.79	118.33	108.02
1	C	115	LYS	N-CA-C	-5.79	106.05	113.23
1	A	277	LEU	N-CA-C	5.79	118.33	108.90
1	B	178	THR	CB-CA-C	-5.78	101.51	111.23
1	D	123	VAL	N-CA-C	5.78	118.07	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	TYR	CB-CA-C	-5.76	103.05	111.23
1	B	166	PRO	CB-CA-C	-5.76	103.21	111.62
1	A	146	ARG	CD-NE-CZ	5.75	132.45	124.40
1	C	215	ILE	CB-CA-C	-5.75	101.87	111.29
1	C	85	LEU	CA-C-N	5.71	131.97	121.70
1	C	85	LEU	C-N-CA	5.71	131.97	121.70
1	A	180	PRO	CA-C-O	-5.70	114.91	121.86
1	C	156	SER	CB-CA-C	-5.70	103.53	110.08
1	A	81	LYS	N-CA-C	5.67	122.88	110.80
1	A	88	ILE	N-CA-C	-5.66	100.84	109.78
1	C	178	THR	CB-CA-C	-5.64	102.16	111.51
1	B	40	GLY	N-CA-C	5.62	119.40	111.42
1	A	274	GLN	N-CA-C	-5.62	101.73	110.10
1	B	75	LEU	N-CA-CB	5.62	118.62	109.69
1	A	255	GLU	CA-C-N	-5.61	113.24	121.99
1	A	255	GLU	C-N-CA	-5.61	113.24	121.99
1	A	308	GLU	CA-C-N	5.57	132.00	121.97
1	A	308	GLU	C-N-CA	5.57	132.00	121.97
1	C	65	SER	N-CA-C	-5.57	98.93	110.80
1	B	52	ILE	CB-CA-C	-5.55	103.60	111.38
1	A	284	VAL	N-CA-C	5.55	116.84	108.96
1	D	250	ILE	CB-CA-C	-5.55	103.61	111.38
1	B	39	ARG	CB-CA-C	5.54	120.24	109.33
1	D	322	GLY	N-CA-C	-5.53	97.26	113.30
1	A	245	TYR	CB-CA-C	-5.51	103.40	111.23
1	A	123	VAL	N-CA-C	5.50	117.11	109.29
1	A	186	ALA	N-CA-C	5.49	115.79	108.38
1	B	89	ASP	CA-C-N	5.48	127.52	120.89
1	B	89	ASP	C-N-CA	5.48	127.52	120.89
1	C	154	ILE	N-CA-C	5.46	120.70	109.34
1	A	96	ASP	N-CA-C	5.44	119.41	112.34
1	C	236	THR	N-CA-C	-5.44	104.89	112.45
1	C	146	ARG	CD-NE-CZ	5.40	131.96	124.40
1	B	65	SER	N-CA-C	-5.40	99.30	110.80
1	B	186	ALA	N-CA-C	5.37	115.64	108.38
1	A	88	ILE	CA-C-O	-5.37	116.21	121.58
1	B	58	VAL	CB-CA-C	-5.37	104.34	111.80
1	A	328	LYS	N-CA-C	5.36	117.62	109.63
1	D	36	GLU	N-CA-C	-5.35	101.74	109.29
1	A	284	VAL	CB-CA-C	-5.35	103.86	111.19
1	B	94	GLU	N-CA-C	5.33	116.78	111.07
1	D	178	THR	CB-CA-C	-5.33	102.66	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	GLU	N-CA-C	5.33	122.15	110.80
1	B	281	ASN	N-CA-C	5.31	122.11	110.80
1	A	268	ILE	CB-CA-C	-5.29	102.61	111.29
1	D	201	ASP	N-CA-C	-5.28	106.69	113.02
1	C	177	GLN	N-CA-CB	-5.26	102.91	110.65
1	B	245	TYR	CB-CA-C	-5.26	103.76	111.23
1	B	231	ASP	CA-C-N	-5.26	113.27	119.84
1	B	231	ASP	C-N-CA	-5.26	113.27	119.84
1	A	99	SER	N-CA-C	5.26	119.99	111.37
1	B	165	THR	N-CA-C	-5.26	101.19	108.76
1	B	41	ASN	CA-C-N	5.25	129.63	122.34
1	B	41	ASN	C-N-CA	5.25	129.63	122.34
1	B	53	GLU	N-CA-C	5.25	116.78	108.96
1	D	235	THR	N-CA-C	5.24	121.96	110.80
1	A	205	VAL	N-CA-CB	5.24	119.87	111.23
1	A	311	VAL	N-CA-C	5.24	125.66	111.00
1	B	126	GLN	N-CA-C	-5.24	107.44	113.88
1	A	219	ASN	N-CA-C	5.22	117.65	111.33
1	B	153	LYS	N-CA-C	5.22	117.47	109.07
1	C	85	LEU	N-CA-C	5.21	119.27	112.13
1	A	316	GLN	CB-CG-CD	5.20	121.44	112.60
1	D	65	SER	N-CA-C	-5.20	99.74	110.80
1	B	156	SER	N-CA-C	5.19	118.03	108.69
1	A	178	THR	CB-CA-C	-5.19	102.59	111.41
1	A	57	THR	CB-CA-C	-5.19	100.10	110.42
1	B	146	ARG	CD-NE-CZ	5.18	131.66	124.40
1	D	321	SER	N-CA-C	5.18	121.83	110.80
1	A	201	ASP	N-CA-C	-5.17	106.81	113.02
1	A	215	ILE	CB-CA-C	-5.17	102.81	111.29
1	A	77	GLN	N-CA-C	-5.16	101.75	109.95
1	B	99	SER	N-CA-C	5.16	119.88	111.37
1	C	260	ILE	CB-CA-C	5.16	115.97	110.91
1	A	177	GLN	N-CA-C	5.15	119.72	113.38
1	D	125	LYS	N-CA-C	-5.15	105.01	113.50
1	B	274	GLN	N-CA-C	-5.14	102.30	109.96
1	D	39	ARG	N-CA-C	5.14	115.60	108.00
1	B	323	LEU	CB-CG-CD1	-5.13	95.31	110.70
1	D	319	VAL	N-CA-C	5.13	120.00	109.34
1	A	275	ASN	N-CA-C	5.12	121.72	110.80
1	D	274	GLN	N-CA-C	-5.12	102.47	110.10
1	D	100	ALA	N-CA-C	5.09	118.75	112.54
1	C	100	ALA	N-CA-C	5.08	119.19	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	GLN	N-CA-C	-5.07	102.55	110.10
1	C	165	THR	CA-C-N	5.05	124.77	119.82
1	C	165	THR	C-N-CA	5.05	124.77	119.82
1	B	273	VAL	N-CA-CB	5.03	117.63	111.60
1	B	268	ILE	CB-CA-C	-5.01	103.07	111.29
1	D	177	GLN	N-CA-CB	-5.01	103.29	110.65
1	A	52	ILE	CB-CA-C	-5.00	104.59	111.49

There are no chirality outliers.

All (94) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	VAL	Peptide
1	A	153	LYS	Peptide
1	A	180	PRO	Peptide
1	A	181	THR	Peptide
1	A	188	LEU	Peptide
1	A	215	ILE	Peptide
1	A	230	VAL	Peptide
1	A	238	SER	Peptide
1	A	241	SER	Peptide
1	A	259	ARG	Peptide
1	A	280	PRO	Peptide
1	A	281	ASN	Peptide
1	A	308	GLU	Peptide
1	A	311	VAL	Peptide
1	A	312	GLN	Peptide
1	A	317	THR	Peptide
1	A	323	LEU	Peptide
1	A	37	VAL	Peptide
1	A	39	ARG	Peptide
1	A	56	ASN	Peptide
1	A	75	LEU	Peptide
1	A	85	LEU	Mainchain,Peptide
1	B	120	ASP	Peptide
1	B	123	VAL	Peptide
1	B	153	LYS	Peptide
1	B	166	PRO	Peptide
1	B	181	THR	Peptide
1	B	188	LEU	Peptide
1	B	230	VAL	Peptide
1	B	250	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	256	HIS	Peptide
1	B	259	ARG	Peptide
1	B	280	PRO	Peptide
1	B	281	ASN	Peptide
1	B	283	ALA	Peptide
1	B	284	VAL	Peptide
1	B	290	LYS	Peptide
1	B	292	VAL	Peptide
1	B	304	GLU	Peptide
1	B	307	ILE	Peptide
1	B	308	GLU	Peptide
1	B	311	VAL	Peptide
1	B	319	VAL	Peptide
1	B	322	GLY	Peptide
1	B	329	VAL	Peptide
1	B	45	ASN	Peptide
1	B	56	ASN	Peptide
1	C	120	ASP	Peptide
1	C	123	VAL	Peptide
1	C	153	LYS	Peptide
1	C	166	PRO	Peptide
1	C	181	THR	Peptide
1	C	188	LEU	Peptide
1	C	215	ILE	Peptide
1	C	230	VAL	Peptide
1	C	259	ARG	Peptide
1	C	280	PRO	Peptide
1	C	281	ASN	Peptide
1	C	282	LEU	Peptide
1	C	288	GLN	Peptide
1	C	306	GLU	Peptide
1	C	308	GLU	Peptide
1	C	311	VAL	Peptide
1	C	319	VAL	Peptide
1	C	320	LYS	Peptide
1	C	322	GLY	Peptide
1	C	45	ASN	Peptide
1	C	56	ASN	Peptide
1	C	87	GLU	Peptide
1	D	120	ASP	Peptide
1	D	123	VAL	Peptide
1	D	153	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	D	166	PRO	Peptide
1	D	181	THR	Peptide
1	D	188	LEU	Peptide
1	D	230	VAL	Peptide
1	D	256	HIS	Peptide
1	D	259	ARG	Peptide
1	D	280	PRO	Peptide
1	D	281	ASN	Peptide
1	D	288	GLN	Peptide
1	D	291	TYR	Peptide
1	D	308	GLU	Peptide
1	D	311	VAL	Peptide
1	D	318	GLU	Peptide
1	D	319	VAL	Peptide
1	D	322	GLY	Peptide
1	D	323	LEU	Peptide
1	D	326	GLY	Peptide
1	D	45	ASN	Peptide
1	D	47	VAL	Peptide
1	D	56	ASN	Peptide
1	D	87	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2108	0	2133	247	2
1	B	2191	0	2215	272	2
1	C	2135	0	2158	225	1
1	D	2134	0	2156	232	1
All	All	8568	0	8662	940	3

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 55.

All (940) 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:277:LEU:HB2	1:A:319:VAL:HB	1.29	1.15
1:A:67:LYS:NZ	1:A:68:ILE:O	1.89	1.05
1:C:67:LYS:NZ	1:C:68:ILE:O	1.89	1.05
1:D:67:LYS:NZ	1:D:68:ILE:O	1.89	1.05
1:D:197:ILE:HD11	1:D:202:ILE:HD13	1.42	1.01
1:B:57:THR:HA	1:B:186:ALA:HB2	1.43	1.00
1:A:57:THR:HA	1:A:186:ALA:HB2	1.43	0.99
1:B:311:VAL:HG22	1:B:312:GLN:HG3	1.45	0.96
1:A:195:PRO:O	1:A:197:ILE:N	1.97	0.96
1:D:85:LEU:H	1:D:86:ALA:HB2	1.31	0.96
1:B:67:LYS:NZ	1:B:68:ILE:O	1.99	0.95
1:A:201:ASP:OD2	1:A:201:ASP:N	1.94	0.95
1:C:57:THR:HA	1:C:186:ALA:HB2	1.45	0.95
1:C:85:LEU:H	1:C:86:ALA:HB2	1.32	0.95
1:D:57:THR:HA	1:D:186:ALA:HB2	1.46	0.94
1:B:201:ASP:OD2	1:B:201:ASP:N	2.00	0.93
1:C:197:ILE:HD11	1:C:202:ILE:HD13	1.48	0.93
1:B:168:SER:N	1:B:171:GLN:OE1	2.01	0.93
1:B:40:GLY:N	1:B:276:VAL:O	2.00	0.92
1:C:174:ASN:ND2	1:D:176:ASN:O	2.03	0.91
1:B:215:ILE:HD13	1:B:218:ASP:H	1.35	0.91
1:B:198:SER:OG	1:B:199:GLU:N	1.93	0.91
1:A:174:ASN:ND2	1:B:176:ASN:O	2.04	0.91
1:B:85:LEU:H	1:B:86:ALA:HB2	1.37	0.90
1:C:235:THR:HB	1:C:246:TYR:CE1	2.06	0.90
1:A:67:LYS:H	1:B:63:GLN:NE2	1.69	0.89
1:D:235:THR:HB	1:D:246:TYR:CE1	2.08	0.88
1:A:198:SER:OG	1:A:199:GLU:N	2.02	0.86
1:B:235:THR:HB	1:B:246:TYR:CE1	2.11	0.86
1:B:285:GLN:HB3	1:B:290:LYS:H	1.41	0.86
1:A:117:LEU:HD12	1:A:123:VAL:HG22	1.55	0.85
1:A:215:ILE:HD13	1:A:217:SER:H	1.41	0.85
1:C:201:ASP:OD2	1:C:201:ASP:N	2.08	0.85
1:D:201:ASP:OD2	1:D:201:ASP:N	2.10	0.85
1:A:235:THR:HB	1:A:246:TYR:CE1	2.12	0.84
1:D:215:ILE:HD13	1:D:218:ASP:H	1.43	0.83
1:B:68:ILE:HD12	1:B:69:THR:H	1.41	0.83
1:A:197:ILE:HD11	1:A:202:ILE:HD13	1.60	0.83
1:D:278:PHE:CE2	1:D:316:GLN:HB3	2.13	0.83
1:B:151:TYR:O	1:B:153:LYS:N	2.11	0.83
1:A:168:SER:N	1:A:171:GLN:OE1	2.12	0.82
1:B:197:ILE:HG13	1:B:198:SER:N	1.91	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ILE:HA	1:B:322:GLY:H	1.43	0.82
1:B:156:SER:O	1:B:156:SER:OG	1.94	0.82
1:B:117:LEU:HD12	1:B:123:VAL:HG22	1.60	0.81
1:D:282:LEU:HA	1:D:284:VAL:HG23	1.61	0.81
1:D:316:GLN:OE1	1:D:316:GLN:N	2.14	0.81
1:C:76:GLY:H	1:C:162:VAL:HB	1.46	0.81
1:D:164:SER:HB3	1:D:184:LYS:HB2	1.62	0.81
1:B:197:ILE:HD11	1:B:202:ILE:HD13	1.62	0.81
1:C:162:VAL:HA	1:C:185:VAL:HG22	1.63	0.81
1:C:151:TYR:O	1:C:153:LYS:N	2.13	0.81
1:B:178:THR:O	1:B:178:THR:OG1	1.94	0.80
1:D:281:ASN:O	1:D:283:ALA:N	2.15	0.80
1:A:197:ILE:HG13	1:A:198:SER:N	1.95	0.79
1:D:35:GLU:HG3	1:D:280:PRO:HG2	1.65	0.79
1:A:68:ILE:HD12	1:A:69:THR:H	1.46	0.79
1:A:86:ALA:CB	1:A:154:ILE:HB	2.13	0.79
1:C:92:THR:HG22	1:D:147:ILE:HG21	1.65	0.79
1:A:164:SER:HB3	1:A:184:LYS:HB2	1.65	0.78
1:B:195:PRO:O	1:B:197:ILE:N	2.16	0.78
1:D:317:THR:HG22	1:D:318:GLU:H	1.47	0.78
1:D:195:PRO:O	1:D:197:ILE:N	2.15	0.77
1:D:234:THR:O	1:D:236:THR:N	2.17	0.77
1:C:215:ILE:HD13	1:C:218:ASP:H	1.49	0.77
1:C:293:VAL:HG12	1:C:328:LYS:HB2	1.66	0.77
1:D:168:SER:N	1:D:171:GLN:OE1	2.16	0.77
1:D:198:SER:OG	1:D:199:GLU:N	2.14	0.77
1:A:35:GLU:HB2	1:A:280:PRO:HG2	1.66	0.77
1:A:215:ILE:HD13	1:A:218:ASP:H	1.48	0.77
1:A:311:VAL:HG22	1:A:312:GLN:H	1.50	0.77
1:B:164:SER:HB3	1:B:184:LYS:HB2	1.67	0.76
1:C:234:THR:O	1:C:234:THR:OG1	2.01	0.76
1:D:162:VAL:HA	1:D:185:VAL:HG22	1.67	0.76
1:C:195:PRO:O	1:C:197:ILE:N	2.16	0.76
1:A:91:ALA:HB1	1:B:147:ILE:HD11	1.68	0.76
1:C:198:SER:OG	1:C:199:GLU:N	2.17	0.76
1:B:86:ALA:CB	1:B:154:ILE:HB	2.16	0.76
1:C:93:TYR:CE1	1:C:148:ASN:HB3	2.20	0.76
1:A:309:ILE:HD11	1:A:319:VAL:HA	1.66	0.76
1:C:211:VAL:HG11	1:C:249:ILE:HD13	1.68	0.76
1:B:34:THR:HB	1:B:329:VAL:HG21	1.67	0.76
1:B:278:PHE:HE2	1:B:316:GLN:O	1.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ILE:HA	1:D:249:ILE:HG12	1.68	0.76
1:A:40:GLY:HA3	1:A:275:ASN:H	1.50	0.75
1:A:67:LYS:HG2	1:B:63:GLN:HE22	1.51	0.75
1:A:182:ILE:O	1:A:183:ILE:HD12	1.85	0.75
1:D:93:TYR:CE1	1:D:148:ASN:HB3	2.21	0.75
1:A:234:THR:O	1:A:234:THR:OG1	2.01	0.75
1:D:279:ILE:HG21	1:D:283:ALA:HB2	1.66	0.75
1:A:92:THR:HG22	1:B:147:ILE:HG21	1.68	0.75
1:B:211:VAL:HG11	1:B:249:ILE:HD13	1.67	0.75
1:D:66:GLY:O	1:D:88:ILE:HG23	1.87	0.75
1:B:278:PHE:CE2	1:B:316:GLN:HB3	2.21	0.75
1:C:197:ILE:HD13	1:C:205:VAL:HG21	1.69	0.75
1:A:85:LEU:H	1:A:86:ALA:HB2	1.51	0.74
1:B:277:LEU:O	1:B:319:VAL:HG13	1.86	0.74
1:B:281:ASN:HB2	1:B:315:PHE:O	1.87	0.74
1:C:235:THR:HG22	1:C:246:TYR:H	1.51	0.74
1:D:197:ILE:HD13	1:D:205:VAL:HG21	1.67	0.74
1:C:117:LEU:HD12	1:C:123:VAL:HG22	1.69	0.74
1:B:227:ILE:HA	1:B:249:ILE:HG12	1.70	0.74
1:B:235:THR:HG22	1:B:246:TYR:H	1.50	0.74
1:B:264:THR:OG1	1:B:266:ASN:ND2	2.21	0.74
1:C:57:THR:HA	1:C:186:ALA:CB	2.17	0.74
1:D:57:THR:HA	1:D:186:ALA:CB	2.18	0.74
1:D:165:THR:O	1:D:165:THR:OG1	1.99	0.74
1:B:199:GLU:OE1	1:B:243:VAL:HG21	1.87	0.73
1:B:57:THR:HA	1:B:186:ALA:CB	2.18	0.73
1:D:151:TYR:O	1:D:153:LYS:N	2.21	0.73
1:A:151:TYR:O	1:A:153:LYS:N	2.21	0.73
1:D:117:LEU:HD12	1:D:123:VAL:HG22	1.68	0.73
1:D:215:ILE:HD13	1:D:217:SER:H	1.52	0.73
1:D:156:SER:OG	1:D:156:SER:O	2.02	0.73
1:B:204:LYS:O	1:B:205:VAL:HG23	1.87	0.73
1:D:281:ASN:OD1	1:D:315:PHE:CG	2.42	0.73
1:B:182:ILE:O	1:B:183:ILE:HD12	1.88	0.73
1:A:277:LEU:O	1:A:319:VAL:N	2.17	0.72
1:A:93:TYR:CE1	1:A:148:ASN:HB3	2.25	0.72
1:A:75:LEU:HD13	1:A:75:LEU:H	1.52	0.72
1:B:162:VAL:HA	1:B:185:VAL:HG22	1.71	0.72
1:B:93:TYR:C	1:B:149:LEU:HD11	2.15	0.72
1:D:211:VAL:HG11	1:D:249:ILE:HD13	1.71	0.72
1:B:68:ILE:HA	1:B:88:ILE:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ILE:HG13	1:D:198:SER:N	2.01	0.71
1:A:57:THR:HA	1:A:186:ALA:CB	2.20	0.71
1:C:88:ILE:HD12	1:C:88:ILE:H	1.55	0.71
1:A:178:THR:O	1:A:180:PRO:HD3	1.90	0.71
1:C:164:SER:HB3	1:C:184:LYS:HB2	1.71	0.71
1:D:278:PHE:HE2	1:D:316:GLN:HB3	1.53	0.71
1:A:56:ASN:O	1:A:186:ALA:HB1	1.90	0.71
1:A:311:VAL:N	1:A:318:GLU:OE2	2.23	0.71
1:C:227:ILE:HA	1:C:249:ILE:HG12	1.73	0.71
1:A:162:VAL:HA	1:A:185:VAL:HG22	1.71	0.71
1:C:194:LYS:HB3	1:C:246:TYR:CE2	2.26	0.70
1:C:217:SER:OG	1:D:199:GLU:O	2.08	0.70
1:C:234:THR:O	1:C:236:THR:N	2.25	0.70
1:C:197:ILE:CD1	1:C:205:VAL:HG21	2.21	0.70
1:B:164:SER:OG	1:B:166:PRO:HD3	1.91	0.70
1:B:293:VAL:HG13	1:B:330:VAL:H	1.56	0.70
1:D:197:ILE:CD1	1:D:205:VAL:HG21	2.22	0.70
1:A:234:THR:O	1:A:236:THR:N	2.24	0.70
1:C:93:TYR:C	1:C:149:LEU:HD11	2.17	0.70
1:D:264:THR:OG1	1:D:266:ASN:ND2	2.24	0.70
1:A:199:GLU:OE1	1:A:243:VAL:HG21	1.92	0.69
1:A:204:LYS:O	1:A:205:VAL:HG23	1.92	0.69
1:C:168:SER:N	1:C:171:GLN:OE1	2.20	0.69
1:D:68:ILE:HA	1:D:88:ILE:HA	1.74	0.69
1:B:178:THR:O	1:B:180:PRO:HD3	1.92	0.69
1:D:93:TYR:C	1:D:149:LEU:HD11	2.17	0.69
1:A:93:TYR:C	1:A:149:LEU:HD11	2.17	0.69
1:D:283:ALA:O	1:D:291:TYR:HB2	1.91	0.69
1:C:90:PRO:HB3	1:C:152:THR:HG21	1.74	0.69
1:C:156:SER:O	1:C:156:SER:OG	2.08	0.69
1:B:215:ILE:HD13	1:B:217:SER:H	1.58	0.69
1:B:305:ARG:NH2	1:B:327:GLU:OE1	2.25	0.69
1:D:76:GLY:H	1:D:162:VAL:HB	1.58	0.69
1:A:309:ILE:CD1	1:A:320:LYS:H	2.05	0.69
1:D:194:LYS:HB3	1:D:246:TYR:CE2	2.27	0.69
1:C:264:THR:OG1	1:C:266:ASN:ND2	2.26	0.69
1:A:69:THR:OG1	1:A:87:GLU:O	2.09	0.69
1:B:76:GLY:H	1:B:162:VAL:HB	1.58	0.69
1:A:178:THR:O	1:A:178:THR:OG1	2.04	0.68
1:B:77:GLN:O	1:B:162:VAL:HG23	1.93	0.68
1:B:93:TYR:O	1:B:149:LEU:HD11	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ILE:HA	1:C:88:ILE:HA	1.75	0.68
1:C:197:ILE:HG13	1:C:198:SER:N	2.06	0.68
1:B:83:ASP:O	1:B:155:THR:HA	1.94	0.68
1:D:315:PHE:O	1:D:317:THR:N	2.26	0.68
1:C:91:ALA:HB1	1:D:147:ILE:HD11	1.74	0.68
1:A:107:THR:OG1	1:A:135:TYR:HA	1.94	0.68
1:A:213:PHE:CE2	1:A:223:TYR:HB2	2.29	0.68
1:A:67:LYS:N	1:B:63:GLN:NE2	2.41	0.68
1:D:85:LEU:N	1:D:86:ALA:HB2	2.06	0.68
1:D:60:VAL:CG2	1:D:183:ILE:HG22	2.24	0.68
1:B:90:PRO:HB3	1:B:152:THR:HG21	1.76	0.67
1:C:178:THR:O	1:C:178:THR:OG1	2.00	0.67
1:D:197:ILE:HD11	1:D:202:ILE:CD1	2.23	0.67
1:B:52:ILE:HG13	1:B:193:ILE:HG22	1.75	0.67
1:B:93:TYR:CE1	1:B:148:ASN:HB3	2.29	0.67
1:D:234:THR:O	1:D:234:THR:OG1	2.12	0.67
1:A:179:THR:HG22	1:A:180:PRO:O	1.93	0.67
1:A:194:LYS:HB3	1:A:246:TYR:CE2	2.29	0.67
1:C:85:LEU:N	1:C:86:ALA:HB2	2.07	0.67
1:D:227:ILE:HG13	1:D:249:ILE:HD11	1.77	0.67
1:A:260:ILE:HD12	1:B:232:PRO:O	1.95	0.67
1:A:278:PHE:HD2	1:A:317:THR:O	1.78	0.67
1:A:312:GLN:HA	1:A:317:THR:HG23	1.76	0.67
1:D:278:PHE:HE2	1:D:316:GLN:O	1.77	0.67
1:C:177:GLN:NE2	1:D:177:GLN:HE21	1.91	0.67
1:C:178:THR:O	1:C:180:PRO:HD3	1.94	0.67
1:C:293:VAL:HG11	1:C:305:ARG:HH12	1.59	0.66
1:C:52:ILE:CG1	1:C:193:ILE:HG22	2.24	0.66
1:B:68:ILE:HD12	1:B:69:THR:N	2.11	0.66
1:B:107:THR:OG1	1:B:135:TYR:HA	1.95	0.66
1:D:64:VAL:HG21	1:D:88:ILE:HG12	1.75	0.66
1:C:213:PHE:CE2	1:C:223:TYR:HB2	2.31	0.66
1:C:215:ILE:HD13	1:C:217:SER:H	1.60	0.66
1:A:175:SER:OG	1:A:176:ASN:N	2.24	0.66
1:B:234:THR:O	1:B:236:THR:N	2.29	0.66
1:D:281:ASN:OD1	1:D:315:PHE:CD2	2.49	0.66
1:B:197:ILE:CD1	1:B:205:VAL:HG21	2.25	0.66
1:B:283:ALA:O	1:B:291:TYR:HA	1.96	0.66
1:C:93:TYR:O	1:C:149:LEU:HD11	1.96	0.66
1:B:36:GLU:HG2	1:B:38:LYS:H	1.60	0.65
1:C:69:THR:OG1	1:C:87:GLU:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:N	1:B:239:ASP:OD2	2.29	0.65
1:C:67:LYS:HG2	1:D:63:GLN:HE22	1.60	0.65
1:A:83:ASP:O	1:A:155:THR:HA	1.96	0.65
1:A:227:ILE:HA	1:A:249:ILE:HG12	1.79	0.65
1:A:264:THR:OG1	1:A:266:ASN:ND2	2.28	0.65
1:A:266:ASN:N	1:A:266:ASN:OD1	2.27	0.65
1:A:235:THR:HG22	1:A:246:TYR:H	1.61	0.65
1:C:266:ASN:N	1:C:266:ASN:OD1	2.29	0.65
1:D:71:LEU:HB3	1:D:169:GLU:HG2	1.78	0.65
1:A:214:THR:OG1	1:A:215:ILE:N	2.27	0.65
1:A:278:PHE:HE2	1:A:316:GLN:O	1.80	0.65
1:B:213:PHE:CE2	1:B:223:TYR:HB2	2.32	0.65
1:C:278:PHE:HE2	1:C:316:GLN:HB3	1.61	0.65
1:D:179:THR:HG22	1:D:180:PRO:O	1.97	0.65
1:C:77:GLN:O	1:C:162:VAL:HG23	1.96	0.65
1:D:107:THR:OG1	1:D:135:TYR:HA	1.97	0.65
1:B:168:SER:O	1:B:170:GLY:N	2.29	0.65
1:A:173:VAL:CG2	1:A:174:ASN:N	2.60	0.64
1:B:135:TYR:HD2	1:B:136:LEU:HD13	1.61	0.64
1:C:165:THR:O	1:C:165:THR:OG1	2.12	0.64
1:D:235:THR:HG22	1:D:246:TYR:H	1.63	0.64
1:A:68:ILE:HA	1:A:88:ILE:HA	1.79	0.64
1:D:204:LYS:HB3	1:D:270:ILE:HD13	1.79	0.64
1:A:77:GLN:O	1:A:162:VAL:HG23	1.97	0.64
1:B:311:VAL:HG22	1:B:312:GLN:CG	2.23	0.64
1:B:278:PHE:HE2	1:B:316:GLN:HB3	1.61	0.64
1:C:66:GLY:O	1:C:88:ILE:HG23	1.97	0.64
1:A:38:LYS:HG2	1:A:277:LEU:HD23	1.78	0.64
1:B:163:ILE:HG22	1:B:164:SER:N	2.12	0.64
1:B:227:ILE:HG13	1:B:249:ILE:HD11	1.79	0.64
1:B:75:LEU:HB3	1:B:163:ILE:O	1.97	0.64
1:C:179:THR:HG22	1:C:180:PRO:O	1.97	0.64
1:C:259:ARG:HD3	1:D:245:TYR:HE1	1.62	0.64
1:A:281:ASN:HB2	1:A:315:PHE:O	1.97	0.63
1:B:266:ASN:OD1	1:B:266:ASN:N	2.31	0.63
1:C:93:TYR:HE1	1:C:148:ASN:HB3	1.61	0.63
1:A:52:ILE:CG1	1:A:193:ILE:HG22	2.29	0.63
1:A:147:ILE:HG22	1:A:148:ASN:OD1	1.99	0.63
1:C:204:LYS:HB3	1:C:270:ILE:HD13	1.81	0.63
1:A:64:VAL:HG23	1:A:65:SER:O	1.97	0.63
1:B:174:ASN:OD1	1:B:174:ASN:C	2.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:OE2	1:B:326:GLY:N	2.27	0.63
1:D:90:PRO:HB3	1:D:152:THR:HG21	1.80	0.63
1:D:317:THR:HG22	1:D:318:GLU:N	2.12	0.63
1:D:278:PHE:CE2	1:D:316:GLN:O	2.52	0.63
1:C:52:ILE:HG12	1:C:193:ILE:HG22	1.80	0.63
1:C:60:VAL:CG2	1:C:183:ILE:HG22	2.28	0.63
1:A:64:VAL:HG23	1:A:65:SER:N	2.14	0.63
1:C:313:ASN:HB3	1:C:314:ASP:HA	1.79	0.63
1:B:69:THR:OG1	1:B:87:GLU:O	2.15	0.63
1:B:72:TYR:N	1:B:85:LEU:O	2.29	0.63
1:C:87:GLU:HG3	1:C:153:LYS:HG3	1.80	0.63
1:A:197:ILE:HD13	1:A:205:VAL:HG21	1.81	0.62
1:B:52:ILE:CG1	1:B:193:ILE:HG22	2.29	0.62
1:D:178:THR:O	1:D:180:PRO:HD3	1.99	0.62
1:B:44:LYS:HD3	1:B:313:ASN:ND2	2.14	0.62
1:C:68:ILE:HD12	1:C:69:THR:H	1.64	0.62
1:C:71:LEU:HB3	1:C:169:GLU:HG2	1.81	0.62
1:D:178:THR:O	1:D:178:THR:OG1	2.06	0.62
1:B:39:ARG:HB3	1:B:275:ASN:C	2.23	0.62
1:B:194:LYS:HB3	1:B:246:TYR:CE2	2.33	0.62
1:D:52:ILE:CG1	1:D:193:ILE:HG22	2.29	0.62
1:A:68:ILE:HD12	1:A:69:THR:N	2.13	0.62
1:B:46:VAL:HG12	1:B:47:VAL:H	1.64	0.62
1:B:85:LEU:N	1:B:86:ALA:HB2	2.12	0.62
1:D:56:ASN:O	1:D:186:ALA:HB1	2.00	0.62
1:D:93:TYR:HE1	1:D:148:ASN:HB3	1.63	0.62
1:C:204:LYS:O	1:C:205:VAL:HG23	2.00	0.62
1:C:64:VAL:O	1:C:175:SER:HB3	2.00	0.62
1:D:199:GLU:OE1	1:D:243:VAL:HG21	1.98	0.62
1:D:213:PHE:CE2	1:D:223:TYR:HB2	2.35	0.62
1:A:309:ILE:HD13	1:A:320:LYS:H	1.63	0.61
1:C:86:ALA:CB	1:C:154:ILE:HB	2.30	0.61
1:C:111:ALA:HB2	1:C:131:ALA:HB1	1.82	0.61
1:C:199:GLU:OE1	1:C:243:VAL:HG21	1.99	0.61
1:C:227:ILE:HG13	1:C:249:ILE:HD11	1.81	0.61
1:A:52:ILE:HG13	1:A:193:ILE:HG22	1.82	0.61
1:B:81:LYS:O	1:B:83:ASP:N	2.33	0.61
1:B:71:LEU:HB3	1:B:169:GLU:HG2	1.83	0.61
1:D:68:ILE:HD12	1:D:69:THR:H	1.65	0.61
1:A:107:THR:HG1	1:A:135:TYR:HA	1.65	0.61
1:C:171:GLN:O	1:C:173:VAL:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:VAL:HG11	1:D:157:PRO:HD2	1.83	0.61
1:A:45:ASN:HD22	1:A:267:ASN:HB2	1.65	0.61
1:D:88:ILE:HD12	1:D:88:ILE:H	1.66	0.61
1:A:86:ALA:HB1	1:A:154:ILE:HB	1.83	0.61
1:D:69:THR:OG1	1:D:87:GLU:O	2.18	0.61
1:A:93:TYR:HE1	1:A:148:ASN:HB3	1.65	0.60
1:B:308:GLU:O	1:B:320:LYS:N	2.26	0.60
1:C:45:ASN:HD22	1:C:267:ASN:HB2	1.66	0.60
1:D:278:PHE:CZ	1:D:316:GLN:HB3	2.36	0.60
1:A:87:GLU:HG3	1:A:153:LYS:HG3	1.83	0.60
1:C:64:VAL:HG21	1:C:88:ILE:HG12	1.82	0.60
1:D:83:ASP:O	1:D:155:THR:HA	2.01	0.60
1:A:109:GLU:OE2	1:B:125:LYS:NZ	2.29	0.60
1:B:285:GLN:HG2	1:B:289:ASP:HA	1.84	0.60
1:A:310:GLY:O	1:A:320:LYS:HE3	2.01	0.60
1:B:278:PHE:CZ	1:B:316:GLN:HB3	2.37	0.60
1:B:327:GLU:O	1:B:329:VAL:HG22	1.99	0.60
1:C:305:ARG:O	1:C:305:ARG:NH1	2.34	0.60
1:B:34:THR:O	1:B:329:VAL:HG21	2.01	0.60
1:C:60:VAL:HG11	1:C:157:PRO:HD2	1.83	0.60
1:D:64:VAL:O	1:D:175:SER:HB3	2.02	0.60
1:D:93:TYR:O	1:D:149:LEU:HD11	2.00	0.60
1:B:135:TYR:CD2	1:B:136:LEU:HD13	2.37	0.60
1:D:204:LYS:O	1:D:205:VAL:HG23	2.02	0.60
1:D:311:VAL:N	1:D:318:GLU:OE1	2.34	0.60
1:A:66:GLY:O	1:A:88:ILE:HG23	2.02	0.60
1:A:178:THR:O	1:A:179:THR:C	2.43	0.60
1:A:278:PHE:CE2	1:A:316:GLN:HB3	2.36	0.60
1:D:277:LEU:HB2	1:D:319:VAL:HG11	1.83	0.60
1:A:93:TYR:O	1:A:149:LEU:HD11	2.01	0.59
1:A:46:VAL:HG12	1:A:47:VAL:H	1.66	0.59
1:A:211:VAL:HG11	1:A:249:ILE:HD13	1.83	0.59
1:C:191:MSE:HE1	1:C:260:ILE:HG22	1.84	0.59
1:A:47:VAL:HG22	1:A:267:ASN:HB3	1.85	0.59
1:C:107:THR:OG1	1:C:135:TYR:HA	2.03	0.59
1:C:163:ILE:HG22	1:C:164:SER:N	2.18	0.59
1:D:86:ALA:CB	1:D:154:ILE:HB	2.32	0.59
1:B:165:THR:O	1:B:165:THR:OG1	2.08	0.59
1:D:34:THR:OG1	1:D:326:GLY:O	2.19	0.59
1:A:53:GLU:O	1:A:191:MSE:HB3	2.02	0.59
1:A:60:VAL:CG2	1:A:183:ILE:HG22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLN:O	1:D:162:VAL:HG23	2.03	0.59
1:C:56:ASN:O	1:C:186:ALA:HB1	2.03	0.59
1:D:52:ILE:HG12	1:D:193:ILE:HG22	1.83	0.59
1:B:64:VAL:O	1:B:175:SER:HB3	2.03	0.59
1:A:197:ILE:CD1	1:A:205:VAL:HG21	2.32	0.58
1:B:47:VAL:HG22	1:B:267:ASN:HB3	1.84	0.58
1:B:293:VAL:HA	1:B:330:VAL:HG22	1.85	0.58
1:C:83:ASP:O	1:C:155:THR:HA	2.03	0.58
1:A:47:VAL:CG2	1:A:267:ASN:HB3	2.33	0.58
1:D:36:GLU:OE1	1:D:38:LYS:NZ	2.33	0.58
1:D:182:ILE:O	1:D:183:ILE:HD12	2.03	0.58
1:D:111:ALA:HB2	1:D:131:ALA:HB1	1.86	0.58
1:A:308:GLU:C	1:A:309:ILE:HG23	2.28	0.58
1:A:278:PHE:CE2	1:A:316:GLN:O	2.57	0.58
1:B:39:ARG:HB3	1:B:275:ASN:O	2.03	0.58
1:B:325:GLU:O	1:B:327:GLU:N	2.30	0.58
1:A:173:VAL:HG23	1:A:174:ASN:N	2.19	0.58
1:B:86:ALA:HB1	1:B:154:ILE:HB	1.85	0.58
1:A:71:LEU:HB3	1:A:169:GLU:HG2	1.86	0.58
1:A:181:THR:OG1	1:A:182:ILE:N	2.35	0.57
1:B:173:VAL:CG2	1:B:174:ASN:N	2.67	0.57
1:C:231:ASP:HB3	1:C:233:ALA:H	1.69	0.57
1:D:277:LEU:HB2	1:D:319:VAL:CG1	2.33	0.57
1:B:277:LEU:HB2	1:B:319:VAL:CG2	2.33	0.57
1:C:281:ASN:HD22	1:C:282:LEU:HG	1.67	0.57
1:C:281:ASN:OD1	1:C:315:PHE:O	2.22	0.57
1:D:191:MSE:HE1	1:D:260:ILE:HG22	1.86	0.57
1:B:215:ILE:CD1	1:B:218:ASP:H	2.15	0.57
1:C:194:LYS:HB3	1:C:246:TYR:CD2	2.39	0.57
1:B:279:ILE:HG13	1:B:319:VAL:HG12	1.87	0.57
1:C:67:LYS:H	1:D:63:GLN:NE2	2.02	0.57
1:D:34:THR:HG21	1:D:328:LYS:O	2.04	0.57
1:A:39:ARG:O	1:A:275:ASN:HA	2.04	0.57
1:C:76:GLY:N	1:C:162:VAL:HB	2.18	0.57
1:D:45:ASN:HD22	1:D:267:ASN:HB2	1.70	0.57
1:D:163:ILE:HG22	1:D:164:SER:N	2.18	0.57
1:B:36:GLU:HG2	1:B:38:LYS:N	2.20	0.57
1:B:173:VAL:HG23	1:B:180:PRO:HG2	1.87	0.57
1:D:68:ILE:HD11	1:D:169:GLU:HA	1.87	0.56
1:B:147:ILE:O	1:B:150:ARG:N	2.39	0.56
1:C:235:THR:HB	1:C:246:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PHE:CE2	1:B:316:GLN:O	2.55	0.56
1:A:46:VAL:O	1:A:268:ILE:HG12	2.05	0.56
1:A:60:VAL:HG11	1:A:157:PRO:HD2	1.88	0.56
1:C:168:SER:O	1:C:170:GLY:N	2.38	0.56
1:C:305:ARG:NH2	1:C:327:GLU:HG2	2.19	0.56
1:A:90:PRO:HB3	1:A:152:THR:HG21	1.85	0.56
1:B:312:GLN:HA	1:B:317:THR:HA	1.87	0.56
1:C:147:ILE:HG22	1:C:148:ASN:OD1	2.05	0.56
1:A:177:GLN:NE2	1:B:177:GLN:HE21	2.03	0.56
1:B:64:VAL:HG23	1:B:65:SER:O	2.06	0.56
1:C:173:VAL:CG2	1:C:174:ASN:N	2.69	0.56
1:D:173:VAL:CG2	1:D:174:ASN:N	2.69	0.56
1:D:266:ASN:OD1	1:D:266:ASN:N	2.39	0.56
1:C:311:VAL:H	1:C:318:GLU:HG2	1.71	0.56
1:A:60:VAL:O	1:A:182:ILE:HB	2.06	0.56
1:A:199:GLU:O	1:A:199:GLU:HG2	2.05	0.56
1:A:40:GLY:CA	1:A:275:ASN:H	2.19	0.55
1:A:86:ALA:HB2	1:A:154:ILE:HB	1.88	0.55
1:A:156:SER:O	1:A:156:SER:OG	2.23	0.55
1:A:135:TYR:HD2	1:A:136:LEU:HD13	1.71	0.55
1:B:47:VAL:CG2	1:B:267:ASN:HB3	2.37	0.55
1:D:108:GLN:HG3	1:D:135:TYR:HE1	1.70	0.55
1:A:204:LYS:HB3	1:A:270:ILE:HD13	1.87	0.55
1:D:64:VAL:HG23	1:D:65:SER:N	2.21	0.55
1:D:87:GLU:HG3	1:D:153:LYS:HG3	1.86	0.55
1:D:231:ASP:HB3	1:D:233:ALA:H	1.71	0.55
1:B:82:GLY:O	1:B:155:THR:OG1	2.18	0.55
1:B:179:THR:HG22	1:B:180:PRO:O	2.06	0.55
1:C:228:ASP:OD2	1:C:229:SER:OG	2.23	0.55
1:C:260:ILE:HD12	1:D:232:PRO:O	2.06	0.55
1:D:244:TYR:O	1:D:245:TYR:HD2	1.90	0.55
1:A:313:ASN:HA	1:A:314:ASP:C	2.30	0.55
1:D:47:VAL:HG22	1:D:267:ASN:HB3	1.88	0.55
1:A:163:ILE:HG22	1:A:164:SER:N	2.22	0.55
1:B:93:TYR:HE1	1:B:148:ASN:HB3	1.68	0.55
1:D:281:ASN:C	1:D:281:ASN:HD22	2.15	0.55
1:A:162:VAL:HA	1:A:185:VAL:CG2	2.37	0.55
1:C:47:VAL:HG22	1:C:267:ASN:HB3	1.88	0.55
1:C:46:VAL:HG12	1:C:47:VAL:H	1.71	0.55
1:D:282:LEU:HD12	1:D:282:LEU:H	1.71	0.55
1:B:199:GLU:HB2	1:B:243:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:TYR:C	1:B:245:TYR:HD2	2.15	0.54
1:A:168:SER:O	1:A:170:GLY:N	2.39	0.54
1:B:56:ASN:O	1:B:186:ALA:HB1	2.06	0.54
1:B:214:THR:OG1	1:B:215:ILE:N	2.37	0.54
1:A:67:LYS:N	1:B:63:GLN:HE21	2.04	0.54
1:A:227:ILE:HG13	1:A:249:ILE:HD11	1.90	0.54
1:B:111:ALA:HB2	1:B:131:ALA:HB1	1.89	0.54
1:D:194:LYS:HB3	1:D:246:TYR:CD2	2.42	0.54
1:A:259:ARG:HB2	1:A:262:MSE:HE3	1.87	0.54
1:C:177:GLN:CD	1:D:177:GLN:HE21	2.14	0.54
1:D:199:GLU:HB2	1:D:243:VAL:HG23	1.89	0.54
1:B:209:GLN:H	1:B:227:ILE:HG22	1.72	0.54
1:D:64:VAL:HG23	1:D:65:SER:O	2.07	0.54
1:B:184:LYS:O	1:B:185:VAL:HG23	2.07	0.54
1:D:37:VAL:HG23	1:D:325:GLU:HA	1.90	0.54
1:D:50:GLY:HA2	1:D:195:PRO:HA	1.90	0.54
1:B:102:ALA:O	1:B:105:ALA:N	2.40	0.54
1:D:167:VAL:HA	1:D:171:GLN:OE1	2.08	0.54
1:C:108:GLN:HG3	1:C:135:TYR:HE1	1.73	0.54
1:A:167:VAL:HA	1:A:171:GLN:OE1	2.07	0.54
1:A:228:ASP:OD2	1:A:229:SER:OG	2.26	0.54
1:A:135:TYR:CD2	1:A:136:LEU:HD13	2.43	0.54
1:D:214:THR:OG1	1:D:215:ILE:N	2.40	0.54
1:A:111:ALA:HB2	1:A:131:ALA:HB1	1.89	0.53
1:C:64:VAL:HG23	1:C:65:SER:O	2.08	0.53
1:B:60:VAL:HG22	1:B:183:ILE:O	2.08	0.53
1:C:211:VAL:HG23	1:C:268:ILE:HG23	1.90	0.53
1:D:178:THR:O	1:D:179:THR:C	2.50	0.53
1:A:309:ILE:C	1:A:309:ILE:HD12	2.33	0.53
1:B:165:THR:N	1:B:166:PRO:HD3	2.22	0.53
1:B:281:ASN:HD22	1:B:282:LEU:HG	1.73	0.53
1:D:168:SER:O	1:D:170:GLY:N	2.40	0.53
1:B:292:VAL:HG22	1:B:293:VAL:O	2.09	0.53
1:A:38:LYS:CG	1:A:277:LEU:HD23	2.39	0.53
1:C:50:GLY:HA2	1:C:195:PRO:HA	1.91	0.53
1:D:162:VAL:HA	1:D:185:VAL:CG2	2.39	0.53
1:B:194:LYS:HB3	1:B:246:TYR:CD2	2.44	0.53
1:C:167:VAL:HA	1:C:171:GLN:OE1	2.09	0.53
1:D:147:ILE:HG22	1:D:148:ASN:OD1	2.09	0.53
1:A:184:LYS:O	1:A:185:VAL:HG23	2.09	0.53
1:B:191:MSE:HE1	1:B:260:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:HG23	1:B:268:ILE:HG23	1.89	0.53
1:D:61:GLY:HA3	1:D:182:ILE:HD12	1.91	0.53
1:B:237:ILE:C	1:B:238:SER:O	2.49	0.53
1:B:244:TYR:O	1:B:245:TYR:HD2	1.91	0.53
1:D:228:ASP:OD2	1:D:229:SER:OG	2.25	0.53
1:B:164:SER:OG	1:B:165:THR:N	2.42	0.53
1:C:281:ASN:HD21	1:C:284:VAL:CG2	2.21	0.53
1:A:192:ARG:HA	1:A:250:ILE:HA	1.90	0.52
1:B:228:ASP:OD2	1:B:229:SER:OG	2.26	0.52
1:D:279:ILE:HG22	1:D:279:ILE:O	2.08	0.52
1:A:147:ILE:O	1:A:150:ARG:N	2.42	0.52
1:C:184:LYS:O	1:C:185:VAL:HG23	2.09	0.52
1:D:47:VAL:CG2	1:D:267:ASN:HB3	2.39	0.52
1:B:277:LEU:C	1:B:319:VAL:HG13	2.34	0.52
1:A:88:ILE:HD12	1:A:88:ILE:H	1.74	0.52
1:A:77:GLN:H	1:A:162:VAL:CG2	2.23	0.52
1:B:270:ILE:HD12	1:B:270:ILE:O	2.09	0.52
1:C:117:LEU:CD1	1:C:123:VAL:HG22	2.39	0.52
1:A:281:ASN:HD22	1:A:282:LEU:HG	1.75	0.52
1:B:175:SER:OG	1:B:176:ASN:N	2.40	0.52
1:C:64:VAL:HG23	1:C:65:SER:N	2.23	0.52
1:A:165:THR:N	1:A:166:PRO:HD3	2.24	0.52
1:C:117:LEU:N	1:C:117:LEU:HD23	2.25	0.52
1:A:198:SER:HB2	1:A:244:TYR:CD1	2.45	0.52
1:A:278:PHE:HE2	1:A:316:GLN:HB3	1.75	0.52
1:B:107:THR:HG1	1:B:135:TYR:HA	1.73	0.52
1:C:289:ASP:N	1:C:289:ASP:OD1	2.42	0.52
1:D:190:LYS:HA	1:D:252:GLU:HA	1.92	0.52
1:D:57:THR:O	1:D:57:THR:OG1	2.12	0.52
1:B:60:VAL:HG11	1:B:157:PRO:HD2	1.92	0.52
1:A:117:LEU:HD23	1:A:117:LEU:N	2.25	0.51
1:B:87:GLU:HG3	1:B:153:LYS:HG3	1.91	0.51
1:D:93:TYR:HB3	1:D:149:LEU:CD1	2.39	0.51
1:C:85:LEU:HD23	1:C:155:THR:N	2.26	0.51
1:D:46:VAL:HG12	1:D:47:VAL:H	1.75	0.51
1:B:46:VAL:O	1:B:268:ILE:HG12	2.10	0.51
1:B:102:ALA:O	1:B:104:LEU:N	2.44	0.51
1:B:293:VAL:HG23	1:B:304:GLU:HA	1.91	0.51
1:C:52:ILE:HG13	1:C:193:ILE:HG22	1.91	0.51
1:A:55:ILE:HG23	1:A:56:ASN:H	1.75	0.51
1:B:195:PRO:O	1:B:197:ILE:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLU:O	1:B:199:GLU:HG2	2.10	0.51
1:C:244:TYR:O	1:C:245:TYR:HD2	1.93	0.51
1:C:316:GLN:H	1:C:316:GLN:CD	2.15	0.51
1:D:235:THR:HB	1:D:246:TYR:CD1	2.44	0.51
1:A:211:VAL:HG22	1:A:212:THR:N	2.26	0.51
1:C:93:TYR:CD1	1:C:148:ASN:HB3	2.45	0.51
1:A:64:VAL:O	1:A:175:SER:HB3	2.11	0.51
1:A:147:ILE:HG22	1:A:148:ASN:N	2.26	0.51
1:B:64:VAL:HG23	1:B:65:SER:N	2.23	0.51
1:C:47:VAL:CG2	1:C:267:ASN:HB3	2.41	0.51
1:C:97:TYR:OH	1:C:146:ARG:NH1	2.43	0.51
1:A:61:GLY:HA3	1:A:182:ILE:HD12	1.93	0.51
1:B:64:VAL:HG21	1:B:88:ILE:HG12	1.93	0.51
1:B:323:LEU:HD21	1:B:327:GLU:HB2	1.93	0.51
1:A:231:ASP:HB3	1:A:233:ALA:H	1.75	0.51
1:A:244:TYR:O	1:A:245:TYR:HD2	1.94	0.51
1:C:46:VAL:O	1:C:268:ILE:HG12	2.10	0.51
1:C:147:ILE:O	1:C:150:ARG:N	2.44	0.51
1:D:282:LEU:C	1:D:284:VAL:H	2.18	0.51
1:B:66:GLY:O	1:B:88:ILE:HG23	2.10	0.51
1:B:282:LEU:HA	1:B:284:VAL:HG13	1.93	0.51
1:C:214:THR:OG1	1:C:215:ILE:N	2.43	0.51
1:D:37:VAL:HG21	1:D:324:THR:O	2.11	0.51
1:D:135:TYR:CD2	1:D:136:LEU:HD13	2.46	0.51
1:D:171:GLN:O	1:D:173:VAL:HG12	2.10	0.51
1:D:277:LEU:HD12	1:D:321:SER:OG	2.11	0.51
1:B:52:ILE:HG12	1:B:53:GLU:H	1.76	0.50
1:D:76:GLY:N	1:D:162:VAL:HB	2.24	0.50
1:D:164:SER:OG	1:D:166:PRO:HD3	2.10	0.50
1:A:190:LYS:HA	1:A:252:GLU:HA	1.92	0.50
1:A:195:PRO:C	1:A:197:ILE:N	2.69	0.50
1:A:177:GLN:CD	1:B:177:GLN:HE21	2.20	0.50
1:B:57:THR:O	1:B:58:VAL:HG13	2.11	0.50
1:B:231:ASP:HB3	1:B:233:ALA:H	1.77	0.50
1:B:259:ARG:HB2	1:B:262:MSE:HE3	1.92	0.50
1:C:151:TYR:O	1:C:152:THR:C	2.54	0.50
1:D:93:TYR:HB3	1:D:149:LEU:HD12	1.92	0.50
1:D:281:ASN:HD22	1:D:282:LEU:HA	1.75	0.50
1:A:74:LYS:HB2	1:A:75:LEU:HD13	1.94	0.50
1:B:117:LEU:CD1	1:B:123:VAL:HG22	2.35	0.50
1:B:151:TYR:O	1:B:152:THR:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HA	1:B:252:GLU:HA	1.94	0.50
1:B:305:ARG:HH12	1:B:327:GLU:CD	2.19	0.50
1:A:117:LEU:CD1	1:A:123:VAL:HG22	2.35	0.50
1:C:81:LYS:O	1:C:83:ASP:N	2.44	0.50
1:A:244:TYR:C	1:A:245:TYR:HD2	2.20	0.50
1:B:60:VAL:O	1:B:182:ILE:HB	2.11	0.49
1:B:293:VAL:HG13	1:B:328:LYS:O	2.12	0.49
1:D:82:GLY:O	1:D:155:THR:OG1	2.27	0.49
1:A:206:LYS:O	1:A:227:ILE:HG21	2.11	0.49
1:B:93:TYR:HB3	1:B:149:LEU:CD1	2.42	0.49
1:B:234:THR:O	1:B:234:THR:OG1	2.29	0.49
1:C:60:VAL:O	1:C:182:ILE:HB	2.11	0.49
1:C:93:TYR:HB3	1:C:149:LEU:HD12	1.94	0.49
1:A:194:LYS:HB3	1:A:246:TYR:CD2	2.46	0.49
1:B:322:GLY:HA2	1:B:323:LEU:HB2	1.94	0.49
1:D:46:VAL:O	1:D:268:ILE:HG12	2.13	0.49
1:B:197:ILE:HD11	1:B:202:ILE:CD1	2.38	0.49
1:B:285:GLN:CG	1:B:289:ASP:HA	2.41	0.49
1:A:106:SER:OG	1:A:107:THR:N	2.45	0.49
1:C:88:ILE:H	1:C:88:ILE:CD1	2.24	0.49
1:C:322:GLY:CA	1:C:323:LEU:HB2	2.43	0.49
1:D:68:ILE:HD12	1:D:69:THR:N	2.26	0.49
1:D:318:GLU:HG2	1:D:319:VAL:H	1.77	0.49
1:A:67:LYS:HZ3	1:A:67:LYS:HB2	1.78	0.49
1:A:164:SER:OG	1:A:166:PRO:HD3	2.12	0.49
1:B:181:THR:OG1	1:B:182:ILE:N	2.44	0.49
1:A:311:VAL:HG13	1:A:313:ASN:OD1	2.12	0.49
1:B:174:ASN:OD1	1:B:175:SER:O	2.30	0.49
1:C:68:ILE:HD11	1:C:169:GLU:HA	1.94	0.49
1:C:135:TYR:CD2	1:C:136:LEU:HD13	2.48	0.49
1:D:316:GLN:H	1:D:316:GLN:CD	2.17	0.49
1:A:68:ILE:HD11	1:A:169:GLU:HA	1.94	0.48
1:B:76:GLY:N	1:B:162:VAL:HB	2.25	0.48
1:C:102:ALA:O	1:C:105:ALA:N	2.46	0.48
1:A:93:TYR:HB3	1:A:149:LEU:HD12	1.95	0.48
1:A:250:ILE:HD13	1:A:250:ILE:H	1.78	0.48
1:A:174:ASN:OD1	1:A:174:ASN:C	2.57	0.48
1:A:239:ASP:OD2	1:A:239:ASP:N	2.36	0.48
1:B:293:VAL:CG2	1:B:304:GLU:HA	2.43	0.48
1:B:293:VAL:HG22	1:B:328:LYS:O	2.13	0.48
1:C:244:TYR:C	1:C:245:TYR:HD2	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:GLN:HB2	1:D:289:ASP:HB2	1.95	0.48
1:B:147:ILE:HG22	1:B:148:ASN:OD1	2.13	0.48
1:C:68:ILE:HD12	1:C:69:THR:N	2.27	0.48
1:D:215:ILE:HD13	1:D:218:ASP:N	2.22	0.48
1:D:192:ARG:HA	1:D:250:ILE:HA	1.95	0.48
1:A:278:PHE:CZ	1:A:316:GLN:HB3	2.49	0.48
1:B:117:LEU:N	1:B:117:LEU:HD23	2.28	0.48
1:B:197:ILE:HD13	1:B:205:VAL:HG21	1.92	0.48
1:C:61:GLY:HA3	1:C:182:ILE:HD12	1.95	0.48
1:C:309:ILE:O	1:C:320:LYS:NZ	2.42	0.48
1:C:281:ASN:ND2	1:C:284:VAL:CG2	2.77	0.48
1:A:199:GLU:HB2	1:A:243:VAL:HG23	1.96	0.48
1:A:215:ILE:CD1	1:A:218:ASP:H	2.23	0.48
1:A:256:HIS:O	1:A:258:LEU:O	2.32	0.48
1:C:270:ILE:HD12	1:C:270:ILE:O	2.13	0.48
1:A:81:LYS:NZ	1:A:82:GLY:H	2.12	0.48
1:A:279:ILE:HG22	1:A:279:ILE:O	2.13	0.48
1:B:155:THR:O	1:B:157:PRO:HD3	2.14	0.48
1:C:330:VAL:O	1:C:331:ILE:HG23	2.14	0.48
1:A:88:ILE:HD12	1:A:88:ILE:N	2.29	0.48
1:C:192:ARG:HA	1:C:250:ILE:HA	1.95	0.48
1:D:77:GLN:H	1:D:162:VAL:CG2	2.27	0.48
1:A:93:TYR:HB3	1:A:149:LEU:CD1	2.44	0.47
1:A:174:ASN:OD1	1:A:174:ASN:O	2.31	0.47
1:B:313:ASN:HA	1:B:314:ASP:HA	1.66	0.47
1:C:77:GLN:H	1:C:162:VAL:CG2	2.27	0.47
1:A:86:ALA:HB1	1:A:154:ILE:CB	2.42	0.47
1:A:171:GLN:O	1:A:173:VAL:HG12	2.14	0.47
1:C:83:ASP:O	1:C:85:LEU:HD22	2.13	0.47
1:C:93:TYR:HB3	1:C:149:LEU:CD1	2.44	0.47
1:D:277:LEU:O	1:D:319:VAL:HG22	2.15	0.47
1:A:208:GLY:N	1:A:227:ILE:HG22	2.29	0.47
1:A:259:ARG:HB3	1:A:260:ILE:H	1.61	0.47
1:D:60:VAL:O	1:D:182:ILE:HB	2.14	0.47
1:A:102:ALA:O	1:A:105:ALA:N	2.47	0.47
1:B:238:SER:O	1:B:239:ASP:C	2.56	0.47
1:C:235:THR:CG2	1:C:246:TYR:H	2.21	0.47
1:D:184:LYS:O	1:D:185:VAL:HG23	2.14	0.47
1:A:108:GLN:HG3	1:A:135:TYR:HE1	1.79	0.47
1:A:211:VAL:HG23	1:A:268:ILE:HG23	1.95	0.47
1:A:282:LEU:HD12	1:A:282:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HA	1:B:171:GLN:OE1	2.14	0.47
1:C:92:THR:CG2	1:D:147:ILE:HG21	2.40	0.47
1:D:165:THR:N	1:D:166:PRO:HD3	2.30	0.47
1:D:174:ASN:OD1	1:D:174:ASN:C	2.57	0.47
1:A:270:ILE:HD12	1:A:270:ILE:O	2.15	0.47
1:B:70:LYS:O	1:B:86:ALA:O	2.33	0.47
1:C:162:VAL:HA	1:C:185:VAL:CG2	2.38	0.47
1:D:173:VAL:HG23	1:D:180:PRO:HG2	1.95	0.47
1:D:211:VAL:HG23	1:D:268:ILE:HG23	1.96	0.47
1:D:234:THR:OG1	1:D:236:THR:OG1	2.32	0.47
1:B:325:GLU:CD	1:B:326:GLY:H	2.21	0.47
1:A:215:ILE:HB	1:A:216:LEU:H	1.30	0.47
1:B:108:GLN:HG3	1:B:135:TYR:HE1	1.80	0.47
1:B:310:GLY:HA2	1:B:311:VAL:HA	1.60	0.47
1:C:259:ARG:CD	1:D:245:TYR:HE1	2.28	0.47
1:D:46:VAL:O	1:D:267:ASN:HA	2.15	0.47
1:D:85:LEU:HD23	1:D:155:THR:N	2.30	0.47
1:D:244:TYR:C	1:D:245:TYR:HD2	2.23	0.47
1:A:235:THR:HB	1:A:246:TYR:CD1	2.48	0.47
1:C:329:VAL:HG22	1:C:330:VAL:HG12	1.96	0.47
1:A:38:LYS:HB3	1:A:39:ARG:H	1.40	0.46
1:A:50:GLY:HA2	1:A:195:PRO:HA	1.97	0.46
1:B:291:TYR:HD1	1:B:306:GLU:HB3	1.78	0.46
1:C:174:ASN:C	1:C:174:ASN:OD1	2.57	0.46
1:C:269:LYS:HE2	1:C:269:LYS:HB3	1.61	0.46
1:A:282:LEU:HB3	1:A:284:VAL:HG22	1.97	0.46
1:D:307:ILE:HD12	1:D:320:LYS:HG3	1.96	0.46
1:A:39:ARG:HB3	1:A:40:GLY:H	1.40	0.46
1:B:69:THR:HG1	1:B:70:LYS:H	1.62	0.46
1:C:182:ILE:O	1:C:183:ILE:HD12	2.15	0.46
1:D:89:ASP:HA	1:D:90:PRO:HD3	1.65	0.46
1:D:135:TYR:HD2	1:D:136:LEU:HD13	1.79	0.46
1:A:213:PHE:HA	1:A:266:ASN:HA	1.97	0.46
1:A:327:GLU:HB3	1:A:328:LYS:H	1.42	0.46
1:B:37:VAL:CG1	1:B:278:PHE:HB3	2.45	0.46
1:B:163:ILE:HD13	1:B:163:ILE:N	2.30	0.46
1:B:235:THR:CG2	1:B:246:TYR:H	2.23	0.46
1:C:238:SER:O	1:C:239:ASP:C	2.58	0.46
1:D:279:ILE:O	1:D:280:PRO:C	2.58	0.46
1:A:52:ILE:HG12	1:A:193:ILE:HG22	1.96	0.46
1:A:217:SER:OG	1:B:199:GLU:O	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HA	1:B:85:LEU:HD13	1.52	0.46
1:B:199:GLU:HB2	1:B:243:VAL:CG2	2.46	0.46
1:B:313:ASN:HA	1:B:314:ASP:C	2.35	0.46
1:C:178:THR:O	1:C:179:THR:C	2.58	0.46
1:D:83:ASP:O	1:D:85:LEU:HD22	2.15	0.46
1:D:93:TYR:CD1	1:D:148:ASN:HB3	2.50	0.46
1:D:204:LYS:CB	1:D:270:ILE:HD13	2.43	0.46
1:A:64:VAL:HG21	1:A:88:ILE:HG12	1.98	0.46
1:B:250:ILE:HD13	1:B:250:ILE:H	1.80	0.46
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.75	0.46
1:B:86:ALA:HA	1:B:154:ILE:HG13	1.98	0.46
1:A:191:MSE:HE1	1:A:260:ILE:HG22	1.96	0.46
1:A:257:VAL:HG13	1:A:258:LEU:H	1.80	0.46
1:B:37:VAL:HG11	1:B:278:PHE:HB3	1.98	0.46
1:B:204:LYS:HB3	1:B:270:ILE:HD13	1.97	0.46
1:D:311:VAL:HG22	1:D:312:GLN:H	1.81	0.46
1:A:215:ILE:HD13	1:A:218:ASP:N	2.25	0.46
1:B:106:SER:OG	1:B:107:THR:N	2.48	0.46
1:B:215:ILE:HB	1:B:216:LEU:H	1.20	0.46
1:B:312:GLN:HB2	1:B:313:ASN:H	1.20	0.46
1:C:311:VAL:N	1:C:318:GLU:HG2	2.31	0.46
1:A:93:TYR:CD1	1:A:148:ASN:HB3	2.50	0.46
1:C:215:ILE:HD13	1:C:218:ASP:N	2.26	0.46
1:D:220:LYS:H	1:D:220:LYS:HG2	1.50	0.46
1:C:197:ILE:HD11	1:C:202:ILE:CD1	2.35	0.45
1:C:237:ILE:HD12	1:C:237:ILE:HA	1.62	0.45
1:B:202:ILE:O	1:B:204:LYS:O	2.34	0.45
1:B:321:SER:HA	1:B:322:GLY:HA3	1.54	0.45
1:D:250:ILE:HD13	1:D:250:ILE:H	1.81	0.45
1:D:308:GLU:HB2	1:D:320:LYS:HD3	1.98	0.45
1:A:66:GLY:HA2	1:B:63:GLN:HG2	1.99	0.45
1:A:151:TYR:O	1:A:152:THR:C	2.60	0.45
1:B:191:MSE:O	1:B:251:VAL:N	2.39	0.45
1:C:155:THR:O	1:C:157:PRO:HD3	2.16	0.45
1:C:163:ILE:HG22	1:C:164:SER:CB	2.47	0.45
1:D:102:ALA:O	1:D:105:ALA:N	2.50	0.45
1:C:199:GLU:HB2	1:C:243:VAL:HG23	1.98	0.45
1:C:277:LEU:HD12	1:C:319:VAL:HG21	1.98	0.45
1:C:293:VAL:HG11	1:C:305:ARG:HH22	1.81	0.45
1:D:293:VAL:HG22	1:D:307:ILE:N	2.31	0.45
1:A:40:GLY:HA3	1:A:275:ASN:N	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASP:HA	1:B:90:PRO:HD3	1.66	0.45
1:B:269:LYS:HE2	1:B:269:LYS:HB3	1.63	0.45
1:C:67:LYS:HB3	1:C:172:THR:HA	1.97	0.45
1:C:308:GLU:HB2	1:C:309:ILE:CA	2.46	0.45
1:C:310:GLY:HA2	1:C:311:VAL:HA	1.85	0.45
1:C:311:VAL:H	1:C:318:GLU:CD	2.25	0.45
1:A:226:LYS:O	1:A:249:ILE:HG23	2.17	0.45
1:B:50:GLY:HA2	1:B:195:PRO:HA	1.99	0.45
1:B:93:TYR:HB3	1:B:149:LEU:HD12	1.99	0.45
1:B:179:THR:HG22	1:B:180:PRO:C	2.42	0.45
1:B:322:GLY:CA	1:B:323:LEU:HB2	2.46	0.45
1:C:81:LYS:NZ	1:C:82:GLY:H	2.15	0.45
1:D:211:VAL:HG22	1:D:212:THR:N	2.32	0.45
1:A:165:THR:O	1:A:165:THR:OG1	2.04	0.45
1:B:282:LEU:HD12	1:B:282:LEU:H	1.81	0.45
1:C:83:ASP:HB3	1:C:84:LEU:H	1.45	0.45
1:C:290:LYS:HA	1:C:308:GLU:OE2	2.17	0.45
1:D:167:VAL:HG11	1:D:182:ILE:HG23	1.98	0.45
1:A:155:THR:O	1:A:157:PRO:HD3	2.17	0.44
1:C:190:LYS:HA	1:C:252:GLU:HA	1.99	0.44
1:C:213:PHE:CB	1:C:266:ASN:HB3	2.48	0.44
1:C:259:ARG:HB2	1:C:262:MSE:HE3	1.98	0.44
1:D:269:LYS:HE2	1:D:269:LYS:HB3	1.62	0.44
1:A:237:ILE:C	1:A:238:SER:O	2.61	0.44
1:B:206:LYS:O	1:B:227:ILE:HG21	2.16	0.44
1:C:315:PHE:O	1:C:316:GLN:O	2.36	0.44
1:D:151:TYR:O	1:D:152:THR:C	2.59	0.44
1:D:289:ASP:OD1	1:D:289:ASP:N	2.49	0.44
1:A:167:VAL:HG11	1:A:182:ILE:HG23	1.99	0.44
1:B:206:LYS:H	1:B:209:GLN:CD	2.26	0.44
1:B:235:THR:HB	1:B:246:TYR:CD1	2.52	0.44
1:C:209:GLN:H	1:C:227:ILE:HG22	1.82	0.44
1:A:215:ILE:CD1	1:A:216:LEU:H	2.30	0.44
1:B:283:ALA:HB1	1:B:291:TYR:C	2.42	0.44
1:C:199:GLU:O	1:C:199:GLU:HG2	2.16	0.44
1:B:277:LEU:HB2	1:B:319:VAL:HG22	1.99	0.44
1:B:293:VAL:HG13	1:B:330:VAL:N	2.30	0.44
1:B:293:VAL:N	1:B:304:GLU:HB3	2.32	0.44
1:C:52:ILE:HG21	1:C:262:MSE:HB2	1.98	0.44
1:C:92:THR:HG22	1:D:147:ILE:HD13	1.98	0.44
1:C:311:VAL:H	1:C:318:GLU:CG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ILE:O	1:D:270:ILE:HD12	2.17	0.44
1:A:92:THR:HG22	1:B:147:ILE:HD13	2.00	0.44
1:B:147:ILE:HG22	1:B:148:ASN:N	2.33	0.44
1:B:158:ILE:HD12	1:B:158:ILE:HA	1.88	0.44
1:C:259:ARG:HD3	1:D:245:TYR:CE1	2.49	0.44
1:A:199:GLU:HB2	1:A:243:VAL:CG2	2.48	0.44
1:A:250:ILE:O	1:A:251:VAL:HB	2.17	0.44
1:B:259:ARG:HH11	1:B:259:ARG:HD2	1.65	0.44
1:C:85:LEU:HB2	1:C:154:ILE:HB	2.00	0.44
1:C:282:LEU:HA	1:C:284:VAL:HG23	1.99	0.44
1:C:324:THR:OG1	1:C:325:GLU:N	2.49	0.44
1:D:52:ILE:HG21	1:D:262:MSE:HB2	1.99	0.44
1:D:173:VAL:HG23	1:D:174:ASN:N	2.32	0.44
1:D:198:SER:HB2	1:D:244:TYR:CD1	2.52	0.44
1:D:199:GLU:HB2	1:D:243:VAL:CG2	2.48	0.44
1:A:331:ILE:HA	1:A:332:SER:HA	1.89	0.44
1:B:65:SER:HB3	1:B:66:GLY:H	1.48	0.44
1:C:283:ALA:O	1:C:291:TYR:CG	2.71	0.44
1:D:250:ILE:O	1:D:251:VAL:HB	2.18	0.44
1:A:81:LYS:O	1:A:83:ASP:N	2.50	0.44
1:A:175:SER:OG	1:A:176:ASN:O	2.36	0.44
1:A:179:THR:HG22	1:A:180:PRO:C	2.43	0.44
1:D:117:LEU:HD23	1:D:117:LEU:N	2.32	0.44
1:D:237:ILE:C	1:D:238:SER:O	2.60	0.44
1:D:282:LEU:C	1:D:284:VAL:N	2.75	0.44
1:A:198:SER:HB2	1:A:244:TYR:HD1	1.83	0.43
1:B:53:GLU:HG2	1:B:54:SER:H	1.83	0.43
1:B:211:VAL:HG22	1:B:212:THR:N	2.33	0.43
1:D:52:ILE:HG13	1:D:193:ILE:HG22	2.00	0.43
1:A:213:PHE:CB	1:A:266:ASN:HB3	2.49	0.43
1:B:213:PHE:HB3	1:B:266:ASN:HB3	2.00	0.43
1:C:85:LEU:HD13	1:C:85:LEU:HA	1.51	0.43
1:D:60:VAL:HG22	1:D:183:ILE:HG22	1.98	0.43
1:B:53:GLU:O	1:B:191:MSE:HB3	2.18	0.43
1:C:215:ILE:HB	1:C:216:LEU:H	1.29	0.43
1:D:35:GLU:HB3	1:D:36:GLU:H	1.62	0.43
1:A:57:THR:O	1:A:58:VAL:HG13	2.19	0.43
1:A:154:ILE:HD12	1:A:154:ILE:HG23	1.66	0.43
1:B:36:GLU:HG3	1:B:325:GLU:HG2	2.01	0.43
1:B:324:THR:OG1	1:B:325:GLU:N	2.52	0.43
1:C:257:VAL:HG13	1:C:258:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LYS:O	1:D:88:ILE:HA	2.18	0.43
1:D:85:LEU:H	1:D:86:ALA:CB	2.16	0.43
1:D:164:SER:HB3	1:D:184:LYS:CB	2.41	0.43
1:D:179:THR:HG22	1:D:180:PRO:C	2.43	0.43
1:A:173:VAL:HG23	1:A:180:PRO:HG2	2.00	0.43
1:A:315:PHE:N	1:A:316:GLN:OE1	2.44	0.43
1:D:97:TYR:OH	1:D:146:ARG:NH1	2.50	0.43
1:B:46:VAL:O	1:B:267:ASN:HA	2.18	0.43
1:C:202:ILE:O	1:C:204:LYS:O	2.37	0.43
1:C:250:ILE:O	1:C:251:VAL:HB	2.18	0.43
1:D:314:ASP:OD1	1:D:316:GLN:NE2	2.51	0.43
1:B:60:VAL:CG2	1:B:183:ILE:HG22	2.49	0.43
1:B:86:ALA:HB2	1:B:154:ILE:HB	1.98	0.43
1:B:192:ARG:HA	1:B:250:ILE:HA	2.00	0.43
1:A:156:SER:O	1:A:158:ILE:N	2.52	0.43
1:A:268:ILE:HG12	1:A:268:ILE:H	1.65	0.43
1:B:37:VAL:HG22	1:B:278:PHE:H	1.83	0.43
1:C:69:THR:HG1	1:C:70:LYS:H	1.67	0.43
1:C:156:SER:O	1:C:158:ILE:N	2.52	0.43
1:C:198:SER:HB2	1:C:244:TYR:CD1	2.53	0.43
1:C:198:SER:HB2	1:C:244:TYR:HD1	1.84	0.43
1:C:282:LEU:HD12	1:C:282:LEU:H	1.84	0.43
1:A:87:GLU:HA	1:A:152:THR:O	2.19	0.43
1:B:55:ILE:HG23	1:B:56:ASN:H	1.83	0.43
1:C:327:GLU:O	1:C:329:VAL:N	2.52	0.43
1:D:75:LEU:HG	1:D:165:THR:HG23	2.01	0.43
1:D:156:SER:O	1:D:158:ILE:N	2.52	0.43
1:D:199:GLU:O	1:D:199:GLU:HG2	2.17	0.43
1:D:278:PHE:HE2	1:D:316:GLN:C	2.26	0.43
1:D:75:LEU:HD23	1:D:163:ILE:O	2.19	0.43
1:D:85:LEU:HB2	1:D:154:ILE:HB	2.01	0.43
1:D:163:ILE:HG22	1:D:164:SER:CB	2.49	0.43
1:A:80:LYS:H	1:A:80:LYS:HD2	1.84	0.42
1:A:269:LYS:HB3	1:A:269:LYS:HE2	1.66	0.42
1:B:277:LEU:HB2	1:B:319:VAL:HG21	2.01	0.42
1:B:285:GLN:HE22	1:B:288:GLN:HG2	1.84	0.42
1:B:305:ARG:NH1	1:B:327:GLU:OE2	2.44	0.42
1:C:135:TYR:HD2	1:C:136:LEU:HD13	1.83	0.42
1:A:152:THR:HG22	1:A:153:LYS:HD2	2.01	0.42
1:B:50:GLY:O	1:B:264:THR:N	2.43	0.42
1:B:304:GLU:O	1:B:305:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ASN:C	1:D:283:ALA:H	2.22	0.42
1:D:281:ASN:ND2	1:D:282:LEU:HA	2.34	0.42
1:A:313:ASN:HB3	1:A:314:ASP:HA	2.01	0.42
1:B:67:LYS:HB3	1:B:172:THR:HA	2.00	0.42
1:C:173:VAL:HG23	1:C:174:ASN:N	2.33	0.42
1:D:51:SER:O	1:D:194:LYS:HB2	2.19	0.42
1:D:322:GLY:HA3	1:D:323:LEU:O	2.19	0.42
1:B:34:THR:CB	1:B:329:VAL:HG11	2.49	0.42
1:B:86:ALA:HB1	1:B:154:ILE:CB	2.48	0.42
1:C:315:PHE:HD2	1:C:315:PHE:HA	1.79	0.42
1:D:117:LEU:CD1	1:D:123:VAL:HG22	2.43	0.42
1:A:52:ILE:O	1:A:260:ILE:O	2.38	0.42
1:A:195:PRO:O	1:A:197:ILE:HG23	2.20	0.42
1:B:40:GLY:O	1:B:275:ASN:N	2.52	0.42
1:B:75:LEU:H	1:B:75:LEU:HG	1.40	0.42
1:B:85:LEU:HB2	1:B:154:ILE:HB	2.02	0.42
1:B:215:ILE:HD13	1:B:218:ASP:N	2.16	0.42
1:C:158:ILE:HD12	1:C:158:ILE:HA	1.90	0.42
1:C:176:ASN:HB2	1:C:177:GLN:H	1.57	0.42
1:C:259:ARG:H	1:C:262:MSE:SE	2.52	0.42
1:D:281:ASN:HD22	1:D:282:LEU:CA	2.33	0.42
1:C:67:LYS:O	1:C:88:ILE:HA	2.19	0.42
1:D:163:ILE:HD13	1:D:163:ILE:N	2.35	0.42
1:D:259:ARG:HB2	1:D:262:MSE:HE3	2.01	0.42
1:D:308:GLU:C	1:D:320:LYS:HB3	2.44	0.42
1:A:59:ASP:C	1:A:60:VAL:HG13	2.44	0.42
1:A:70:LYS:O	1:A:86:ALA:O	2.38	0.42
1:B:156:SER:O	1:B:158:ILE:N	2.52	0.42
1:C:65:SER:HB3	1:C:66:GLY:H	1.60	0.42
1:C:77:GLN:H	1:C:162:VAL:HG23	1.84	0.42
1:D:309:ILE:N	1:D:320:LYS:HB3	2.35	0.42
1:D:315:PHE:N	1:D:316:GLN:OE1	2.50	0.42
1:A:259:ARG:HD3	1:B:245:TYR:HE1	1.83	0.42
1:C:86:ALA:HB1	1:C:154:ILE:HB	2.02	0.42
1:A:158:ILE:HD12	1:A:158:ILE:HA	1.90	0.42
1:A:198:SER:O	1:A:200:GLY:N	2.53	0.42
1:A:260:ILE:CD1	1:B:233:ALA:HA	2.49	0.42
1:B:85:LEU:HD23	1:B:155:THR:N	2.35	0.42
1:B:198:SER:HB2	1:B:244:TYR:CD1	2.54	0.42
1:B:213:PHE:CB	1:B:266:ASN:HB3	2.50	0.42
1:C:70:LYS:O	1:C:86:ALA:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:H	1:C:209:GLN:NE2	2.18	0.42
1:A:52:ILE:HG21	1:A:262:MSE:HB2	2.02	0.42
1:B:205:VAL:HA	1:B:209:GLN:OE1	2.20	0.42
1:D:237:ILE:HA	1:D:237:ILE:HD12	1.58	0.42
1:A:72:TYR:N	1:A:85:LEU:O	2.43	0.41
1:C:179:THR:HG22	1:C:180:PRO:C	2.44	0.41
1:A:66:GLY:HA2	1:B:63:GLN:CG	2.49	0.41
1:B:87:GLU:HA	1:B:152:THR:O	2.20	0.41
1:B:147:ILE:O	1:B:149:LEU:N	2.53	0.41
1:B:226:LYS:O	1:B:249:ILE:HG23	2.19	0.41
1:C:113:ARG:HG3	1:C:114:TYR:N	2.35	0.41
1:C:204:LYS:CB	1:C:270:ILE:HD13	2.49	0.41
1:D:88:ILE:H	1:D:88:ILE:CD1	2.31	0.41
1:B:102:ALA:C	1:B:104:LEU:N	2.78	0.41
1:C:147:ILE:HG22	1:C:148:ASN:N	2.36	0.41
1:D:34:THR:OG1	1:D:327:GLU:O	2.33	0.41
1:A:260:ILE:HD11	1:B:233:ALA:HA	2.02	0.41
1:A:279:ILE:O	1:A:280:PRO:C	2.58	0.41
1:B:88:ILE:HD12	1:B:88:ILE:H	1.85	0.41
1:B:162:VAL:HA	1:B:185:VAL:CG2	2.48	0.41
1:A:74:LYS:O	1:A:76:GLY:N	2.52	0.41
1:A:220:LYS:H	1:A:220:LYS:HG2	1.50	0.41
1:C:234:THR:OG1	1:C:236:THR:OG1	2.36	0.41
1:C:317:THR:HG22	1:C:318:GLU:N	2.36	0.41
1:D:72:TYR:N	1:D:85:LEU:O	2.41	0.41
1:A:67:LYS:HZ2	1:A:67:LYS:HG3	1.64	0.41
1:A:85:LEU:HD13	1:A:85:LEU:HA	1.49	0.41
1:A:253:ASN:HD21	1:A:256:HIS:HA	1.85	0.41
1:C:202:ILE:C	1:C:204:LYS:N	2.79	0.41
1:C:213:PHE:HB3	1:C:266:ASN:HB3	2.02	0.41
1:A:259:ARG:CB	1:B:245:TYR:HE1	2.34	0.41
1:A:309:ILE:HD11	1:A:320:LYS:H	1.84	0.41
1:C:202:ILE:HD13	1:C:202:ILE:HA	1.84	0.41
1:C:259:ARG:HB3	1:C:260:ILE:H	1.59	0.41
1:A:168:SER:O	1:A:171:GLN:HB2	2.21	0.41
1:B:34:THR:HB	1:B:329:VAL:CG2	2.45	0.41
1:B:59:ASP:C	1:B:60:VAL:HG13	2.44	0.41
1:B:61:GLY:HA3	1:B:182:ILE:HD12	2.02	0.41
1:B:165:THR:N	1:B:166:PRO:CD	2.82	0.41
1:B:291:TYR:CG	1:B:307:ILE:HG12	2.56	0.41
1:C:167:VAL:HG12	1:C:182:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:VAL:HG23	1:C:174:ASN:H	1.84	0.41
1:C:237:ILE:C	1:C:238:SER:O	2.62	0.41
1:D:69:THR:HG1	1:D:70:LYS:H	1.69	0.41
1:A:36:GLU:HG3	1:A:37:VAL:HG22	2.02	0.41
1:A:117:LEU:C	1:A:119:ALA:H	2.28	0.41
1:C:195:PRO:C	1:C:197:ILE:N	2.78	0.41
1:A:147:ILE:CG2	1:A:148:ASN:N	2.84	0.40
1:A:197:ILE:CG1	1:A:198:SER:N	2.75	0.40
1:B:279:ILE:O	1:B:279:ILE:HG22	2.21	0.40
1:C:84:LEU:O	1:C:85:LEU:HD13	2.21	0.40
1:C:211:VAL:HG22	1:C:212:THR:N	2.36	0.40
1:C:215:ILE:CD1	1:C:216:LEU:H	2.34	0.40
1:D:215:ILE:CD1	1:D:216:LEU:H	2.34	0.40
1:A:67:LYS:CG	1:B:63:GLN:HE22	2.28	0.40
1:A:147:ILE:HG22	1:A:148:ASN:H	1.86	0.40
1:B:83:ASP:HB3	1:B:84:LEU:H	1.50	0.40
1:C:163:ILE:HG23	1:D:237:ILE:HG23	2.02	0.40
1:C:220:LYS:H	1:C:220:LYS:HG2	1.51	0.40
1:D:81:LYS:O	1:D:83:ASP:N	2.53	0.40
1:D:147:ILE:O	1:D:150:ARG:N	2.55	0.40
1:D:308:GLU:H	1:D:320:LYS:HG2	1.85	0.40
1:A:67:LYS:NZ	1:A:67:LYS:HB2	2.36	0.40
1:C:293:VAL:HG12	1:C:328:LYS:CB	2.43	0.40
1:D:313:ASN:CG	1:D:314:ASP:O	2.64	0.40
1:A:252:GLU:O	1:A:254:PRO:HD2	2.21	0.40
1:B:195:PRO:C	1:B:197:ILE:N	2.77	0.40
1:B:317:THR:HG22	1:B:318:GLU:N	2.36	0.40
1:C:89:ASP:HA	1:C:90:PRO:HD3	1.69	0.40
1:C:177:GLN:OE1	1:C:178:THR:HG23	2.22	0.40
1:D:213:PHE:HD1	1:D:264:THR:HB	1.85	0.40
1:D:215:ILE:CD1	1:D:218:ASP:H	2.23	0.40
1:B:293:VAL:H	1:B:304:GLU:HB3	1.85	0.40
1:C:46:VAL:O	1:C:267:ASN:HA	2.22	0.40
1:C:55:ILE:HG23	1:C:56:ASN:H	1.86	0.40
1:C:261:GLY:CA	1:D:234:THR:HG21	2.51	0.40
1:D:52:ILE:O	1:D:260:ILE:O	2.39	0.40
1:D:313:ASN:HB3	1:D:314:ASP:HA	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASN:O	1:D:174:ASN:ND2[3_565]	1.97	0.23
1:A:199:GLU:O	1:B:217:SER:OG[2_665]	2.11	0.09
1:A:176:ASN:O	1:B:174:ASN:ND2[2_665]	2.12	0.08

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	270/341 (79%)	163 (60%)	51 (19%)	56 (21%)	0	1
1	B	277/341 (81%)	170 (61%)	56 (20%)	51 (18%)	0	1
1	C	270/341 (79%)	164 (61%)	49 (18%)	57 (21%)	0	1
1	D	270/341 (79%)	161 (60%)	59 (22%)	50 (18%)	0	1
All	All	1087/1364 (80%)	658 (60%)	215 (20%)	214 (20%)	0	1

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	75	LEU
1	A	82	GLY
1	A	121	GLN
1	A	122	ALA
1	A	124	SER
1	A	152	THR
1	A	169	GLU
1	A	190	LYS
1	A	196	GLU
1	A	215	ILE
1	A	216	LEU
1	A	232	PRO
1	A	235	THR
1	A	238	SER

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Mol	Chain	Res	Type
1	A	242	ALA
1	A	257	VAL
1	A	281	ASN
1	A	309	ILE
1	A	317	THR
1	B	81	LYS
1	B	82	GLY
1	B	121	GLN
1	B	122	ALA
1	B	124	SER
1	B	152	THR
1	B	169	GLU
1	B	173	VAL
1	B	190	LYS
1	B	196	GLU
1	B	215	ILE
1	B	216	LEU
1	B	232	PRO
1	B	235	THR
1	B	257	VAL
1	B	281	ASN
1	B	317	THR
1	B	323	LEU
1	B	326	GLY
1	B	327	GLU
1	B	331	ILE
1	C	82	GLY
1	C	121	GLN
1	C	122	ALA
1	C	124	SER
1	C	151	TYR
1	C	152	THR
1	C	169	GLU
1	C	173	VAL
1	C	196	GLU
1	C	216	LEU
1	C	232	PRO
1	C	235	THR
1	C	238	SER
1	C	258	LEU
1	C	281	ASN
1	C	282	LEU

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Mol	Chain	Res	Type
1	C	307	ILE
1	C	308	GLU
1	C	316	GLN
1	C	323	LEU
1	C	328	LYS
1	C	329	VAL
1	D	82	GLY
1	D	121	GLN
1	D	122	ALA
1	D	124	SER
1	D	152	THR
1	D	169	GLU
1	D	173	VAL
1	D	196	GLU
1	D	215	ILE
1	D	216	LEU
1	D	232	PRO
1	D	235	THR
1	D	238	SER
1	D	258	LEU
1	D	281	ASN
1	D	282	LEU
1	D	316	GLN
1	D	317	THR
1	A	45	ASN
1	A	103	ASN
1	A	114	TYR
1	A	151	TYR
1	A	258	LEU
1	A	329	VAL
1	B	45	ASN
1	B	66	GLY
1	B	83	ASP
1	B	103	ASN
1	B	114	TYR
1	B	151	TYR
1	B	182	ILE
1	B	246	TYR
1	B	275	ASN
1	C	45	ASN
1	C	103	ASN
1	C	114	TYR

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Mol	Chain	Res	Type
1	C	182	ILE
1	C	190	LYS
1	C	215	ILE
1	C	246	TYR
1	C	262	MSE
1	C	269	LYS
1	C	310	GLY
1	D	45	ASN
1	D	103	ASN
1	D	182	ILE
1	D	190	LYS
1	D	257	VAL
1	D	269	LYS
1	A	81	LYS
1	A	95	ALA
1	A	106	SER
1	A	140	ALA
1	A	141	ALA
1	A	222	VAL
1	A	269	LYS
1	A	275	ASN
1	A	282	LEU
1	B	86	ALA
1	B	87	GLU
1	B	95	ALA
1	B	106	SER
1	B	140	ALA
1	B	205	VAL
1	B	258	LEU
1	C	83	ASP
1	C	86	ALA
1	C	148	ASN
1	C	257	VAL
1	C	306	GLU
1	C	331	ILE
1	D	66	GLY
1	D	81	LYS
1	D	86	ALA
1	D	106	SER
1	D	151	TYR
1	D	222	VAL
1	D	262	MSE

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Mol	Chain	Res	Type
1	D	275	ASN
1	D	321	SER
1	A	76	GLY
1	A	83	ASP
1	A	110	GLN
1	A	148	ASN
1	A	155	THR
1	A	173	VAL
1	A	182	ILE
1	B	222	VAL
1	B	269	LYS
1	C	81	LYS
1	C	106	SER
1	C	197	ILE
1	C	205	VAL
1	C	222	VAL
1	C	275	ASN
1	C	327	GLU
1	D	87	GLU
1	D	140	ALA
1	D	205	VAL
1	D	234	THR
1	D	246	TYR
1	D	327	GLU
1	A	36	GLU
1	A	87	GLU
1	A	170	GLY
1	A	205	VAL
1	A	221	THR
1	A	234	THR
1	B	110	GLN
1	B	155	THR
1	B	170	GLY
1	B	230	VAL
1	B	313	ASN
1	C	118	VAL
1	C	140	ALA
1	C	155	THR
1	C	157	PRO
1	C	170	GLY
1	C	221	THR
1	D	114	TYR

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Mol	Chain	Res	Type
1	D	155	THR
1	D	197	ILE
1	A	66	GLY
1	A	118	VAL
1	A	176	ASN
1	B	118	VAL
1	C	66	GLY
1	C	87	GLU
1	D	118	VAL
1	D	170	GLY
1	D	230	VAL
1	A	40	GLY
1	A	230	VAL
1	D	157	PRO
1	D	251	VAL
1	A	276	VAL
1	C	64	VAL
1	C	276	VAL
1	D	64	VAL
1	D	276	VAL
1	D	284	VAL
1	A	64	VAL
1	A	197	ILE
1	C	251	VAL
1	B	64	VAL
1	B	157	PRO
1	B	253	ASN
1	B	276	VAL
1	B	329	VAL
1	C	230	VAL
1	B	37	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/288 (82%)	129 (55%)	107 (45%)	0	0
1	B	245/288 (85%)	136 (56%)	109 (44%)	0	0
1	C	239/288 (83%)	133 (56%)	106 (44%)	0	0
1	D	238/288 (83%)	132 (56%)	106 (44%)	0	0
All	All	958/1152 (83%)	530 (55%)	428 (45%)	0	0

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	35	GLU
1	A	37	VAL
1	A	38	LYS
1	A	39	ARG
1	A	42	ILE
1	A	44	LYS
1	A	46	VAL
1	A	49	THR
1	A	52	ILE
1	A	56	ASN
1	A	58	VAL
1	A	64	VAL
1	A	67	LYS
1	A	68	ILE
1	A	69	THR
1	A	75	LEU
1	A	80	LYS
1	A	81	LYS
1	A	84	LEU
1	A	85	LEU
1	A	89	ASP
1	A	92	THR
1	A	101	GLN
1	A	106	SER
1	A	107	THR
1	A	109	GLU
1	A	113	ARG
1	A	116	LEU
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	125	LYS
1	A	127	GLN
1	A	136	LEU
1	A	139	LYS
1	A	142	VAL
1	A	146	ARG
1	A	147	ILE
1	A	148	ASN
1	A	149	LEU
1	A	150	ARG
1	A	152	THR
1	A	153	LYS
1	A	155	THR
1	A	156	SER
1	A	161	THR
1	A	163	ILE
1	A	167	VAL
1	A	173	VAL
1	A	174	ASN
1	A	176	ASN
1	A	177	GLN
1	A	180	PRO
1	A	181	THR
1	A	182	ILE
1	A	183	ILE
1	A	185	VAL
1	A	188	LEU
1	A	191	MSE
1	A	192	ARG
1	A	193	ILE
1	A	197	ILE
1	A	198	SER
1	A	201	ASP
1	A	202	ILE
1	A	203	THR
1	A	204	LYS
1	A	205	VAL
1	A	206	LYS
1	A	210	ASP
1	A	212	THR
1	A	215	ILE
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	220	LYS
1	A	221	THR
1	A	224	HIS
1	A	227	ILE
1	A	228	ASP
1	A	229	SER
1	A	234	THR
1	A	235	THR
1	A	236	THR
1	A	237	ILE
1	A	239	ASP
1	A	241	SER
1	A	248	ASN
1	A	250	ILE
1	A	251	VAL
1	A	252	GLU
1	A	256	HIS
1	A	258	LEU
1	A	259	ARG
1	A	260	ILE
1	A	263	THR
1	A	266	ASN
1	A	267	ASN
1	A	268	ILE
1	A	270	ILE
1	A	273	VAL
1	A	276	VAL
1	A	277	LEU
1	A	285	GLN
1	A	309	ILE
1	A	311	VAL
1	A	312	GLN
1	A	317	THR
1	A	327	GLU
1	A	329	VAL
1	B	34	THR
1	B	35	GLU
1	B	36	GLU
1	B	37	VAL
1	B	41	ASN
1	B	42	ILE
1	B	44	LYS

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Mol	Chain	Res	Type
1	B	46	VAL
1	B	49	THR
1	B	52	ILE
1	B	56	ASN
1	B	58	VAL
1	B	64	VAL
1	B	67	LYS
1	B	68	ILE
1	B	69	THR
1	B	74	LYS
1	B	75	LEU
1	B	80	LYS
1	B	81	LYS
1	B	84	LEU
1	B	85	LEU
1	B	89	ASP
1	B	92	THR
1	B	101	GLN
1	B	106	SER
1	B	107	THR
1	B	109	GLU
1	B	113	ARG
1	B	116	LEU
1	B	127	GLN
1	B	136	LEU
1	B	139	LYS
1	B	142	VAL
1	B	146	ARG
1	B	147	ILE
1	B	149	LEU
1	B	150	ARG
1	B	152	THR
1	B	153	LYS
1	B	155	THR
1	B	156	SER
1	B	161	THR
1	B	163	ILE
1	B	167	VAL
1	B	173	VAL
1	B	174	ASN
1	B	176	ASN
1	B	177	GLN

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Mol	Chain	Res	Type
1	B	180	PRO
1	B	181	THR
1	B	182	ILE
1	B	183	ILE
1	B	185	VAL
1	B	188	LEU
1	B	192	ARG
1	B	197	ILE
1	B	201	ASP
1	B	202	ILE
1	B	203	THR
1	B	205	VAL
1	B	206	LYS
1	B	210	ASP
1	B	212	THR
1	B	215	ILE
1	B	216	LEU
1	B	220	LYS
1	B	221	THR
1	B	224	HIS
1	B	227	ILE
1	B	228	ASP
1	B	229	SER
1	B	234	THR
1	B	235	THR
1	B	236	THR
1	B	237	ILE
1	B	239	ASP
1	B	248	ASN
1	B	250	ILE
1	B	251	VAL
1	B	252	GLU
1	B	256	HIS
1	B	258	LEU
1	B	259	ARG
1	B	260	ILE
1	B	263	THR
1	B	266	ASN
1	B	267	ASN
1	B	268	ILE
1	B	270	ILE
1	B	273	VAL

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Mol	Chain	Res	Type
1	B	276	VAL
1	B	277	LEU
1	B	291	TYR
1	B	292	VAL
1	B	304	GLU
1	B	305	ARG
1	B	309	ILE
1	B	311	VAL
1	B	312	GLN
1	B	315	PHE
1	B	316	GLN
1	B	319	VAL
1	B	320	LYS
1	B	321	SER
1	B	323	LEU
1	B	325	GLU
1	B	329	VAL
1	B	331	ILE
1	C	41	ASN
1	C	42	ILE
1	C	44	LYS
1	C	46	VAL
1	C	49	THR
1	C	52	ILE
1	C	56	ASN
1	C	58	VAL
1	C	64	VAL
1	C	67	LYS
1	C	68	ILE
1	C	69	THR
1	C	74	LYS
1	C	75	LEU
1	C	80	LYS
1	C	81	LYS
1	C	84	LEU
1	C	85	LEU
1	C	89	ASP
1	C	92	THR
1	C	101	GLN
1	C	106	SER
1	C	109	GLU
1	C	113	ARG

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Mol	Chain	Res	Type
1	C	116	LEU
1	C	121	GLN
1	C	125	LYS
1	C	127	GLN
1	C	136	LEU
1	C	139	LYS
1	C	142	VAL
1	C	146	ARG
1	C	147	ILE
1	C	149	LEU
1	C	150	ARG
1	C	152	THR
1	C	153	LYS
1	C	155	THR
1	C	156	SER
1	C	161	THR
1	C	163	ILE
1	C	167	VAL
1	C	173	VAL
1	C	174	ASN
1	C	176	ASN
1	C	177	GLN
1	C	180	PRO
1	C	181	THR
1	C	182	ILE
1	C	183	ILE
1	C	185	VAL
1	C	188	LEU
1	C	192	ARG
1	C	193	ILE
1	C	197	ILE
1	C	198	SER
1	C	201	ASP
1	C	202	ILE
1	C	205	VAL
1	C	206	LYS
1	C	210	ASP
1	C	212	THR
1	C	215	ILE
1	C	216	LEU
1	C	220	LYS
1	C	221	THR

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Mol	Chain	Res	Type
1	C	224	HIS
1	C	227	ILE
1	C	228	ASP
1	C	229	SER
1	C	234	THR
1	C	235	THR
1	C	236	THR
1	C	237	ILE
1	C	239	ASP
1	C	248	ASN
1	C	250	ILE
1	C	251	VAL
1	C	252	GLU
1	C	258	LEU
1	C	259	ARG
1	C	260	ILE
1	C	263	THR
1	C	266	ASN
1	C	267	ASN
1	C	268	ILE
1	C	270	ILE
1	C	273	VAL
1	C	276	VAL
1	C	277	LEU
1	C	284	VAL
1	C	289	ASP
1	C	290	LYS
1	C	293	VAL
1	C	307	ILE
1	C	308	GLU
1	C	309	ILE
1	C	312	GLN
1	C	315	PHE
1	C	316	GLN
1	C	318	GLU
1	C	320	LYS
1	C	323	LEU
1	C	325	GLU
1	C	327	GLU
1	C	331	ILE
1	D	34	THR
1	D	36	GLU

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Mol	Chain	Res	Type
1	D	37	VAL
1	D	42	ILE
1	D	44	LYS
1	D	46	VAL
1	D	49	THR
1	D	52	ILE
1	D	56	ASN
1	D	58	VAL
1	D	67	LYS
1	D	68	ILE
1	D	69	THR
1	D	80	LYS
1	D	81	LYS
1	D	84	LEU
1	D	85	LEU
1	D	89	ASP
1	D	92	THR
1	D	101	GLN
1	D	106	SER
1	D	109	GLU
1	D	113	ARG
1	D	116	LEU
1	D	121	GLN
1	D	125	LYS
1	D	127	GLN
1	D	136	LEU
1	D	139	LYS
1	D	142	VAL
1	D	146	ARG
1	D	147	ILE
1	D	149	LEU
1	D	150	ARG
1	D	152	THR
1	D	153	LYS
1	D	155	THR
1	D	156	SER
1	D	161	THR
1	D	163	ILE
1	D	167	VAL
1	D	173	VAL
1	D	174	ASN
1	D	176	ASN

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Mol	Chain	Res	Type
1	D	177	GLN
1	D	180	PRO
1	D	181	THR
1	D	182	ILE
1	D	183	ILE
1	D	185	VAL
1	D	188	LEU
1	D	191	MSE
1	D	192	ARG
1	D	193	ILE
1	D	197	ILE
1	D	198	SER
1	D	201	ASP
1	D	202	ILE
1	D	203	THR
1	D	205	VAL
1	D	206	LYS
1	D	210	ASP
1	D	212	THR
1	D	215	ILE
1	D	216	LEU
1	D	220	LYS
1	D	221	THR
1	D	224	HIS
1	D	227	ILE
1	D	228	ASP
1	D	229	SER
1	D	234	THR
1	D	235	THR
1	D	236	THR
1	D	237	ILE
1	D	239	ASP
1	D	248	ASN
1	D	250	ILE
1	D	251	VAL
1	D	252	GLU
1	D	256	HIS
1	D	258	LEU
1	D	259	ARG
1	D	260	ILE
1	D	263	THR
1	D	266	ASN

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Mol	Chain	Res	Type
1	D	267	ASN
1	D	268	ILE
1	D	270	ILE
1	D	273	VAL
1	D	276	VAL
1	D	277	LEU
1	D	281	ASN
1	D	284	VAL
1	D	288	GLN
1	D	289	ASP
1	D	290	LYS
1	D	292	VAL
1	D	307	ILE
1	D	311	VAL
1	D	312	GLN
1	D	315	PHE
1	D	319	VAL
1	D	320	LYS
1	D	323	LEU
1	D	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	45	ASN
1	A	121	GLN
1	A	174	ASN
1	A	253	ASN
1	A	281	ASN
1	B	45	ASN
1	B	63	GLN
1	B	177	GLN
1	B	275	ASN
1	B	285	GLN
1	C	45	ASN
1	C	121	GLN
1	C	256	HIS
1	C	281	ASN
1	C	313	ASN
1	D	45	ASN
1	D	63	GLN

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Mol	Chain	Res	Type
1	D	177	GLN
1	D	281	ASN
1	D	285	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	274/341 (80%)	-0.58	0	100 100	7, 60, 178, 245	1 (0%)
1	B	283/341 (82%)	-0.53	0	100 100	7, 63, 166, 285	1 (0%)
1	C	276/341 (80%)	-0.32	1 (0%)	88 72	27, 99, 200, 277	1 (0%)
1	D	276/341 (80%)	-0.37	0	100 100	27, 93, 190, 275	1 (0%)
All	All	1109/1364 (81%)	-0.45	1 (0%)	92 86	7, 82, 185, 285	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	GLN	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.