



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:08 PM UTC

PDB ID : 3FOA / pdb_00003foa
Title : Crystal structure of the bacteriophage T4 tail sheath protein, deletion mutant gp18M
Authors : Aksyuk, A.A.; Leiman, P.G.; Kurochkina, L.P.; Shneider, M.M.; Kostyuchenko, V.A.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on : 2008-12-29
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
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

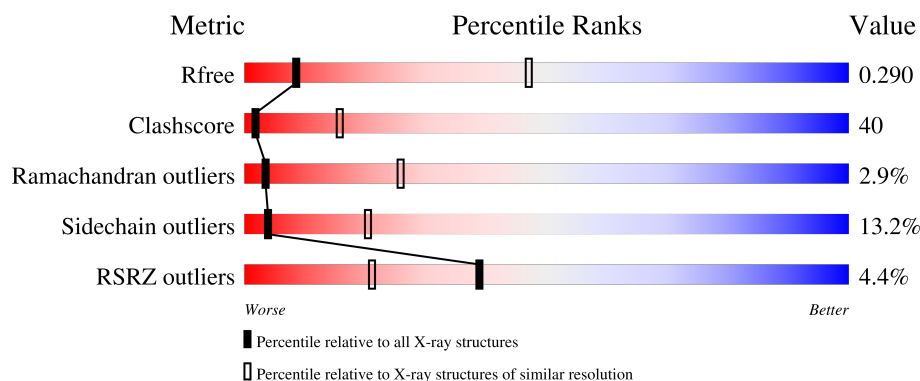
1 Overall quality at a glance

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	510	2% 36% 46% 11% 6%
1	B	510	5% 35% 45% 11% 6%
1	C	510	3% 37% 44% 11% 6%
1	D	510	6% 37% 44% 10% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14406 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 Tail sheath protein Gp18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3613	2279	600	726	8			
1	B	478	Total	C	N	O	S	0	0	0
			3605	2275	598	724	8			
1	C	477	Total	C	N	O	S	0	0	0
			3597	2271	596	722	8			
1	D	476	Total	C	N	O	S	0	0	0
			3591	2268	595	720	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLU	ASP	variant	UNP P13332
A	148	ALA	GLY	variant	UNP P13332
A	150	ILE	ASN	variant	UNP P13332
A	151	ILE	TYR	variant	UNP P13332
A	301	GLY	GLU	variant	UNP P13332
A	399	VAL	ALA	variant	UNP P13332
A	454	TYR	HIS	variant	UNP P13332
A	510	PRO	ARG	engineered mutation	UNP P13332
B	100	GLU	ASP	variant	UNP P13332
B	148	ALA	GLY	variant	UNP P13332
B	150	ILE	ASN	variant	UNP P13332
B	151	ILE	TYR	variant	UNP P13332
B	301	GLY	GLU	variant	UNP P13332
B	399	VAL	ALA	variant	UNP P13332
B	454	TYR	HIS	variant	UNP P13332
B	510	PRO	ARG	engineered mutation	UNP P13332
C	100	GLU	ASP	variant	UNP P13332
C	148	ALA	GLY	variant	UNP P13332
C	150	ILE	ASN	variant	UNP P13332
C	151	ILE	TYR	variant	UNP P13332
C	301	GLY	GLU	variant	UNP P13332

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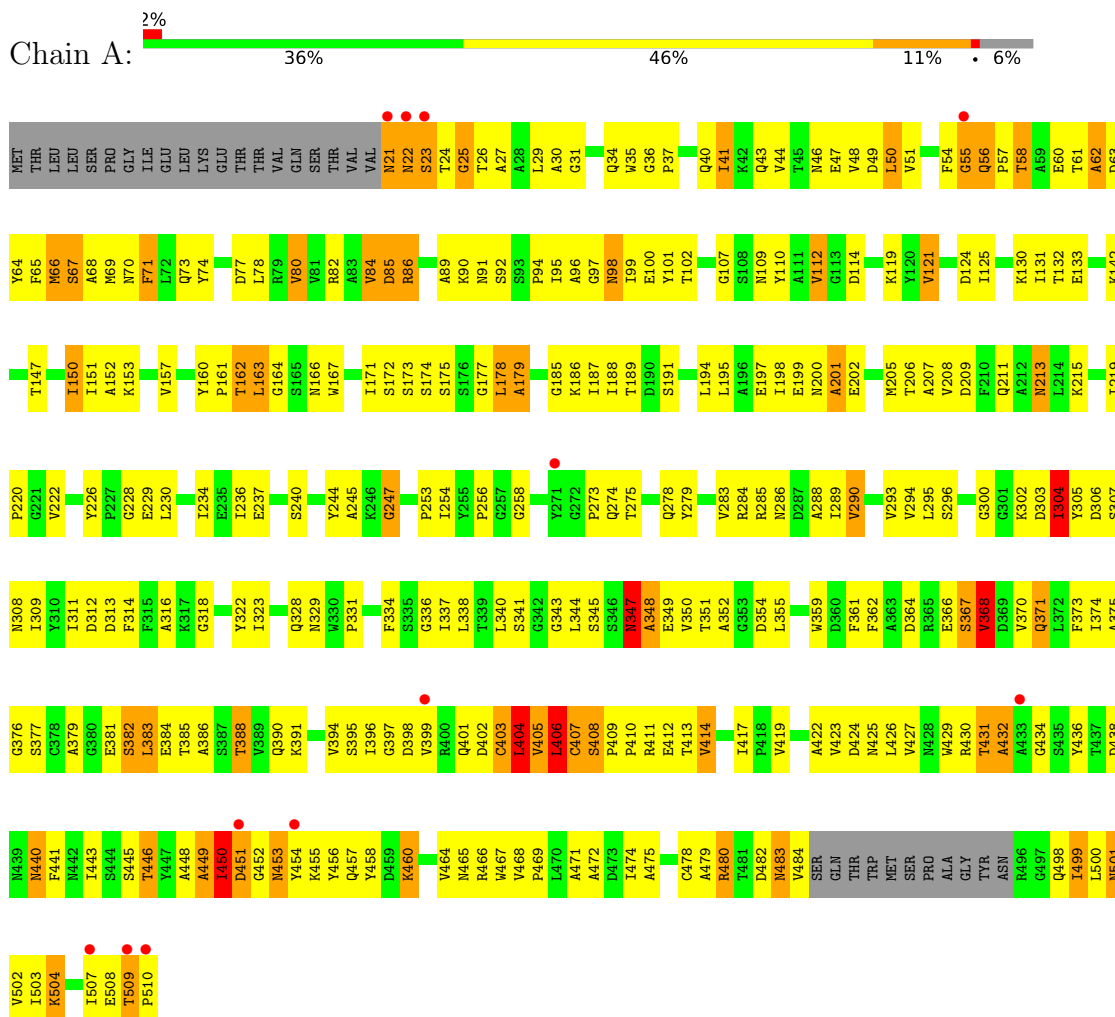
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Chain	Residue	Modelled	Actual	Comment	Reference
C	399	VAL	ALA	variant	UNP P13332
C	454	TYR	HIS	variant	UNP P13332
C	510	PRO	ARG	engineered mutation	UNP P13332
D	100	GLU	ASP	variant	UNP P13332
D	148	ALA	GLY	variant	UNP P13332
D	150	ILE	ASN	variant	UNP P13332
D	151	ILE	TYR	variant	UNP P13332
D	301	GLY	GLU	variant	UNP P13332
D	399	VAL	ALA	variant	UNP P13332
D	454	TYR	HIS	variant	UNP P13332
D	510	PRO	ARG	engineered mutation	UNP P13332

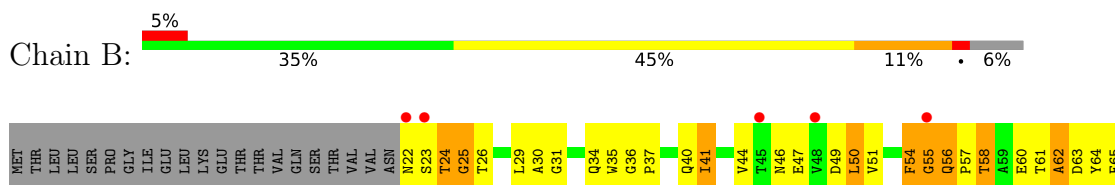
3 Residue-property plots

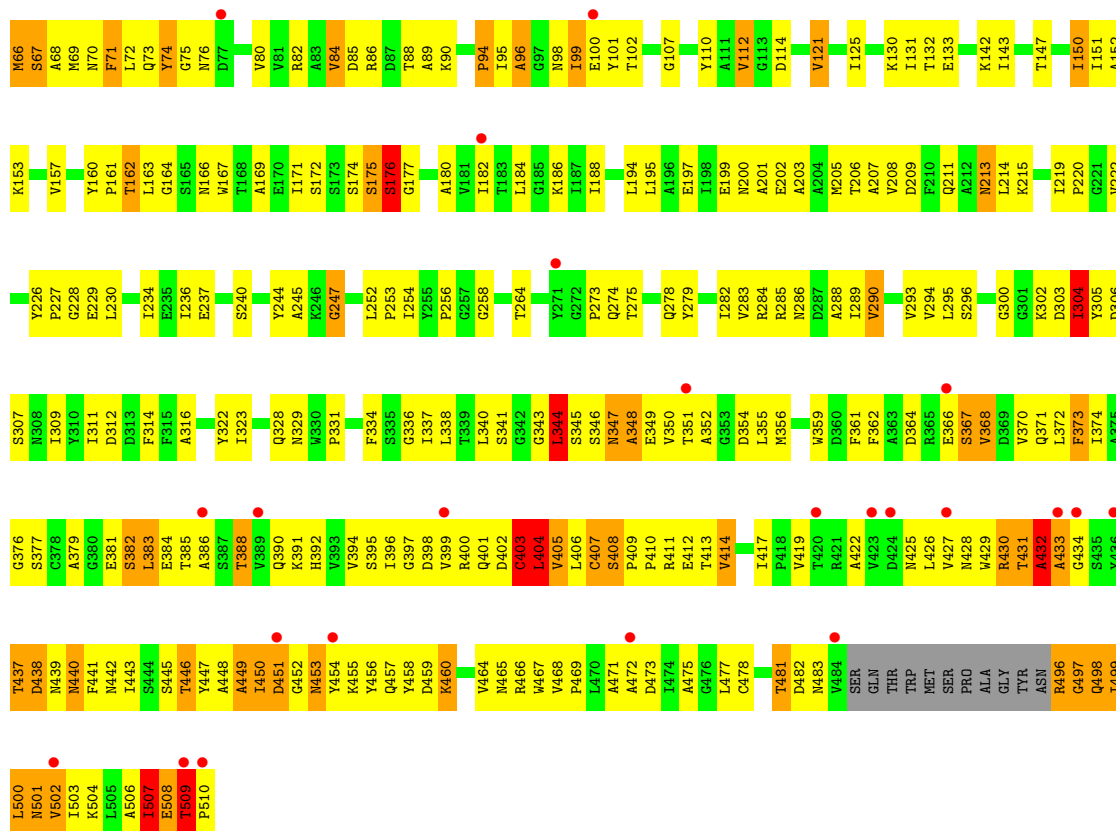
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tail sheath protein Gp18

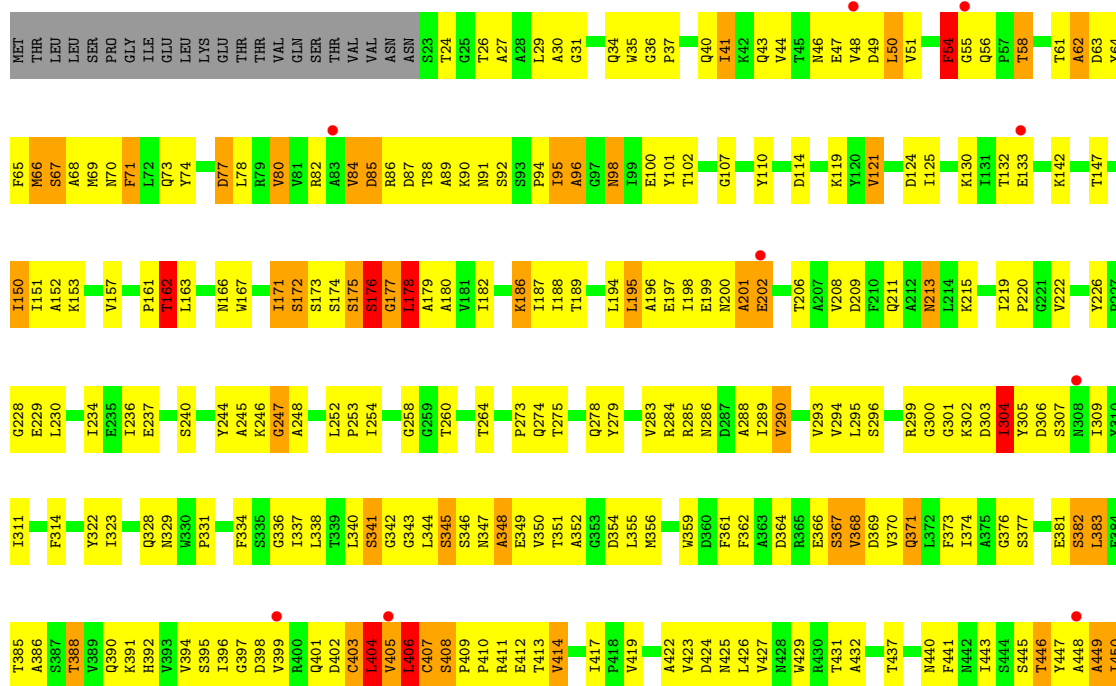


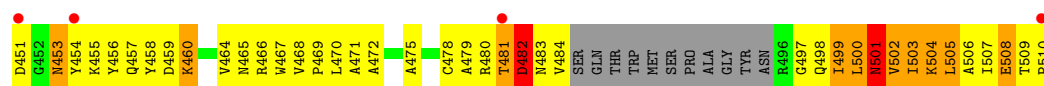
• Molecule 1: Tail sheath protein Gp18



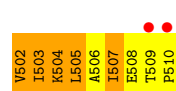
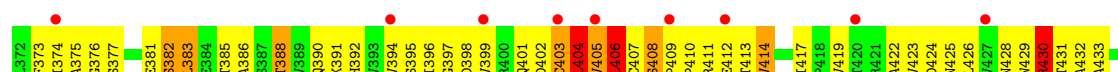
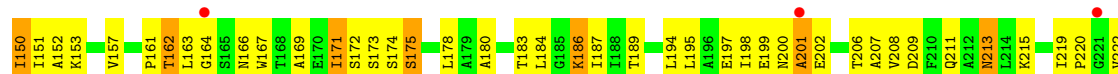
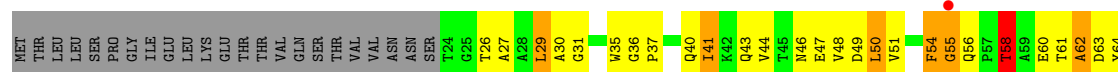


• Molecule 1: Tail sheath protein Gp18





• Molecule 1: Tail sheath protein Gp18



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.59Å 116.29Å 433.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.50 49.80 – 3.50	Depositor EDS
% Data completeness (in resolution range)	87.8 (49.80-3.50) 87.8 (49.80-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.267 , 0.299 0.281 , 0.290	Depositor DCC
R_{free} test set	5405 reflections (16.72%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14406	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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	0.47	4/3677 (0.1%)	1.09	30/5001 (0.6%)
1	B	0.38	1/3669 (0.0%)	1.20	45/4990 (0.9%)
1	C	0.40	0/3661	1.08	35/4979 (0.7%)
1	D	0.38	0/3655	1.29	48/4971 (1.0%)
All	All	0.41	5/14662 (0.0%)	1.17	158/19941 (0.8%)

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	13
1	C	0	5
1	D	0	2
All	All	0	24

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	ASN	C-N	-7.18	1.23	1.33
1	A	23	SER	C-N	-6.90	1.24	1.33
1	A	23	SER	C-O	6.82	1.32	1.24
1	B	432	ALA	C-N	6.65	1.42	1.33
1	A	22	ASN	C-O	5.52	1.30	1.24

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	GLY	N-CA-C	33.86	153.61	112.64
1	C	195	LEU	N-CA-C	21.34	134.23	110.97
1	B	96	ALA	N-CA-CB	-21.11	78.81	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	503	ILE	CB-CA-C	20.59	129.38	111.05
1	A	55	GLY	N-CA-C	18.96	158.11	113.18
1	D	500	LEU	CB-CA-C	-18.50	75.86	109.71
1	C	405	VAL	N-CA-C	-17.62	83.51	108.17
1	A	112	VAL	N-CA-C	17.38	136.65	112.50
1	B	112	VAL	N-CA-C	16.20	125.48	110.74
1	D	405	VAL	N-CA-C	-15.82	85.14	108.71
1	A	405	VAL	N-CA-C	-15.51	85.11	107.75
1	B	55	GLY	N-CA-C	14.29	147.05	113.18
1	B	201	ALA	N-CA-C	14.19	134.78	111.37
1	D	85	ASP	N-CA-C	-13.19	90.96	110.48
1	B	498	GLN	N-CA-C	-12.73	89.35	109.72
1	B	407	CYS	CB-CA-C	-12.67	84.26	109.35
1	D	367	SER	N-CA-CB	-12.42	91.82	110.07
1	D	366	GLU	CB-CA-C	12.18	130.29	110.92
1	B	403	CYS	CB-CA-C	-12.04	86.46	110.42
1	C	85	ASP	N-CA-C	-12.03	91.19	110.20
1	B	367	SER	N-CA-CB	-11.77	92.73	110.26
1	D	56	GLN	N-CA-CB	-11.33	90.11	110.39
1	B	366	GLU	CB-CA-C	11.14	128.64	110.81
1	D	482	ASP	N-CA-C	-11.04	93.51	109.96
1	D	501	ASN	N-CA-C	10.96	130.50	113.28
1	C	196	ALA	N-CA-C	10.96	124.96	108.31
1	B	201	ALA	CB-CA-C	-10.78	92.85	110.74
1	A	404	LEU	N-CA-C	-10.76	90.68	108.32
1	C	85	ASP	CB-CA-C	10.74	127.68	109.53
1	A	56	GLN	N-CA-CB	-10.60	90.17	110.10
1	B	56	GLN	N-CA-CB	-10.51	91.58	110.39
1	B	99	ILE	N-CA-C	10.40	123.23	108.36
1	D	366	GLU	N-CA-C	-10.34	98.41	111.02
1	A	85	ASP	N-CA-C	-10.32	93.36	109.76
1	C	86	ARG	N-CA-C	-10.29	99.04	111.69
1	C	114	ASP	N-CA-C	-10.28	92.52	109.07
1	D	407	CYS	CB-CA-C	-10.15	88.78	109.38
1	D	85	ASP	CB-CA-C	10.14	128.12	109.46
1	B	114	ASP	N-CA-C	-10.13	92.75	109.07
1	C	404	LEU	N-CA-C	-10.01	91.91	108.32
1	B	404	LEU	N-CA-CB	-10.00	94.01	110.52
1	D	503	ILE	N-CA-C	-9.89	103.81	111.62
1	B	432	ALA	CA-C-N	9.88	134.73	120.71
1	B	432	ALA	C-N-CA	9.88	134.73	120.71
1	B	99	ILE	N-CA-CB	-9.85	99.17	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	503	ILE	CB-CA-C	9.52	120.24	110.91
1	B	367	SER	N-CA-C	9.40	125.52	112.45
1	A	367	SER	N-CA-CB	-9.39	94.55	110.33
1	D	367	SER	N-CA-C	9.37	123.33	111.24
1	B	497	GLY	N-CA-C	-9.36	96.08	112.55
1	B	373	PHE	N-CA-C	9.34	125.69	107.57
1	D	504	LYS	N-CA-CB	-9.26	96.20	111.66
1	A	407	CYS	CB-CA-C	-9.22	91.42	109.68
1	C	407	CYS	CB-CA-C	-9.18	91.25	109.33
1	B	366	GLU	N-CA-C	-9.17	100.11	111.11
1	B	96	ALA	N-CA-C	9.02	124.99	112.45
1	B	408	SER	N-CA-CB	-8.97	93.23	110.10
1	A	366	GLU	CB-CA-C	8.71	125.25	110.79
1	C	367	SER	N-CA-CB	-8.70	97.79	110.40
1	D	86	ARG	N-CA-C	-8.66	101.55	112.90
1	D	246	LYS	N-CA-C	-8.46	96.92	109.62
1	D	450	ILE	CB-CA-C	-8.46	97.97	110.33
1	D	404	LEU	N-CA-C	-8.37	94.12	107.93
1	C	502	VAL	N-CA-C	-8.30	95.34	108.86
1	D	54	PHE	CB-CA-C	-8.24	99.38	112.07
1	D	449	ALA	CB-CA-C	8.21	124.74	109.71
1	D	408	SER	N-CA-CB	-8.20	95.71	110.39
1	D	449	ALA	N-CA-C	-8.09	95.71	108.90
1	D	498	GLN	CB-CA-C	7.95	122.50	109.70
1	A	406	LEU	N-CA-C	-7.89	96.53	109.40
1	A	404	LEU	CB-CA-C	7.88	123.20	109.89
1	D	449	ALA	CA-C-N	-7.78	112.17	122.99
1	D	449	ALA	C-N-CA	-7.78	112.17	122.99
1	A	366	GLU	N-CA-C	-7.61	102.98	111.28
1	B	54	PHE	N-CA-C	-7.61	94.60	110.80
1	D	405	VAL	CB-CA-C	7.54	121.61	110.98
1	A	347	ASN	N-CA-C	-7.43	104.01	113.23
1	A	85	ASP	CB-CA-C	7.36	121.83	109.84
1	B	54	PHE	CB-CA-C	-7.33	95.83	110.42
1	C	87	ASP	N-CA-C	7.27	120.25	111.82
1	C	502	VAL	CB-CA-C	-7.21	99.16	110.69
1	C	408	SER	N-CA-CB	-7.20	97.31	110.63
1	C	345	SER	N-CA-C	-7.07	101.72	110.41
1	D	114	ASP	N-CA-C	-7.01	97.82	109.46
1	B	372	LEU	CB-CA-C	-6.97	97.09	109.70
1	B	498	GLN	N-CA-CB	6.93	122.94	111.08
1	B	449	ALA	N-CA-C	-6.93	97.12	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	505	LEU	N-CA-C	6.90	120.40	109.50
1	C	404	LEU	CB-CA-C	6.90	121.54	109.89
1	C	482	ASP	N-CA-C	-6.88	104.75	113.01
1	B	180	ALA	N-CA-CB	6.88	122.80	110.83
1	A	86	ARG	N-CA-C	-6.84	104.40	112.89
1	A	405	VAL	N-CA-CB	6.84	120.54	111.64
1	C	347	ASN	N-CA-C	-6.78	105.09	113.15
1	A	449	ALA	N-CA-C	-6.77	97.37	108.41
1	D	246	LYS	CB-CA-C	-6.75	101.99	112.12
1	B	405	VAL	N-CA-C	-6.75	95.99	106.72
1	A	179	ALA	N-CA-C	6.74	125.16	110.80
1	B	404	LEU	CB-CA-C	6.72	120.77	109.48
1	C	179	ALA	N-CA-C	6.72	125.11	110.80
1	B	407	CYS	N-CA-C	6.71	120.44	109.24
1	A	21	ASN	CA-C-N	6.70	134.33	121.54
1	A	21	ASN	C-N-CA	6.70	134.33	121.54
1	B	347	ASN	N-CA-C	-6.68	104.08	111.82
1	A	408	SER	N-CA-CB	-6.67	97.22	110.70
1	B	372	LEU	N-CA-C	6.63	119.96	108.76
1	D	504	LYS	CB-CA-C	-6.62	96.22	110.45
1	D	406	LEU	N-CA-C	-6.60	97.01	108.69
1	C	405	VAL	CB-CA-C	6.58	120.64	110.83
1	A	406	LEU	CB-CA-C	6.57	121.92	109.37
1	B	408	SER	N-CA-C	6.55	120.46	110.50
1	B	180	ALA	N-CA-C	-6.40	98.97	109.40
1	D	404	LEU	CB-CA-C	6.35	119.23	110.34
1	D	345	SER	N-CA-C	-6.32	98.11	108.41
1	A	163	LEU	CB-CA-C	-6.19	107.72	115.89
1	A	178	LEU	N-CA-CB	-6.18	100.05	110.49
1	C	497	GLY	N-CA-C	-6.05	104.33	112.14
1	A	449	ALA	CB-CA-C	6.04	120.18	110.16
1	D	344	LEU	CB-CA-C	5.89	119.85	109.89
1	B	400	ARG	CB-CA-C	5.86	119.29	110.08
1	C	449	ALA	N-CA-C	-5.82	97.83	108.02
1	A	446	THR	N-CA-C	-5.80	106.05	113.01
1	D	505	LEU	CB-CA-C	-5.79	97.29	109.38
1	B	449	ALA	CB-CA-C	5.76	119.73	110.16
1	D	58	THR	CB-CA-C	-5.76	99.76	109.83
1	C	405	VAL	N-CA-CB	5.75	119.06	111.25
1	C	366	GLU	CB-CA-C	5.63	121.04	110.63
1	D	406	LEU	N-CA-CB	5.62	120.25	110.81
1	C	446	THR	N-CA-C	-5.61	106.28	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ALA	N-CA-C	5.56	118.30	110.23
1	D	368	VAL	N-CA-C	5.53	115.83	107.75
1	B	405	VAL	N-CA-CB	5.47	118.77	112.15
1	D	450	ILE	N-CA-CB	5.47	119.50	111.52
1	C	505	LEU	N-CA-C	5.46	117.80	108.90
1	B	433	ALA	N-CA-CB	-5.40	101.68	109.83
1	A	368	VAL	N-CA-C	5.37	115.59	107.75
1	A	112	VAL	CB-CA-C	-5.37	96.96	111.34
1	C	501	ASN	N-CA-C	-5.36	97.18	107.57
1	C	196	ALA	CB-CA-C	-5.33	110.41	116.54
1	C	396	ILE	N-CA-C	-5.29	107.67	112.12
1	D	446	THR	N-CA-C	-5.29	106.66	113.01
1	C	342	GLY	N-CA-C	-5.23	108.62	115.47
1	A	396	ILE	N-CA-C	-5.22	107.74	112.12
1	B	85	ASP	N-CA-C	-5.20	101.29	109.25
1	B	373	PHE	N-CA-CB	-5.16	101.96	110.53
1	B	446	THR	N-CA-C	-5.16	106.82	113.01
1	A	367	SER	N-CA-C	5.14	119.52	112.68
1	D	347	ASN	N-CA-C	-5.14	105.68	111.28
1	C	505	LEU	N-CA-CB	-5.13	102.05	110.68
1	D	506	ALA	N-CA-C	5.13	117.53	111.33
1	D	456	TYR	N-CA-C	-5.12	100.17	108.52
1	C	406	LEU	N-CA-CB	5.12	118.62	110.84
1	B	396	ILE	N-CA-C	-5.10	107.83	112.12
1	D	396	ILE	N-CA-C	-5.08	107.85	112.12
1	D	449	ALA	O-C-N	5.06	129.32	123.30
1	C	95	ILE	N-CA-C	-5.05	105.47	110.62
1	C	504	LYS	CB-CA-C	-5.05	99.18	109.94
1	D	248	ALA	N-CA-C	-5.05	100.04	110.80

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ASN	Peptide
1	A	450	ILE	Peptide
1	A	451	ASP	Peptide
1	A	452	GLY	Peptide
1	B	175	SER	Peptide
1	B	176	SER	Peptide
1	B	177	GLY	Peptide
1	B	22	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	23	SER	Peptide
1	B	24	THR	Peptide
1	B	432	ALA	Peptide
1	B	451	ASP	Peptide
1	B	496	ARG	Peptide
1	B	501	ASN	Peptide
1	B	509	THR	Peptide
1	B	74	TYR	Peptide
1	B	76	ASN	Peptide
1	C	176	SER	Peptide
1	C	177	GLY	Peptide
1	C	178	LEU	Peptide
1	C	508	GLU	Peptide
1	C	54	PHE	Peptide
1	D	430	ARG	Peptide
1	D	496	ARG	Peptide

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	3613	0	3554	323	2
1	B	3605	0	3548	304	1
1	C	3597	0	3541	272	1
1	D	3591	0	3536	249	0
All	All	14406	0	14179	1135	2

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 40.

All (1135) 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:409:PRO:O	1:A:454:TYR:CE1	1.65	1.48
1:A:409:PRO:CD	1:A:451:ASP:O	1.75	1.33
1:B:496:ARG:HG3	1:B:497:GLY:O	1.16	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ALA:CB	1:A:454:TYR:OH	1.84	1.25
1:B:496:ARG:CG	1:B:497:GLY:O	1.89	1.21
1:B:24:THR:OG1	1:B:25:GLY:HA3	1.38	1.20
1:B:501:ASN:O	1:B:502:VAL:HG12	1.40	1.20
1:B:24:THR:O	1:B:482:ASP:OD2	1.62	1.16
1:B:379:ALA:HB1	1:B:454:TYR:OH	1.46	1.16
1:A:409:PRO:HD3	1:A:451:ASP:O	0.98	1.14
1:A:379:ALA:HB2	1:A:454:TYR:OH	1.37	1.14
1:A:379:ALA:HB1	1:A:454:TYR:CZ	1.83	1.13
1:D:84:VAL:HG13	1:D:85:ASP:O	1.47	1.12
1:B:409:PRO:O	1:B:454:TYR:OH	1.64	1.11
1:C:51:VAL:HA	1:C:55:GLY:HA2	1.27	1.10
1:A:454:TYR:CE2	1:A:469:PRO:HA	1.84	1.10
1:A:409:PRO:O	1:A:454:TYR:CZ	2.06	1.09
1:C:178:LEU:H	1:C:178:LEU:HD23	0.94	1.09
1:A:450:ILE:HG12	1:A:451:ASP:H	0.94	1.09
1:B:409:PRO:O	1:B:454:TYR:CZ	2.05	1.08
1:A:379:ALA:CB	1:A:454:TYR:CZ	2.35	1.08
1:C:178:LEU:HD23	1:C:178:LEU:N	1.63	1.08
1:A:454:TYR:CD2	1:A:469:PRO:HA	1.89	1.07
1:C:55:GLY:O	1:C:65:PHE:CE1	2.09	1.06
1:C:84:VAL:HG13	1:C:85:ASP:O	1.56	1.05
1:D:84:VAL:CG1	1:D:85:ASP:O	2.04	1.05
1:B:51:VAL:HA	1:B:55:GLY:HA2	1.38	1.04
1:A:51:VAL:HA	1:A:55:GLY:HA2	1.36	1.04
1:A:450:ILE:HG12	1:A:451:ASP:N	1.67	1.03
1:D:51:VAL:HA	1:D:55:GLY:HA2	1.38	1.03
1:C:55:GLY:O	1:C:65:PHE:HE1	1.42	1.02
1:B:112:VAL:O	1:B:131:ILE:O	1.77	1.02
1:C:171:ILE:HG22	1:C:172:SER:H	1.24	1.02
1:B:379:ALA:HB1	1:B:454:TYR:CZ	1.96	1.01
1:B:440:ASN:HD22	1:B:442:ASN:H	1.07	0.99
1:B:499:ILE:CG1	1:B:502:VAL:HG21	1.95	0.97
1:B:499:ILE:HG13	1:B:502:VAL:HG21	1.44	0.97
1:D:73:GLN:HB3	1:D:500:LEU:HD12	1.48	0.96
1:A:112:VAL:O	1:A:112:VAL:CG1	2.14	0.95
1:D:454:TYR:CE2	1:D:469:PRO:HA	2.02	0.95
1:C:51:VAL:CA	1:C:55:GLY:HA2	1.98	0.94
1:A:228:GLY:HA2	1:A:345:SER:HB3	1.47	0.94
1:B:51:VAL:HG13	1:B:55:GLY:O	1.68	0.93
1:A:409:PRO:O	1:A:454:TYR:HE1	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:H	1:C:178:LEU:CD2	1.79	0.93
1:C:94:PRO:HB2	1:C:219:ILE:HD12	1.49	0.92
1:A:408:SER:CA	1:A:451:ASP:HB3	2.00	0.91
1:C:84:VAL:CG1	1:C:85:ASP:O	2.18	0.91
1:B:496:ARG:CB	1:B:497:GLY:O	2.18	0.91
1:B:24:THR:HG1	1:B:25:GLY:HA3	1.33	0.90
1:B:498:GLN:HE21	1:B:510:PRO:HB3	1.33	0.90
1:A:408:SER:HA	1:A:451:ASP:HB3	1.54	0.90
1:A:23:SER:OG	1:A:483:ASN:CB	2.19	0.90
1:A:508:GLU:HG2	1:A:509:THR:HG22	1.55	0.89
1:B:379:ALA:HB1	1:B:454:TYR:CE2	2.09	0.89
1:D:503:ILE:O	1:D:510:PRO:HG2	1.72	0.88
1:D:41:ILE:HD11	1:D:361:PHE:HB3	1.54	0.88
1:C:41:ILE:HD11	1:C:361:PHE:HB3	1.56	0.88
1:C:178:LEU:N	1:C:178:LEU:CD2	2.33	0.87
1:A:41:ILE:HD11	1:A:361:PHE:HB3	1.57	0.87
1:A:391:LYS:HE3	1:A:440:ASN:O	1.76	0.86
1:B:507:ILE:O	1:B:508:GLU:HB2	1.73	0.86
1:C:409:PRO:O	1:C:454:TYR:CE1	2.28	0.86
1:D:455:LYS:HG3	1:D:502:VAL:HG22	1.54	0.86
1:A:23:SER:CB	1:A:483:ASN:HB3	2.04	0.86
1:B:379:ALA:CB	1:B:454:TYR:OH	2.22	0.86
1:A:509:THR:OG1	1:A:510:PRO:OXT	1.93	0.86
1:B:502:VAL:HG13	1:B:502:VAL:O	1.75	0.85
1:A:391:LYS:NZ	1:A:440:ASN:ND2	2.23	0.85
1:B:24:THR:HG23	1:B:25:GLY:N	1.89	0.85
1:B:41:ILE:HD11	1:B:361:PHE:HB3	1.55	0.85
1:D:499:ILE:HD13	1:D:499:ILE:H	1.42	0.85
1:D:331:PRO:HB2	1:D:334:PHE:HB2	1.59	0.84
1:D:496:ARG:HA	1:D:497:GLY:O	1.76	0.84
1:D:94:PRO:HB2	1:D:219:ILE:HD12	1.57	0.84
1:C:331:PRO:HB2	1:C:334:PHE:HB2	1.58	0.84
1:D:454:TYR:CE2	1:D:469:PRO:CA	2.60	0.84
1:A:23:SER:CB	1:A:483:ASN:CB	2.55	0.83
1:B:24:THR:HG23	1:B:25:GLY:CA	2.08	0.83
1:A:23:SER:OG	1:A:483:ASN:HB3	1.76	0.83
1:B:509:THR:HG22	1:B:510:PRO:C	2.03	0.83
1:A:94:PRO:HB2	1:A:219:ILE:HD12	1.61	0.83
1:A:331:PRO:HB2	1:A:334:PHE:HB2	1.60	0.82
1:D:454:TYR:HE2	1:D:469:PRO:N	1.78	0.81
1:D:478:CYS:HA	1:D:481:THR:HB	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:TYR:HE2	1:A:469:PRO:HA	1.43	0.81
1:A:110:TYR:CE1	1:A:178:LEU:O	2.33	0.81
1:B:328:GLN:HE21	1:C:299:ARG:NE	1.78	0.81
1:B:95:ILE:HD11	1:B:214:LEU:HD23	1.61	0.81
1:D:455:LYS:HE2	1:D:502:VAL:HG23	1.60	0.80
1:B:331:PRO:HB2	1:B:334:PHE:HB2	1.62	0.80
1:B:431:THR:HG23	1:B:432:ALA:H	1.45	0.80
1:C:228:GLY:HA2	1:C:345:SER:HB3	1.64	0.80
1:A:112:VAL:O	1:A:112:VAL:HG12	1.82	0.79
1:A:23:SER:HB3	1:A:483:ASN:HB3	1.64	0.79
1:A:509:THR:OG1	1:A:510:PRO:CA	2.32	0.78
1:B:440:ASN:HD22	1:B:442:ASN:N	1.80	0.78
1:D:499:ILE:H	1:D:499:ILE:CD1	1.96	0.78
1:B:409:PRO:O	1:B:454:TYR:CE1	2.35	0.78
1:D:100:GLU:HG3	1:D:186:LYS:H	1.48	0.78
1:B:24:THR:C	1:B:482:ASP:OD2	2.26	0.78
1:A:454:TYR:CE2	1:A:469:PRO:CA	2.67	0.78
1:A:479:ALA:HA	1:A:484:VAL:HG11	1.65	0.78
1:B:453:ASN:HB2	1:B:506:ALA:HB3	1.64	0.77
1:B:328:GLN:HG2	1:C:299:ARG:HE	1.48	0.77
1:A:172:SER:C	1:A:174:SER:HA	2.09	0.77
1:A:84:VAL:HG13	1:A:85:ASP:O	1.85	0.77
1:A:178:LEU:CD2	1:A:178:LEU:H	1.98	0.77
1:A:407:CYS:O	1:A:451:ASP:CB	2.32	0.77
1:A:178:LEU:H	1:A:178:LEU:HD23	1.48	0.77
1:B:496:ARG:HB2	1:B:497:GLY:O	1.83	0.77
1:A:379:ALA:HB1	1:A:454:TYR:OH	1.73	0.76
1:B:456:TYR:HB3	1:B:504:LYS:HB3	1.67	0.76
1:B:501:ASN:O	1:B:502:VAL:CG1	2.30	0.76
1:A:407:CYS:O	1:A:451:ASP:HB2	1.85	0.76
1:B:406:LEU:HD11	1:B:475:ALA:HB2	1.65	0.76
1:B:509:THR:HG22	1:B:510:PRO:OXT	1.84	0.76
1:C:410:PRO:O	1:C:413:THR:HG22	1.86	0.76
1:A:451:ASP:OD1	1:A:474:ILE:HD13	1.86	0.76
1:D:428:ASN:HA	1:D:433:ALA:HB3	1.68	0.76
1:C:509:THR:O	1:C:509:THR:HG22	1.83	0.76
1:A:171:ILE:HG22	1:A:172:SER:H	1.50	0.75
1:A:379:ALA:HB2	1:A:454:TYR:CZ	2.11	0.75
1:A:110:TYR:HE1	1:A:178:LEU:O	1.69	0.75
1:A:509:THR:OG1	1:A:510:PRO:HA	1.87	0.75
1:A:24:THR:O	1:A:371:GLN:OE1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LYS:HZ1	1:A:440:ASN:ND2	1.83	0.75
1:C:450:ILE:HG12	1:C:451:ASP:N	2.00	0.75
1:B:228:GLY:HA2	1:B:345:SER:HB3	1.66	0.74
1:A:112:VAL:O	1:A:131:ILE:O	2.04	0.74
1:B:382:SER:HB2	1:B:385:THR:HG22	1.68	0.74
1:C:406:LEU:HD11	1:C:475:ALA:HB2	1.69	0.74
1:A:454:TYR:HD2	1:A:469:PRO:HA	1.53	0.74
1:B:379:ALA:CB	1:B:454:TYR:CE2	2.70	0.74
1:B:498:GLN:NE2	1:B:510:PRO:HB3	2.03	0.74
1:D:406:LEU:HD11	1:D:475:ALA:HB2	1.69	0.74
1:B:440:ASN:ND2	1:B:442:ASN:H	1.85	0.74
1:A:112:VAL:O	1:A:112:VAL:HG13	1.88	0.74
1:C:453:ASN:HB2	1:C:506:ALA:HB3	1.70	0.74
1:A:26:THR:HA	1:A:77:ASP:OD1	1.87	0.73
1:D:410:PRO:O	1:D:413:THR:HG22	1.89	0.73
1:D:496:ARG:O	1:D:496:ARG:HG3	1.88	0.73
1:C:456:TYR:HB3	1:C:504:LYS:HB3	1.69	0.73
1:C:36:GLY:HA2	1:C:82:ARG:HD2	1.71	0.73
1:C:31:GLY:HA3	1:C:64:TYR:CD2	2.24	0.73
1:D:36:GLY:HA2	1:D:82:ARG:HD2	1.71	0.73
1:A:509:THR:H	1:A:510:PRO:HA	1.52	0.73
1:A:409:PRO:O	1:A:454:TYR:OH	2.06	0.72
1:B:413:THR:HG23	1:B:414:VAL:HG23	1.71	0.72
1:B:200:ASN:O	1:B:203:ALA:HB3	1.89	0.72
1:B:24:THR:O	1:B:482:ASP:CG	2.32	0.72
1:D:172:SER:C	1:D:174:SER:HA	2.15	0.72
1:A:509:THR:OG1	1:A:510:PRO:C	2.32	0.72
1:D:171:ILE:HG22	1:D:172:SER:H	1.54	0.72
1:A:51:VAL:HG13	1:A:55:GLY:O	1.89	0.72
1:D:454:TYR:HE2	1:D:469:PRO:CA	2.02	0.72
1:B:410:PRO:O	1:B:413:THR:HG22	1.90	0.72
1:A:409:PRO:C	1:A:454:TYR:HE1	1.98	0.71
1:A:413:THR:HG23	1:A:414:VAL:HG23	1.72	0.71
1:A:410:PRO:O	1:A:413:THR:HG22	1.89	0.71
1:B:31:GLY:HA3	1:B:64:TYR:CD2	2.26	0.71
1:C:54:PHE:CD2	1:C:54:PHE:N	2.57	0.71
1:B:36:GLY:HA2	1:B:82:ARG:HD2	1.72	0.71
1:C:382:SER:HB2	1:C:385:THR:HG22	1.71	0.71
1:A:31:GLY:HA3	1:A:64:TYR:CD2	2.26	0.71
1:D:51:VAL:HG13	1:D:55:GLY:O	1.90	0.71
1:A:36:GLY:HA2	1:A:82:ARG:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:VAL:HG11	1:A:443:ILE:HD12	1.73	0.71
1:D:289:ILE:HD12	1:D:289:ILE:H	1.54	0.71
1:D:382:SER:HB2	1:D:385:THR:HG22	1.71	0.71
1:A:499:ILE:HD13	1:A:499:ILE:H	1.55	0.71
1:B:407:CYS:O	1:B:450:ILE:HA	1.90	0.71
1:A:406:LEU:HD11	1:A:475:ALA:HB2	1.73	0.70
1:D:499:ILE:HD13	1:D:499:ILE:N	2.05	0.70
1:A:114:ASP:OD2	1:A:175:SER:HB2	1.91	0.70
1:D:428:ASN:O	1:D:431:THR:O	2.06	0.70
1:A:382:SER:HB2	1:A:385:THR:HG22	1.72	0.70
1:B:24:THR:HG23	1:B:25:GLY:C	2.15	0.70
1:C:413:THR:HG23	1:C:414:VAL:HG23	1.73	0.70
1:D:58:THR:O	1:D:61:THR:N	2.17	0.70
1:A:23:SER:CB	1:A:483:ASN:HB2	2.21	0.70
1:D:413:THR:HG23	1:D:414:VAL:HG23	1.74	0.70
1:D:246:LYS:O	1:D:250:ALA:HB2	1.90	0.70
1:B:47:GLU:HG3	1:B:69:MET:HG3	1.73	0.69
1:C:47:GLU:HG3	1:C:69:MET:HG3	1.74	0.69
1:C:215:LYS:HE3	1:C:329:ASN:HD21	1.57	0.69
1:D:31:GLY:HA3	1:D:64:TYR:CD2	2.26	0.69
1:D:47:GLU:HG3	1:D:69:MET:HG3	1.74	0.69
1:A:409:PRO:HD2	1:A:451:ASP:O	1.88	0.69
1:A:450:ILE:CG1	1:A:451:ASP:H	1.89	0.69
1:B:456:TYR:CD2	1:B:503:ILE:HD11	2.27	0.69
1:C:394:VAL:HG11	1:C:443:ILE:HD12	1.75	0.69
1:D:450:ILE:O	1:D:450:ILE:HG23	1.90	0.69
1:A:47:GLU:HG3	1:A:69:MET:HG3	1.74	0.69
1:D:394:VAL:HG11	1:D:443:ILE:HD12	1.75	0.69
1:A:22:ASN:O	1:A:23:SER:OG	2.04	0.69
1:A:23:SER:HB3	1:A:483:ASN:CB	2.22	0.69
1:A:228:GLY:CA	1:A:345:SER:HB3	2.23	0.68
1:D:26:THR:H	1:D:371:GLN:HB2	1.56	0.68
1:B:96:ALA:O	1:B:188:ILE:O	2.11	0.68
1:B:289:ILE:H	1:B:289:ILE:HD12	1.58	0.68
1:C:407:CYS:O	1:C:450:ILE:HA	1.93	0.68
1:B:24:THR:CB	1:B:25:GLY:HA3	2.23	0.68
1:B:351:THR:HG23	1:B:354:ASP:H	1.58	0.68
1:A:55:GLY:O	1:A:65:PHE:CE1	2.46	0.68
1:D:169:ALA:HB2	1:D:184:LEU:HD11	1.75	0.68
1:A:289:ILE:HD12	1:A:289:ILE:H	1.58	0.68
1:A:454:TYR:HE2	1:A:469:PRO:CA	2.03	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:THR:OG1	1:B:25:GLY:CA	2.30	0.68
1:C:51:VAL:HA	1:C:55:GLY:CA	2.16	0.68
1:C:351:THR:HG23	1:C:354:ASP:H	1.59	0.68
1:A:455:LYS:HG3	1:A:502:VAL:HG22	1.75	0.67
1:D:85:ASP:HB2	1:D:349:GLU:O	1.94	0.67
1:A:171:ILE:HG22	1:A:172:SER:N	2.09	0.67
1:A:215:LYS:HE3	1:A:329:ASN:HD21	1.58	0.67
1:D:428:ASN:HB3	1:D:433:ALA:O	1.94	0.67
1:A:427:VAL:O	1:A:431:THR:HG22	1.94	0.67
1:B:403:CYS:SG	1:B:403:CYS:O	2.51	0.67
1:D:96:ALA:HB1	1:D:341:SER:OG	1.95	0.67
1:B:394:VAL:HG11	1:B:443:ILE:HD12	1.76	0.67
1:A:96:ALA:HB2	1:A:191:SER:HA	1.77	0.67
1:C:50:LEU:O	1:C:54:PHE:N	2.23	0.67
1:D:55:GLY:O	1:D:65:PHE:CE1	2.48	0.67
1:A:304:ILE:HG13	1:A:305:TYR:CE2	2.30	0.67
1:A:391:LYS:NZ	1:A:440:ASN:HD21	1.92	0.67
1:B:373:PHE:HB2	1:B:405:VAL:HA	1.76	0.67
1:A:500:LEU:HB2	1:A:501:ASN:OD1	1.95	0.67
1:C:100:GLU:HG3	1:C:186:LYS:H	1.59	0.67
1:C:509:THR:N	1:C:510:PRO:HD3	2.09	0.67
1:D:215:LYS:HE3	1:D:329:ASN:HD21	1.59	0.67
1:B:379:ALA:CB	1:B:454:TYR:HE2	2.08	0.67
1:B:456:TYR:O	1:B:503:ILE:HG12	1.95	0.67
1:D:351:THR:HG23	1:D:354:ASP:H	1.60	0.66
1:C:289:ILE:HD12	1:C:289:ILE:H	1.61	0.66
1:B:208:VAL:HG11	1:C:202:GLU:OE1	1.96	0.66
1:C:408:SER:HB2	1:C:471:ALA:HB2	1.77	0.66
1:A:55:GLY:O	1:A:65:PHE:HE1	1.78	0.66
1:B:121:VAL:HG22	1:B:166:ASN:HB3	1.78	0.66
1:C:304:ILE:HG13	1:C:305:TYR:CE2	2.29	0.66
1:A:51:VAL:CA	1:A:55:GLY:HA2	2.20	0.66
1:B:211:GLN:HG3	1:C:299:ARG:HH21	1.59	0.66
1:C:481:THR:HA	1:C:484:VAL:HA	1.78	0.66
1:D:84:VAL:HG12	1:D:85:ASP:O	1.94	0.66
1:B:215:LYS:HE3	1:B:329:ASN:HD21	1.59	0.66
1:B:228:GLY:HA2	1:B:345:SER:H	1.60	0.66
1:D:408:SER:HB2	1:D:471:ALA:HB2	1.78	0.66
1:A:379:ALA:CB	1:A:454:TYR:CE2	2.79	0.66
1:A:121:VAL:HG22	1:A:166:ASN:HB3	1.78	0.65
1:B:408:SER:HB2	1:B:471:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:MET:HG2	1:D:468:VAL:HG11	1.78	0.65
1:A:351:THR:HG23	1:A:354:ASP:H	1.60	0.65
1:D:304:ILE:HG13	1:D:305:TYR:CE2	2.31	0.65
1:A:391:LYS:HZ3	1:A:440:ASN:HD21	1.42	0.65
1:B:66:MET:HG2	1:B:468:VAL:HG11	1.79	0.65
1:D:55:GLY:O	1:D:65:PHE:HE1	1.79	0.65
1:D:89:ALA:HB3	1:D:194:LEU:HD11	1.78	0.65
1:A:408:SER:HB2	1:A:471:ALA:HB2	1.77	0.65
1:B:50:LEU:C	1:B:50:LEU:HD12	2.21	0.65
1:B:304:ILE:HG13	1:B:305:TYR:CE2	2.31	0.65
1:C:121:VAL:HG22	1:C:166:ASN:HB3	1.78	0.65
1:D:454:TYR:CE2	1:D:469:PRO:N	2.62	0.64
1:D:121:VAL:HG22	1:D:166:ASN:HB3	1.78	0.64
1:D:504:LYS:HA	1:D:510:PRO:HD2	1.79	0.64
1:B:24:THR:CG2	1:B:25:GLY:CA	2.75	0.64
1:B:427:VAL:O	1:B:431:THR:HG22	1.97	0.64
1:C:176:SER:HB3	1:C:177:GLY:CA	2.28	0.64
1:D:100:GLU:HG3	1:D:186:LYS:N	2.12	0.64
1:C:406:LEU:HD12	1:C:406:LEU:O	1.98	0.64
1:A:66:MET:HG2	1:A:468:VAL:HG11	1.80	0.63
1:A:100:GLU:HG3	1:A:186:LYS:H	1.63	0.63
1:B:498:GLN:HA	1:B:498:GLN:OE1	1.98	0.63
1:C:174:SER:OG	1:C:175:SER:N	2.30	0.63
1:C:66:MET:HG2	1:C:468:VAL:HG11	1.80	0.63
1:C:107:GLY:HA3	1:C:110:TYR:CE1	2.34	0.63
1:A:215:LYS:HE3	1:A:329:ASN:ND2	2.13	0.62
1:A:509:THR:H	1:A:510:PRO:CA	2.12	0.62
1:B:74:TYR:OH	1:B:500:LEU:N	2.22	0.62
1:B:496:ARG:HG3	1:B:497:GLY:C	2.15	0.62
1:D:51:VAL:CA	1:D:55:GLY:HA2	2.22	0.62
1:A:213:ASN:N	1:A:213:ASN:HD22	1.98	0.62
1:B:206:THR:O	1:B:206:THR:HG22	1.99	0.62
1:A:407:CYS:O	1:A:450:ILE:HA	2.00	0.62
1:C:88:THR:O	1:C:90:LYS:HG2	1.99	0.62
1:D:480:ARG:O	1:D:482:ASP:O	2.18	0.62
1:D:161:PRO:HB3	1:D:187:ILE:HB	1.81	0.62
1:D:114:ASP:CG	1:D:175:SER:HB2	2.24	0.62
1:D:151:ILE:HG22	1:D:187:ILE:HD12	1.82	0.62
1:A:107:GLY:HA3	1:A:110:TYR:CE1	2.35	0.62
1:B:215:LYS:HE3	1:B:329:ASN:ND2	2.15	0.62
1:C:174:SER:O	1:C:176:SER:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LYS:HE3	1:C:329:ASN:ND2	2.13	0.61
1:A:107:GLY:HA3	1:A:110:TYR:HE1	1.65	0.61
1:A:499:ILE:HG13	1:A:502:VAL:HG21	1.81	0.61
1:B:229:GLU:HG3	1:B:344:LEU:HA	1.82	0.61
1:C:107:GLY:HA3	1:C:110:TYR:HE1	1.65	0.61
1:D:107:GLY:HA3	1:D:110:TYR:CE1	2.35	0.61
1:A:455:LYS:HE2	1:A:502:VAL:HG22	1.82	0.61
1:B:453:ASN:OD1	1:B:507:ILE:HG12	1.99	0.61
1:D:215:LYS:HE3	1:D:329:ASN:ND2	2.14	0.61
1:D:278:GLN:HG2	1:D:296:SER:HB2	1.82	0.61
1:B:107:GLY:HA3	1:B:110:TYR:CE1	2.35	0.61
1:C:176:SER:HB3	1:C:177:GLY:C	2.26	0.61
1:B:107:GLY:HA3	1:B:110:TYR:HE1	1.66	0.61
1:D:133:GLU:HB3	1:D:142:LYS:HB3	1.83	0.61
1:C:66:MET:HE3	1:C:66:MET:HA	1.83	0.61
1:C:409:PRO:O	1:C:454:TYR:HE1	1.80	0.61
1:A:161:PRO:HB3	1:A:187:ILE:HB	1.83	0.61
1:B:88:THR:O	1:B:90:LYS:HG2	2.01	0.60
1:C:278:GLN:HG2	1:C:296:SER:HB2	1.83	0.60
1:D:453:ASN:HB3	1:D:507:ILE:HG12	1.83	0.60
1:C:479:ALA:O	1:C:483:ASN:HB3	2.02	0.60
1:B:175:SER:N	1:B:176:SER:OG	2.33	0.60
1:B:406:LEU:O	1:B:406:LEU:HD12	2.02	0.60
1:C:51:VAL:O	1:C:55:GLY:HA2	2.02	0.60
1:A:278:GLN:HG2	1:A:296:SER:HB2	1.83	0.60
1:B:431:THR:O	1:B:442:ASN:HB2	2.01	0.60
1:A:97:GLY:HA3	1:A:256:PRO:HG2	1.84	0.60
1:A:409:PRO:C	1:A:454:TYR:CE1	2.71	0.60
1:A:50:LEU:HD12	1:A:50:LEU:C	2.26	0.59
1:C:213:ASN:N	1:C:213:ASN:HD22	2.00	0.59
1:D:50:LEU:C	1:D:50:LEU:HD12	2.26	0.59
1:A:419:VAL:HA	1:A:422:ALA:HB3	1.84	0.59
1:C:51:VAL:C	1:C:55:GLY:HA2	2.27	0.59
1:C:95:ILE:HG22	1:C:188:ILE:HG21	1.83	0.59
1:B:278:GLN:HG2	1:B:296:SER:HB2	1.84	0.59
1:D:213:ASN:HD22	1:D:213:ASN:N	2.01	0.59
1:B:34:GLN:OE1	1:B:230:LEU:HD11	2.03	0.59
1:A:347:ASN:O	1:A:348:ALA:C	2.45	0.59
1:A:382:SER:O	1:A:383:LEU:C	2.45	0.59
1:C:50:LEU:HD12	1:C:50:LEU:C	2.28	0.59
1:C:236:ILE:HD12	1:C:236:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:MET:HE3	1:A:66:MET:HA	1.85	0.59
1:C:509:THR:N	1:C:510:PRO:CD	2.66	0.59
1:C:133:GLU:HB3	1:C:142:LYS:HB3	1.84	0.59
1:D:246:LYS:O	1:D:250:ALA:CB	2.51	0.59
1:B:133:GLU:HB3	1:B:142:LYS:HB3	1.84	0.58
1:B:429:TRP:CZ2	1:B:441:PHE:HB2	2.38	0.58
1:B:66:MET:HA	1:B:66:MET:HE3	1.84	0.58
1:B:213:ASN:HD22	1:B:213:ASN:N	2.02	0.58
1:B:437:THR:HG23	1:B:438:ASP:OD2	2.03	0.58
1:B:499:ILE:CD1	1:B:502:VAL:HG11	2.34	0.58
1:B:501:ASN:C	1:B:502:VAL:HG12	2.27	0.58
1:C:382:SER:O	1:C:383:LEU:C	2.47	0.58
1:D:107:GLY:HA3	1:D:110:TYR:HE1	1.67	0.58
1:D:419:VAL:HA	1:D:422:ALA:HB3	1.84	0.58
1:C:110:TYR:CE1	1:C:180:ALA:HB2	2.39	0.58
1:C:454:TYR:CE2	1:C:469:PRO:HA	2.39	0.58
1:C:73:GLN:HB3	1:C:500:LEU:HD12	1.86	0.58
1:D:58:THR:C	1:D:60:GLU:H	2.11	0.58
1:A:391:LYS:CE	1:A:440:ASN:O	2.49	0.58
1:A:429:TRP:CZ2	1:A:441:PHE:HB2	2.39	0.58
1:A:501:ASN:OD1	1:A:501:ASN:N	2.36	0.58
1:C:453:ASN:HB3	1:C:507:ILE:HG12	1.86	0.58
1:C:27:ALA:HB2	1:C:71:PHE:CZ	2.38	0.58
1:A:456:TYR:HB3	1:A:504:LYS:HB3	1.85	0.57
1:D:450:ILE:HG12	1:D:451:ASP:N	2.19	0.57
1:A:60:GLU:HG2	1:A:347:ASN:HB2	1.85	0.57
1:B:398:ASP:O	1:B:401:GLN:HG3	2.03	0.57
1:C:478:CYS:O	1:C:481:THR:N	2.37	0.57
1:C:508:GLU:HB3	1:C:509:THR:HB	1.86	0.57
1:B:341:SER:C	1:B:343:GLY:H	2.12	0.57
1:B:509:THR:CG2	1:B:510:PRO:N	2.67	0.57
1:D:429:TRP:CZ2	1:D:441:PHE:HB2	2.39	0.57
1:A:456:TYR:O	1:A:503:ILE:HG12	2.04	0.57
1:D:171:ILE:HG22	1:D:172:SER:N	2.19	0.57
1:D:283:VAL:HG21	1:D:323:ILE:HD13	1.87	0.57
1:A:499:ILE:HG13	1:A:502:VAL:CG2	2.35	0.57
1:B:228:GLY:CA	1:B:345:SER:H	2.17	0.57
1:B:419:VAL:HA	1:B:422:ALA:HB3	1.85	0.57
1:A:373:PHE:HB2	1:A:405:VAL:HA	1.86	0.57
1:A:455:LYS:HG2	1:A:456:TYR:N	2.19	0.57
1:D:455:LYS:HE2	1:D:502:VAL:CG2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HG22	1:B:65:PHE:HZ	1.70	0.57
1:C:419:VAL:HA	1:C:422:ALA:HB3	1.86	0.57
1:D:302:LYS:HD3	1:D:306:ASP:HA	1.86	0.57
1:D:398:ASP:O	1:D:401:GLN:HG3	2.04	0.57
1:A:114:ASP:CG	1:A:175:SER:HB2	2.29	0.56
1:B:382:SER:O	1:B:383:LEU:C	2.47	0.56
1:B:430:ARG:CA	1:B:430:ARG:HE	2.18	0.56
1:B:499:ILE:HG12	1:B:502:VAL:HG21	1.85	0.56
1:A:178:LEU:CD2	1:A:178:LEU:N	2.66	0.56
1:C:398:ASP:O	1:C:401:GLN:HG3	2.05	0.56
1:A:133:GLU:HB3	1:A:142:LYS:HB3	1.86	0.56
1:B:51:VAL:CA	1:B:55:GLY:HA2	2.24	0.56
1:B:74:TYR:CE1	1:B:477:LEU:HD13	2.40	0.56
1:C:46:ASN:HB2	1:C:49:ASP:HB2	1.87	0.56
1:A:431:THR:O	1:A:432:ALA:HB2	2.06	0.56
1:B:211:GLN:HG3	1:C:299:ARG:NH2	2.20	0.56
1:C:150:ILE:HG22	1:C:167:TRP:CZ3	2.40	0.56
1:A:398:ASP:O	1:A:401:GLN:HG3	2.04	0.56
1:B:24:THR:CB	1:B:25:GLY:CA	2.83	0.56
1:C:373:PHE:HB2	1:C:405:VAL:HA	1.88	0.56
1:C:429:TRP:CZ2	1:C:441:PHE:HB2	2.41	0.56
1:C:502:VAL:O	1:C:502:VAL:CG1	2.51	0.56
1:B:328:GLN:HE21	1:C:299:ARG:CZ	2.19	0.56
1:D:66:MET:HE3	1:D:66:MET:HA	1.86	0.56
1:A:373:PHE:HB2	1:A:404:LEU:O	2.04	0.56
1:B:432:ALA:O	1:B:437:THR:HA	2.06	0.56
1:C:228:GLY:HA2	1:C:345:SER:N	2.21	0.56
1:D:58:THR:O	1:D:60:GLU:N	2.39	0.56
1:D:289:ILE:HD12	1:D:289:ILE:N	2.21	0.56
1:A:89:ALA:HB3	1:A:194:LEU:HD11	1.88	0.56
1:A:509:THR:N	1:A:510:PRO:HA	2.14	0.56
1:C:234:ILE:HB	1:C:340:LEU:HD12	1.88	0.56
1:C:373:PHE:HB2	1:C:404:LEU:O	2.06	0.56
1:D:382:SER:O	1:D:383:LEU:C	2.48	0.56
1:B:150:ILE:HG22	1:B:167:TRP:HZ3	1.71	0.55
1:B:150:ILE:HG22	1:B:167:TRP:CZ3	2.41	0.55
1:C:161:PRO:HB3	1:C:187:ILE:HB	1.87	0.55
1:C:171:ILE:HD11	1:C:182:ILE:HD11	1.87	0.55
1:C:481:THR:C	1:C:483:ASN:H	2.14	0.55
1:D:73:GLN:CB	1:D:500:LEU:HD12	2.31	0.55
1:A:84:VAL:CG1	1:A:85:ASP:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LYS:HD3	1:B:306:ASP:HA	1.89	0.55
1:C:150:ILE:HG22	1:C:167:TRP:HZ3	1.70	0.55
1:D:150:ILE:HG22	1:D:167:TRP:HZ3	1.72	0.55
1:D:150:ILE:HG22	1:D:167:TRP:CZ3	2.41	0.55
1:B:228:GLY:HA2	1:B:345:SER:CB	2.35	0.55
1:C:51:VAL:HG22	1:C:65:PHE:HZ	1.71	0.55
1:D:51:VAL:HG22	1:D:65:PHE:HZ	1.72	0.55
1:B:100:GLU:HG3	1:B:186:LYS:H	1.71	0.55
1:C:481:THR:C	1:C:483:ASN:N	2.65	0.55
1:C:483:ASN:O	1:C:484:VAL:O	2.25	0.55
1:D:381:GLU:HB3	1:D:385:THR:HG23	1.89	0.55
1:A:503:ILE:O	1:A:504:LYS:HB2	2.06	0.55
1:C:409:PRO:O	1:C:454:TYR:CZ	2.59	0.55
1:B:35:TRP:CE2	1:B:226:TYR:HD2	2.25	0.55
1:B:51:VAL:HG22	1:B:65:PHE:CZ	2.42	0.55
1:B:274:GLN:H	1:B:278:GLN:NE2	2.05	0.55
1:B:373:PHE:HB2	1:B:404:LEU:O	2.07	0.55
1:A:274:GLN:H	1:A:278:GLN:NE2	2.05	0.55
1:B:430:ARG:HE	1:B:430:ARG:HA	1.72	0.55
1:C:171:ILE:HG22	1:C:172:SER:N	2.06	0.55
1:C:302:LYS:HD3	1:C:306:ASP:HA	1.89	0.55
1:D:46:ASN:HB2	1:D:49:ASP:HB2	1.88	0.55
1:D:430:ARG:HD2	1:D:450:ILE:HD12	1.89	0.55
1:A:236:ILE:HD12	1:A:236:ILE:H	1.71	0.55
1:D:234:ILE:HB	1:D:340:LEU:HD12	1.89	0.55
1:D:373:PHE:HB2	1:D:405:VAL:HA	1.88	0.55
1:A:150:ILE:HG22	1:A:167:TRP:HZ3	1.72	0.54
1:A:245:ALA:C	1:A:247:GLY:H	2.15	0.54
1:A:283:VAL:HG21	1:A:323:ILE:HD13	1.88	0.54
1:A:454:TYR:HE2	1:A:469:PRO:CB	2.19	0.54
1:A:498:GLN:OE1	1:A:498:GLN:HA	2.07	0.54
1:B:46:ASN:HB2	1:B:49:ASP:HB2	1.89	0.54
1:D:453:ASN:HB3	1:D:507:ILE:CG1	2.37	0.54
1:A:302:LYS:HD3	1:A:306:ASP:HA	1.88	0.54
1:B:175:SER:CA	1:B:176:SER:OG	2.55	0.54
1:B:234:ILE:HB	1:B:340:LEU:HD12	1.90	0.54
1:C:451:ASP:OD2	1:C:470:LEU:HB3	2.06	0.54
1:A:51:VAL:HG22	1:A:65:PHE:HZ	1.73	0.54
1:A:71:PHE:C	1:A:71:PHE:CD2	2.85	0.54
1:A:173:SER:N	1:A:174:SER:HA	2.22	0.54
1:C:275:THR:OG1	1:C:278:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:THR:O	1:D:206:THR:HG22	2.07	0.54
1:D:236:ILE:HD12	1:D:236:ILE:H	1.72	0.54
1:D:456:TYR:HB3	1:D:504:LYS:HB3	1.90	0.54
1:A:371:GLN:HB3	1:A:484:VAL:HG23	1.90	0.54
1:C:30:ALA:HB3	1:C:359:TRP:CD2	2.42	0.54
1:D:228:GLY:HA2	1:D:345:SER:HB3	1.90	0.54
1:D:274:GLN:H	1:D:278:GLN:NE2	2.05	0.54
1:D:428:ASN:O	1:D:431:THR:C	2.51	0.54
1:D:507:ILE:O	1:D:508:GLU:HB2	2.07	0.54
1:C:508:GLU:O	1:C:510:PRO:HD3	2.08	0.54
1:A:206:THR:HG22	1:A:206:THR:O	2.07	0.54
1:B:275:THR:OG1	1:B:278:GLN:HG3	2.07	0.54
1:C:274:GLN:H	1:C:278:GLN:NE2	2.06	0.54
1:D:173:SER:N	1:D:174:SER:HA	2.21	0.54
1:D:453:ASN:H	1:D:453:ASN:HD22	1.55	0.54
1:A:381:GLU:HB3	1:A:385:THR:HG23	1.89	0.54
1:A:46:ASN:HB2	1:A:49:ASP:HB2	1.89	0.54
1:D:397:GLY:HA2	1:D:403:CYS:SG	2.47	0.54
1:A:455:LYS:HE2	1:A:502:VAL:CG2	2.37	0.53
1:C:283:VAL:HG21	1:C:323:ILE:HD13	1.90	0.53
1:D:455:LYS:HG2	1:D:456:TYR:N	2.23	0.53
1:A:23:SER:HG	1:A:483:ASN:HB3	1.70	0.53
1:B:98:ASN:ND2	1:B:256:PRO:HB3	2.23	0.53
1:B:236:ILE:HD12	1:B:236:ILE:H	1.72	0.53
1:A:150:ILE:HG22	1:A:167:TRP:CZ3	2.42	0.53
1:A:244:TYR:CD2	1:A:273:PRO:HD2	2.43	0.53
1:B:397:GLY:HA2	1:B:403:CYS:SG	2.49	0.53
1:C:51:VAL:HG22	1:C:65:PHE:CZ	2.43	0.53
1:C:206:THR:HG22	1:C:206:THR:O	2.08	0.53
1:B:381:GLU:HB3	1:B:385:THR:HG23	1.90	0.53
1:B:244:TYR:CD2	1:B:273:PRO:HD2	2.44	0.53
1:B:384:GLU:HA	1:B:439:ASN:OD1	2.09	0.53
1:B:478:CYS:HA	1:B:481:THR:HB	1.90	0.53
1:D:30:ALA:HB3	1:D:359:TRP:CD2	2.43	0.53
1:D:244:TYR:CD2	1:D:273:PRO:HD2	2.44	0.53
1:C:508:GLU:CB	1:C:509:THR:HB	2.39	0.53
1:D:275:THR:OG1	1:D:278:GLN:HG3	2.08	0.53
1:D:453:ASN:H	1:D:453:ASN:ND2	2.07	0.53
1:D:431:THR:OG1	1:D:432:ALA:N	2.42	0.53
1:A:179:ALA:HA	1:B:305:TYR:CD1	2.44	0.53
1:A:234:ILE:HB	1:A:340:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG12	1:A:399:VAL:O	2.09	0.53
1:B:74:TYR:CE2	1:B:473:ASP:OD2	2.62	0.53
1:B:455:LYS:HG2	1:B:456:TYR:N	2.24	0.53
1:C:71:PHE:C	1:C:71:PHE:CD2	2.87	0.53
1:C:236:ILE:HD12	1:C:236:ILE:N	2.24	0.53
1:C:455:LYS:HG2	1:C:456:TYR:N	2.24	0.53
1:D:51:VAL:HG22	1:D:65:PHE:CZ	2.44	0.53
1:A:374:ILE:HG23	1:A:472:ALA:HA	1.91	0.53
1:A:397:GLY:HA2	1:A:403:CYS:SG	2.49	0.53
1:C:29:LEU:O	1:C:80:VAL:HA	2.09	0.53
1:C:254:ILE:HG12	1:C:337:ILE:HB	1.91	0.53
1:C:453:ASN:HD22	1:C:453:ASN:H	1.57	0.53
1:D:29:LEU:O	1:D:80:VAL:HA	2.09	0.53
1:A:451:ASP:OD2	1:A:471:ALA:N	2.42	0.52
1:B:72:LEU:HA	1:B:75:GLY:O	2.09	0.52
1:B:283:VAL:HG21	1:B:323:ILE:HD13	1.92	0.52
1:A:172:SER:O	1:A:174:SER:HA	2.08	0.52
1:B:71:PHE:C	1:B:71:PHE:CD2	2.87	0.52
1:B:328:GLN:HE21	1:C:299:ARG:HE	1.52	0.52
1:B:434:GLY:O	1:B:437:THR:HG22	2.09	0.52
1:C:284:ARG:HA	1:C:288:ALA:O	2.10	0.52
1:A:450:ILE:CG1	1:A:451:ASP:N	2.53	0.52
1:B:194:LEU:HD23	1:B:195:LEU:N	2.24	0.52
1:D:254:ILE:HG12	1:D:337:ILE:HB	1.91	0.52
1:A:228:GLY:HA2	1:A:345:SER:CB	2.32	0.52
1:A:228:GLY:HA2	1:A:345:SER:H	1.74	0.52
1:C:397:GLY:HA2	1:C:403:CYS:SG	2.49	0.52
1:A:90:LYS:HB2	1:A:344:LEU:HB3	1.90	0.52
1:C:399:VAL:HG12	1:C:399:VAL:O	2.09	0.52
1:D:71:PHE:C	1:D:71:PHE:CD2	2.86	0.52
1:D:505:LEU:O	1:D:508:GLU:O	2.27	0.52
1:A:408:SER:CB	1:A:451:ASP:HB3	2.38	0.52
1:A:51:VAL:HG22	1:A:65:PHE:CZ	2.45	0.52
1:A:275:THR:OG1	1:A:278:GLN:HG3	2.10	0.52
1:A:440:ASN:C	1:A:440:ASN:HD22	2.17	0.52
1:B:428:ASN:HB3	1:B:433:ALA:O	2.10	0.52
1:C:508:GLU:C	1:C:510:PRO:HD3	2.34	0.52
1:D:383:LEU:O	1:D:386:ALA:HB3	2.10	0.52
1:D:454:TYR:CD2	1:D:469:PRO:HA	2.45	0.52
1:A:454:TYR:HE2	1:A:469:PRO:HB3	1.75	0.52
1:A:502:VAL:HG12	1:A:504:LYS:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ASN:H	1:B:453:ASN:HD22	1.57	0.52
1:C:51:VAL:O	1:C:55:GLY:CA	2.57	0.52
1:D:237:GLU:HG3	1:D:337:ILE:CD1	2.40	0.52
1:D:399:VAL:HG12	1:D:399:VAL:O	2.09	0.52
1:B:70:ASN:HB3	1:B:457:GLN:HE22	1.75	0.51
1:B:245:ALA:C	1:B:247:GLY:H	2.18	0.51
1:A:352:ALA:O	1:A:355:LEU:HB2	2.10	0.51
1:C:300:GLY:O	1:C:302:LYS:HG3	2.10	0.51
1:D:499:ILE:HG13	1:D:502:VAL:HG21	1.93	0.51
1:B:95:ILE:O	1:B:95:ILE:HG22	2.10	0.51
1:B:399:VAL:HG12	1:B:399:VAL:O	2.09	0.51
1:A:25:GLY:HA2	1:A:484:VAL:HG21	1.93	0.51
1:A:228:GLY:HA2	1:A:345:SER:N	2.25	0.51
1:A:237:GLU:HG3	1:A:337:ILE:CD1	2.41	0.51
1:C:381:GLU:HB3	1:C:385:THR:HG23	1.92	0.51
1:B:328:GLN:NE2	1:C:299:ARG:NE	2.54	0.51
1:B:374:ILE:HG23	1:B:472:ALA:HA	1.90	0.51
1:B:410:PRO:C	1:B:454:TYR:HE1	2.18	0.51
1:D:374:ILE:HG23	1:D:472:ALA:HA	1.91	0.51
1:A:453:ASN:HD22	1:A:453:ASN:H	1.58	0.51
1:C:244:TYR:CD2	1:C:273:PRO:HD2	2.46	0.51
1:D:63:ASP:O	1:D:67:SER:HB2	2.11	0.51
1:D:93:SER:O	1:D:96:ALA:HB2	2.10	0.51
1:B:24:THR:HG23	1:B:26:THR:N	2.25	0.51
1:C:30:ALA:HB3	1:C:359:TRP:CE2	2.46	0.51
1:C:71:PHE:C	1:C:73:GLN:H	2.19	0.51
1:C:502:VAL:O	1:C:502:VAL:HG13	2.07	0.51
1:A:198:ILE:HG23	1:A:201:ALA:HB2	1.92	0.51
1:B:220:PRO:HD2	1:B:338:LEU:HD11	1.93	0.51
1:C:176:SER:CB	1:C:177:GLY:HA2	2.41	0.51
1:D:130:LYS:O	1:D:132:THR:HG23	2.11	0.51
1:A:30:ALA:HB3	1:A:359:TRP:CD2	2.46	0.51
1:C:194:LEU:HD23	1:C:195:LEU:N	2.26	0.51
1:C:198:ILE:HG23	1:C:201:ALA:HB2	1.92	0.51
1:D:300:GLY:O	1:D:302:LYS:HG3	2.11	0.51
1:A:194:LEU:HD23	1:A:195:LEU:N	2.26	0.51
1:A:379:ALA:HB2	1:A:454:TYR:CE2	2.46	0.51
1:A:411:ARG:O	1:A:412:GLU:C	2.54	0.51
1:B:71:PHE:C	1:B:73:GLN:H	2.19	0.51
1:C:176:SER:CB	1:C:177:GLY:CA	2.88	0.51
1:C:215:LYS:CE	1:C:329:ASN:HD21	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:SER:C	1:C:348:ALA:H	2.17	0.51
1:C:431:THR:HG23	1:C:432:ALA:N	2.26	0.51
1:A:29:LEU:O	1:A:80:VAL:HA	2.10	0.50
1:B:24:THR:CG2	1:B:25:GLY:N	2.61	0.50
1:B:94:PRO:O	1:B:219:ILE:CD1	2.59	0.50
1:B:300:GLY:O	1:B:302:LYS:HG3	2.12	0.50
1:B:352:ALA:O	1:B:355:LEU:HB2	2.12	0.50
1:C:130:LYS:O	1:C:132:THR:HG23	2.10	0.50
1:C:220:PRO:HD2	1:C:338:LEU:HD11	1.93	0.50
1:C:245:ALA:C	1:C:247:GLY:H	2.19	0.50
1:B:328:GLN:HG2	1:C:299:ARG:NE	2.22	0.50
1:B:329:ASN:CG	1:C:299:ARG:HD2	2.37	0.50
1:B:499:ILE:HD11	1:B:502:VAL:HG11	1.93	0.50
1:C:73:GLN:HB3	1:C:500:LEU:CD1	2.41	0.50
1:A:70:ASN:HB3	1:A:457:GLN:HE22	1.76	0.50
1:B:347:ASN:HA	1:B:350:VAL:HG23	1.93	0.50
1:D:71:PHE:C	1:D:73:GLN:H	2.19	0.50
1:D:89:ALA:HB3	1:D:194:LEU:CD1	2.40	0.50
1:D:95:ILE:O	1:D:98:ASN:HB2	2.11	0.50
1:A:391:LYS:HE3	1:A:441:PHE:HA	1.92	0.50
1:B:63:ASP:O	1:B:67:SER:HB2	2.12	0.50
1:B:237:GLU:HG3	1:B:337:ILE:CD1	2.42	0.50
1:B:410:PRO:C	1:B:454:TYR:CE1	2.90	0.50
1:B:413:THR:OG1	1:B:425:ASN:HB3	2.12	0.50
1:A:179:ALA:HA	1:B:305:TYR:HD1	1.76	0.50
1:C:498:GLN:HG3	1:C:499:ILE:HD13	1.94	0.50
1:B:254:ILE:HG12	1:B:337:ILE:HB	1.93	0.50
1:A:84:VAL:HG13	1:A:89:ALA:HB2	1.92	0.50
1:A:161:PRO:O	1:A:186:LYS:HB3	2.11	0.50
1:A:300:GLY:O	1:A:302:LYS:HG3	2.11	0.50
1:B:382:SER:CB	1:B:385:THR:HG22	2.39	0.50
1:A:304:ILE:HG13	1:A:305:TYR:CD2	2.47	0.50
1:B:215:LYS:CE	1:B:329:ASN:HD21	2.25	0.50
1:C:70:ASN:HB3	1:C:457:GLN:HE22	1.77	0.50
1:C:508:GLU:CA	1:C:509:THR:HB	2.41	0.50
1:D:58:THR:C	1:D:60:GLU:N	2.69	0.50
1:A:71:PHE:C	1:A:73:GLN:N	2.69	0.50
1:A:382:SER:CB	1:A:385:THR:HG22	2.42	0.50
1:A:362:PHE:HA	1:A:368:VAL:HG21	1.94	0.49
1:A:509:THR:N	1:A:510:PRO:CA	2.73	0.49
1:C:289:ILE:HD12	1:C:289:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ILE:HG23	1:D:201:ALA:HB2	1.94	0.49
1:D:215:LYS:CE	1:D:329:ASN:HD21	2.25	0.49
1:A:407:CYS:N	1:A:449:ALA:O	2.44	0.49
1:A:23:SER:OG	1:A:483:ASN:HB2	2.04	0.49
1:A:254:ILE:HG12	1:A:337:ILE:HB	1.93	0.49
1:C:450:ILE:HG12	1:C:451:ASP:H	1.77	0.49
1:D:37:PRO:HB2	1:D:40:GLN:HB2	1.94	0.49
1:D:290:VAL:HG11	1:D:322:TYR:CD1	2.48	0.49
1:B:71:PHE:C	1:B:73:GLN:N	2.70	0.49
1:B:347:ASN:O	1:B:348:ALA:C	2.55	0.49
1:C:304:ILE:HG13	1:C:305:TYR:CD2	2.48	0.49
1:C:352:ALA:O	1:C:355:LEU:HB2	2.12	0.49
1:D:304:ILE:HG13	1:D:305:TYR:CD2	2.48	0.49
1:B:30:ALA:HB3	1:B:359:TRP:CD2	2.47	0.49
1:B:236:ILE:HD12	1:B:236:ILE:N	2.27	0.49
1:C:478:CYS:C	1:C:480:ARG:N	2.68	0.49
1:A:289:ILE:HD12	1:A:289:ILE:N	2.24	0.49
1:A:456:TYR:HB2	1:A:467:TRP:CZ3	2.48	0.49
1:B:202:GLU:HA	1:B:205:MET:HB2	1.93	0.49
1:C:63:ASP:O	1:C:67:SER:HB2	2.13	0.49
1:D:30:ALA:HB3	1:D:359:TRP:CE2	2.47	0.49
1:A:109:ASN:O	1:A:177:GLY:HA3	2.13	0.49
1:B:50:LEU:HD12	1:B:51:VAL:N	2.27	0.49
1:B:289:ILE:HD12	1:B:289:ILE:N	2.25	0.49
1:B:411:ARG:N	1:B:454:TYR:CE1	2.81	0.49
1:C:374:ILE:HG23	1:C:472:ALA:HA	1.93	0.49
1:D:350:VAL:HG13	1:D:354:ASP:HB2	1.94	0.49
1:B:350:VAL:HG13	1:B:354:ASP:HB2	1.95	0.49
1:B:383:LEU:O	1:B:386:ALA:HB3	2.12	0.49
1:B:445:SER:HB3	1:B:448:ALA:HB2	1.94	0.49
1:D:71:PHE:C	1:D:73:GLN:N	2.70	0.49
1:D:148:ALA:HB2	1:D:257:GLY:C	2.37	0.49
1:A:71:PHE:C	1:A:73:GLN:H	2.19	0.49
1:B:328:GLN:CG	1:C:299:ARG:HE	2.21	0.49
1:D:352:ALA:O	1:D:355:LEU:HB2	2.12	0.49
1:D:362:PHE:HA	1:D:368:VAL:HG21	1.95	0.49
1:A:383:LEU:O	1:A:386:ALA:HB3	2.13	0.49
1:B:431:THR:HG23	1:B:432:ALA:N	2.23	0.49
1:C:24:THR:HG23	1:C:24:THR:O	2.12	0.49
1:C:385:THR:HA	1:C:388:THR:HG23	1.95	0.49
1:A:236:ILE:HD12	1:A:236:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:PRO:HA	1:D:226:TYR:CD1	2.49	0.48
1:C:237:GLU:HG3	1:C:337:ILE:CD1	2.44	0.48
1:C:383:LEU:O	1:C:386:ALA:HB3	2.13	0.48
1:D:70:ASN:HB3	1:D:457:GLN:HE22	1.78	0.48
1:D:35:TRP:HB3	1:D:54:PHE:HA	1.96	0.48
1:D:382:SER:CB	1:D:385:THR:HG22	2.42	0.48
1:D:496:ARG:O	1:D:496:ARG:CG	2.58	0.48
1:A:220:PRO:HD2	1:A:338:LEU:HD11	1.94	0.48
1:C:411:ARG:O	1:C:412:GLU:C	2.56	0.48
1:C:285:ARG:O	1:C:286:ASN:HB2	2.12	0.48
1:A:376:GLY:HA2	1:A:390:GLN:NE2	2.28	0.48
1:A:453:ASN:H	1:A:453:ASN:ND2	2.11	0.48
1:D:211:GLN:OE1	1:D:328:GLN:HG2	2.14	0.48
1:A:408:SER:HA	1:A:451:ASP:O	2.14	0.48
1:B:284:ARG:HA	1:B:288:ALA:O	2.14	0.48
1:C:153:LYS:O	1:C:157:VAL:HG22	2.14	0.48
1:C:456:TYR:CZ	1:C:465:ASN:HB3	2.48	0.48
1:A:413:THR:OG1	1:A:425:ASN:HB3	2.14	0.48
1:B:35:TRP:HB3	1:B:54:PHE:HA	1.96	0.48
1:B:456:TYR:CE2	1:B:503:ILE:HD11	2.48	0.48
1:D:456:TYR:CZ	1:D:465:ASN:HB3	2.48	0.48
1:D:503:ILE:C	1:D:510:PRO:HG2	2.37	0.48
1:A:284:ARG:HA	1:A:288:ALA:O	2.14	0.48
1:A:456:TYR:CZ	1:A:465:ASN:HB3	2.49	0.48
1:B:456:TYR:HB2	1:B:467:TRP:CZ3	2.48	0.48
1:B:456:TYR:HD2	1:B:503:ILE:HD11	1.76	0.48
1:D:236:ILE:HD12	1:D:236:ILE:N	2.28	0.48
1:B:51:VAL:HG13	1:B:55:GLY:C	2.37	0.48
1:C:71:PHE:C	1:C:73:GLN:N	2.69	0.48
1:C:100:GLU:HG3	1:C:186:LYS:HG3	1.96	0.48
1:C:390:GLN:HE22	1:C:408:SER:H	1.62	0.48
1:A:63:ASP:O	1:A:67:SER:HB2	2.14	0.47
1:A:407:CYS:O	1:A:451:ASP:HB3	2.14	0.47
1:B:130:LYS:O	1:B:132:THR:HG23	2.14	0.47
1:B:453:ASN:H	1:B:453:ASN:ND2	2.12	0.47
1:D:284:ARG:HA	1:D:288:ALA:O	2.14	0.47
1:D:411:ARG:O	1:D:412:GLU:C	2.57	0.47
1:B:169:ALA:HB2	1:B:184:LEU:HD11	1.95	0.47
1:D:220:PRO:HD2	1:D:338:LEU:HD11	1.95	0.47
1:D:450:ILE:O	1:D:450:ILE:CG2	2.59	0.47
1:A:445:SER:HB3	1:A:448:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ALA:HB1	1:C:341:SER:OG	2.14	0.47
1:C:505:LEU:O	1:C:506:ALA:C	2.57	0.47
1:B:362:PHE:HA	1:B:368:VAL:HG21	1.95	0.47
1:C:68:ALA:O	1:C:69:MET:C	2.58	0.47
1:C:147:THR:O	1:C:151:ILE:HG23	2.14	0.47
1:C:208:VAL:HG23	1:C:209:ASP:N	2.30	0.47
1:D:456:TYR:HB2	1:D:467:TRP:CZ3	2.49	0.47
1:A:125:ILE:HD12	1:A:153:LYS:HG2	1.96	0.47
1:A:285:ARG:O	1:A:286:ASN:HB2	2.14	0.47
1:B:208:VAL:HG23	1:B:209:ASP:N	2.29	0.47
1:B:408:SER:OG	1:B:409:PRO:HD2	2.15	0.47
1:C:362:PHE:HA	1:C:368:VAL:HG21	1.95	0.47
1:D:68:ALA:O	1:D:69:MET:C	2.58	0.47
1:A:30:ALA:HB3	1:A:359:TRP:CE2	2.49	0.47
1:A:151:ILE:HG13	1:A:152:ALA:N	2.30	0.47
1:A:407:CYS:O	1:A:451:ASP:N	2.48	0.47
1:B:44:VAL:HG11	1:B:50:LEU:HB3	1.96	0.47
1:B:174:SER:O	1:B:175:SER:HB3	2.15	0.47
1:B:293:VAL:HG22	1:B:294:VAL:N	2.29	0.47
1:C:61:THR:O	1:C:62:ALA:C	2.57	0.47
1:C:200:ASN:O	1:C:201:ALA:C	2.57	0.47
1:C:350:VAL:HG13	1:C:354:ASP:HB2	1.95	0.47
1:C:407:CYS:N	1:C:449:ALA:O	2.38	0.47
1:C:413:THR:OG1	1:C:425:ASN:HB3	2.14	0.47
1:C:453:ASN:H	1:C:453:ASN:ND2	2.13	0.47
1:C:456:TYR:CB	1:C:504:LYS:HB3	2.43	0.47
1:D:37:PRO:CA	1:D:226:TYR:CE1	2.97	0.47
1:D:445:SER:HB3	1:D:448:ALA:HB2	1.97	0.47
1:A:509:THR:CB	1:A:510:PRO:HA	2.44	0.47
1:B:100:GLU:HG3	1:B:186:LYS:N	2.29	0.47
1:B:252:LEU:HA	1:B:253:PRO:HD3	1.78	0.47
1:B:285:ARG:O	1:B:286:ASN:HB2	2.15	0.47
1:B:346:SER:HB2	1:B:348:ALA:HB3	1.97	0.47
1:B:402:ASP:CG	1:B:402:ASP:O	2.58	0.47
1:D:58:THR:H	1:D:61:THR:HB	1.79	0.47
1:A:27:ALA:HB2	1:A:71:PHE:CZ	2.50	0.47
1:A:215:LYS:CE	1:A:329:ASN:HD21	2.25	0.47
1:B:304:ILE:HG13	1:B:305:TYR:CD2	2.50	0.47
1:C:88:THR:O	1:C:89:ALA:C	2.58	0.47
1:C:293:VAL:HG22	1:C:294:VAL:N	2.29	0.47
1:C:508:GLU:HA	1:C:509:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:H	1:D:197:GLU:CD	2.22	0.47
1:D:402:ASP:CG	1:D:402:ASP:O	2.57	0.47
1:A:502:VAL:HG12	1:A:503:ILE:N	2.29	0.47
1:D:153:LYS:O	1:D:157:VAL:HG22	2.14	0.47
1:D:385:THR:HA	1:D:388:THR:HG23	1.96	0.47
1:A:453:ASN:ND2	1:A:453:ASN:N	2.62	0.46
1:C:37:PRO:HB2	1:C:40:GLN:HB2	1.97	0.46
1:C:174:SER:O	1:C:175:SER:C	2.58	0.46
1:A:290:VAL:HG11	1:A:322:TYR:CD1	2.50	0.46
1:B:411:ARG:O	1:B:412:GLU:C	2.57	0.46
1:B:508:GLU:O	1:B:509:THR:O	2.33	0.46
1:A:58:THR:H	1:A:61:THR:HB	1.79	0.46
1:A:62:ALA:HB1	1:A:466:ARG:NE	2.30	0.46
1:A:350:VAL:HG13	1:A:354:ASP:HB2	1.97	0.46
1:B:95:ILE:HD11	1:B:214:LEU:CD2	2.39	0.46
1:B:163:LEU:HB3	1:B:164:GLY:H	1.60	0.46
1:C:290:VAL:HG11	1:C:322:TYR:CD1	2.50	0.46
1:C:307:SER:O	1:C:309:ILE:HG23	2.15	0.46
1:C:346:SER:C	1:C:348:ALA:N	2.73	0.46
1:D:37:PRO:HA	1:D:226:TYR:CE1	2.50	0.46
1:D:307:SER:O	1:D:309:ILE:HG23	2.15	0.46
1:A:173:SER:HA	1:A:174:SER:HB3	1.98	0.46
1:C:381:GLU:O	1:C:382:SER:C	2.58	0.46
1:C:445:SER:HB3	1:C:448:ALA:HB2	1.98	0.46
1:D:62:ALA:HB1	1:D:466:ARG:NE	2.30	0.46
1:D:376:GLY:HA2	1:D:390:GLN:NE2	2.31	0.46
1:A:68:ALA:O	1:A:69:MET:C	2.58	0.46
1:B:197:GLU:CD	1:B:197:GLU:H	2.24	0.46
1:B:406:LEU:HA	1:B:449:ALA:O	2.15	0.46
1:B:456:TYR:CZ	1:B:465:ASN:HB3	2.51	0.46
1:C:382:SER:CB	1:C:385:THR:HG22	2.42	0.46
1:C:501:ASN:H	1:C:501:ASN:ND2	2.13	0.46
1:D:173:SER:HA	1:D:174:SER:HB3	1.96	0.46
1:D:194:LEU:HD23	1:D:195:LEU:N	2.29	0.46
1:D:285:ARG:O	1:D:286:ASN:HB2	2.16	0.46
1:A:100:GLU:HG2	1:A:186:LYS:O	2.16	0.46
1:B:509:THR:CG2	1:B:510:PRO:C	2.85	0.46
1:C:51:VAL:HG13	1:C:55:GLY:C	2.40	0.46
1:D:27:ALA:HB3	1:D:78:LEU:HD12	1.96	0.46
1:D:50:LEU:HD12	1:D:51:VAL:N	2.31	0.46
1:D:61:THR:O	1:D:62:ALA:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:HB3	1:A:54:PHE:HA	1.98	0.46
1:A:61:THR:O	1:A:62:ALA:C	2.59	0.46
1:A:208:VAL:HG23	1:A:209:ASP:N	2.31	0.46
1:A:293:VAL:HG22	1:A:294:VAL:N	2.30	0.46
1:B:344:LEU:HD13	1:B:344:LEU:O	2.15	0.46
1:C:456:TYR:HB2	1:C:467:TRP:CZ3	2.50	0.46
1:D:147:THR:O	1:D:151:ILE:HG23	2.15	0.46
1:A:37:PRO:HB2	1:A:40:GLN:HB2	1.97	0.46
1:A:73:GLN:HB3	1:A:500:LEU:HD12	1.98	0.46
1:C:402:ASP:O	1:C:402:ASP:CG	2.57	0.46
1:D:413:THR:OG1	1:D:425:ASN:HB3	2.15	0.46
1:A:458:TYR:CE2	1:A:460:LYS:HA	2.51	0.46
1:C:26:THR:HA	1:C:77:ASP:OD1	2.15	0.46
1:C:215:LYS:HE3	1:C:329:ASN:CG	2.41	0.46
1:D:419:VAL:HA	1:D:422:ALA:CB	2.46	0.46
1:D:454:TYR:HD2	1:D:468:VAL:O	1.99	0.46
1:A:423:VAL:O	1:A:424:ASP:C	2.59	0.46
1:B:66:MET:O	1:B:67:SER:C	2.58	0.46
1:B:376:GLY:HA2	1:B:390:GLN:NE2	2.31	0.46
1:C:174:SER:O	1:C:176:SER:O	2.34	0.46
1:B:385:THR:HA	1:B:388:THR:HG23	1.97	0.45
1:A:419:VAL:HA	1:A:422:ALA:CB	2.46	0.45
1:C:58:THR:H	1:C:61:THR:HB	1.81	0.45
1:C:91:ASN:O	1:C:92:SER:C	2.57	0.45
1:C:252:LEU:HA	1:C:253:PRO:HD3	1.80	0.45
1:D:293:VAL:HG22	1:D:294:VAL:N	2.31	0.45
1:A:130:LYS:O	1:A:132:THR:HG23	2.16	0.45
1:A:215:LYS:HE3	1:A:329:ASN:CG	2.42	0.45
1:A:307:SER:O	1:A:309:ILE:HG23	2.16	0.45
1:B:509:THR:HG22	1:B:510:PRO:N	2.30	0.45
1:C:62:ALA:HB1	1:C:466:ARG:NE	2.31	0.45
1:C:197:GLU:CD	1:C:197:GLU:H	2.24	0.45
1:C:211:GLN:OE1	1:C:328:GLN:HG2	2.15	0.45
1:C:478:CYS:O	1:C:482:ASP:N	2.49	0.45
1:D:73:GLN:HB3	1:D:500:LEU:CD1	2.33	0.45
1:D:453:ASN:ND2	1:D:453:ASN:N	2.65	0.45
1:A:200:ASN:O	1:A:201:ALA:C	2.59	0.45
1:A:402:ASP:O	1:A:402:ASP:CG	2.59	0.45
1:B:58:THR:H	1:B:61:THR:HB	1.81	0.45
1:B:143:ILE:HD13	1:B:182:ILE:HD13	1.99	0.45
1:C:228:GLY:HA2	1:C:345:SER:CB	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:HG2	1:D:186:LYS:O	2.17	0.45
1:D:215:LYS:HE3	1:D:329:ASN:CG	2.41	0.45
1:A:283:VAL:CG2	1:A:323:ILE:HD13	2.47	0.45
1:A:385:THR:HA	1:A:388:THR:HG23	1.98	0.45
1:A:456:TYR:CE2	1:A:503:ILE:HD11	2.52	0.45
1:B:68:ALA:O	1:B:69:MET:C	2.59	0.45
1:B:215:LYS:HE3	1:B:329:ASN:OD1	2.16	0.45
1:B:381:GLU:O	1:B:382:SER:C	2.59	0.45
1:C:35:TRP:NE1	1:C:226:TYR:HD2	2.13	0.45
1:C:89:ALA:O	1:C:194:LEU:HD12	2.17	0.45
1:C:110:TYR:CZ	1:C:180:ALA:HB2	2.52	0.45
1:D:163:LEU:HB3	1:D:164:GLY:H	1.64	0.45
1:A:153:LYS:O	1:A:157:VAL:HG22	2.17	0.45
1:A:197:GLU:CD	1:A:197:GLU:H	2.23	0.45
1:B:62:ALA:HB1	1:B:466:ARG:NE	2.31	0.45
1:C:125:ILE:HD12	1:C:153:LYS:HG2	1.99	0.45
1:C:356:MET:HE3	1:C:392:HIS:CG	2.52	0.45
1:D:200:ASN:O	1:D:201:ALA:C	2.59	0.45
1:D:229:GLU:CD	1:D:229:GLU:H	2.24	0.45
1:D:459:ASP:OD2	1:D:459:ASP:C	2.60	0.45
1:A:50:LEU:HD12	1:A:51:VAL:N	2.32	0.45
1:A:51:VAL:HG13	1:A:55:GLY:C	2.42	0.45
1:D:148:ALA:HB2	1:D:257:GLY:O	2.17	0.45
1:D:208:VAL:HG23	1:D:209:ASP:N	2.32	0.45
1:A:211:GLN:OE1	1:A:328:GLN:HG2	2.16	0.45
1:B:343:GLY:O	1:B:344:LEU:HB2	2.17	0.45
1:C:119:LYS:HE3	1:C:124:ASP:OD1	2.17	0.45
1:D:496:ARG:HD3	1:D:497:GLY:C	2.41	0.45
1:A:66:MET:O	1:A:67:SER:C	2.60	0.45
1:B:215:LYS:HE3	1:B:329:ASN:CG	2.42	0.45
1:C:34:GLN:OE1	1:C:230:LEU:HD11	2.17	0.45
1:D:342:GLY:O	1:D:343:GLY:C	2.60	0.45
1:D:254:ILE:HB	1:D:258:GLY:O	2.17	0.45
1:D:458:TYR:CE2	1:D:460:LYS:HA	2.52	0.45
1:D:478:CYS:C	1:D:480:ARG:N	2.73	0.45
1:B:125:ILE:HD12	1:B:153:LYS:HG2	1.98	0.44
1:B:147:THR:O	1:B:151:ILE:HG23	2.17	0.44
1:B:499:ILE:HG12	1:B:502:VAL:CB	2.47	0.44
1:C:453:ASN:HD22	1:C:453:ASN:N	2.15	0.44
1:D:151:ILE:HG13	1:D:152:ALA:N	2.30	0.44
1:B:35:TRP:NE1	1:B:226:TYR:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG11	1:D:50:LEU:HB3	1.98	0.44
1:D:373:PHE:HB2	1:D:404:LEU:O	2.17	0.44
1:A:44:VAL:HG11	1:A:50:LEU:HB3	1.99	0.44
1:A:147:THR:O	1:A:151:ILE:HG23	2.17	0.44
1:A:454:TYR:O	1:A:467:TRP:CZ3	2.71	0.44
1:B:95:ILE:HG13	1:B:219:ILE:HD11	1.98	0.44
1:C:509:THR:O	1:C:509:THR:CG2	2.56	0.44
1:B:30:ALA:HB3	1:B:359:TRP:CE2	2.51	0.44
1:B:307:SER:O	1:B:309:ILE:HG23	2.17	0.44
1:B:391:LYS:HE3	1:B:440:ASN:HD21	1.82	0.44
1:C:453:ASN:ND2	1:C:453:ASN:N	2.65	0.44
1:D:356:MET:HE3	1:D:392:HIS:CG	2.53	0.44
1:D:365:ARG:O	1:D:366:GLU:C	2.61	0.44
1:D:381:GLU:O	1:D:382:SER:C	2.60	0.44
1:A:27:ALA:HB3	1:A:78:LEU:HD12	1.98	0.44
1:A:229:GLU:H	1:A:229:GLU:CD	2.26	0.44
1:A:375:ALA:HB3	1:A:406:LEU:O	2.17	0.44
1:B:502:VAL:O	1:B:502:VAL:CG1	2.48	0.44
1:D:66:MET:O	1:D:67:SER:C	2.61	0.44
1:A:109:ASN:C	1:A:177:GLY:HA3	2.43	0.44
1:B:61:THR:O	1:B:62:ALA:C	2.60	0.44
1:C:67:SER:OG	1:C:472:ALA:HB2	2.18	0.44
1:C:197:GLU:HB3	1:C:199:GLU:CD	2.43	0.44
1:C:408:SER:OG	1:C:409:PRO:HD2	2.17	0.44
1:C:500:LEU:HB3	1:C:501:ASN:ND2	2.32	0.44
1:D:290:VAL:HG11	1:D:322:TYR:CE1	2.53	0.44
1:A:381:GLU:O	1:A:382:SER:C	2.59	0.44
1:B:419:VAL:HA	1:B:422:ALA:CB	2.48	0.44
1:D:283:VAL:CG2	1:D:323:ILE:HD13	2.46	0.44
1:B:67:SER:OG	1:B:472:ALA:HB2	2.18	0.44
1:B:153:LYS:O	1:B:157:VAL:HG22	2.18	0.44
1:B:161:PRO:O	1:B:162:THR:C	2.60	0.44
1:D:215:LYS:HE3	1:D:329:ASN:OD1	2.18	0.44
1:A:364:ASP:OD1	1:A:364:ASP:N	2.50	0.43
1:A:478:CYS:C	1:A:480:ARG:N	2.72	0.43
1:B:34:GLN:HE21	1:B:58:THR:HG22	1.83	0.43
1:B:37:PRO:HB2	1:B:40:GLN:HB2	2.00	0.43
1:B:84:VAL:HG13	1:B:89:ALA:HB3	2.00	0.43
1:D:240:SER:HB3	1:D:279:TYR:CE1	2.53	0.43
1:A:100:GLU:HB2	1:A:185:GLY:CA	2.48	0.43
1:A:408:SER:OG	1:A:451:ASP:OD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLY:O	1:B:65:PHE:CE1	2.72	0.43
1:B:194:LEU:HD23	1:B:194:LEU:C	2.43	0.43
1:C:66:MET:O	1:C:67:SER:C	2.59	0.43
1:C:215:LYS:HE3	1:C:329:ASN:OD1	2.18	0.43
1:B:60:GLU:HG2	1:B:347:ASN:HB2	2.00	0.43
1:B:290:VAL:HG11	1:B:322:TYR:CD1	2.52	0.43
1:B:508:GLU:C	1:B:509:THR:O	2.62	0.43
1:C:253:PRO:HD2	1:C:336:GLY:HA2	1.99	0.43
1:D:91:ASN:O	1:D:92:SER:C	2.61	0.43
1:D:125:ILE:HD12	1:D:153:LYS:HG2	1.99	0.43
1:A:194:LEU:HD23	1:A:194:LEU:C	2.44	0.43
1:A:254:ILE:HB	1:A:258:GLY:O	2.18	0.43
1:B:499:ILE:CG1	1:B:502:VAL:CG2	2.83	0.43
1:C:161:PRO:O	1:C:162:THR:C	2.61	0.43
1:C:236:ILE:HD11	1:C:340:LEU:HD11	2.00	0.43
1:A:240:SER:HB3	1:A:279:TYR:CE1	2.53	0.43
1:A:508:GLU:HA	1:A:509:THR:HA	1.59	0.43
1:B:450:ILE:HG12	1:B:451:ASP:N	2.31	0.43
1:B:453:ASN:ND2	1:B:453:ASN:N	2.65	0.43
1:C:50:LEU:HD12	1:C:51:VAL:N	2.33	0.43
1:D:222:VAL:HG11	1:D:236:ILE:HG12	2.00	0.43
1:A:253:PRO:HD2	1:A:336:GLY:HA2	2.00	0.43
1:B:407:CYS:N	1:B:449:ALA:O	2.35	0.43
1:C:44:VAL:HG11	1:C:50:LEU:HB3	1.99	0.43
1:C:62:ALA:HB1	1:C:466:ARG:HE	1.84	0.43
1:D:62:ALA:HB1	1:D:466:ARG:HE	1.82	0.43
1:D:502:VAL:CG1	1:D:510:PRO:HG3	2.48	0.43
1:D:502:VAL:CG1	1:D:503:ILE:N	2.80	0.43
1:A:34:GLN:OE1	1:A:230:LEU:HD11	2.19	0.43
1:A:171:ILE:CG2	1:A:172:SER:H	2.25	0.43
1:A:377:SER:HA	1:A:469:PRO:HG3	2.00	0.43
1:A:390:GLN:HE22	1:A:408:SER:H	1.65	0.43
1:B:240:SER:HB3	1:B:279:TYR:CE1	2.53	0.43
1:B:391:LYS:HE3	1:B:440:ASN:ND2	2.33	0.43
1:C:35:TRP:CE2	1:C:226:TYR:HD2	2.37	0.43
1:C:162:THR:O	1:C:163:LEU:HB2	2.18	0.43
1:C:376:GLY:HA2	1:C:390:GLN:NE2	2.34	0.43
1:A:99:ILE:O	1:A:100:GLU:C	2.61	0.43
1:B:312:ASP:O	1:B:316:ALA:HB2	2.19	0.43
1:C:27:ALA:HB3	1:C:78:LEU:HD12	2.01	0.43
1:D:119:LYS:HE3	1:D:124:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:HB3	1:D:199:GLU:CD	2.43	0.43
1:D:390:GLN:O	1:D:391:LYS:C	2.62	0.43
1:A:48:VAL:O	1:A:48:VAL:HG12	2.19	0.43
1:A:90:LYS:N	1:A:344:LEU:O	2.48	0.43
1:A:499:ILE:HD13	1:A:499:ILE:N	2.28	0.43
1:A:508:GLU:CG	1:A:509:THR:HG22	2.36	0.43
1:B:151:ILE:HG13	1:B:152:ALA:N	2.30	0.43
1:B:197:GLU:HB3	1:B:199:GLU:CD	2.43	0.43
1:B:356:MET:HE3	1:B:392:HIS:CG	2.53	0.43
1:C:95:ILE:O	1:C:96:ALA:C	2.61	0.43
1:C:151:ILE:HG13	1:C:152:ALA:N	2.31	0.43
1:A:67:SER:OG	1:A:472:ALA:HB2	2.19	0.43
1:A:197:GLU:HB3	1:A:199:GLU:CD	2.44	0.43
1:A:215:LYS:HE3	1:A:329:ASN:OD1	2.19	0.43
1:A:502:VAL:CG1	1:A:504:LYS:H	2.31	0.43
1:C:390:GLN:O	1:C:391:LYS:C	2.62	0.43
1:A:236:ILE:HD11	1:A:340:LEU:HD11	2.01	0.42
1:A:440:ASN:ND2	1:A:440:ASN:C	2.77	0.42
1:B:175:SER:HA	1:B:176:SER:OG	2.19	0.42
1:B:254:ILE:HB	1:B:258:GLY:O	2.18	0.42
1:B:453:ASN:HD22	1:B:453:ASN:N	2.15	0.42
1:B:499:ILE:HG12	1:B:502:VAL:HG11	2.00	0.42
1:C:423:VAL:O	1:C:424:ASP:C	2.62	0.42
1:C:501:ASN:ND2	1:C:501:ASN:N	2.66	0.42
1:A:295:LEU:HD11	1:A:314:PHE:CD2	2.54	0.42
1:B:481:THR:O	1:B:482:ASP:C	2.62	0.42
1:C:240:SER:HB3	1:C:279:TYR:CE1	2.54	0.42
1:C:501:ASN:H	1:C:501:ASN:HD22	1.67	0.42
1:D:499:ILE:HG13	1:D:502:VAL:CG2	2.48	0.42
1:A:62:ALA:HB1	1:A:466:ARG:HE	1.83	0.42
1:A:91:ASN:ND2	1:A:226:TYR:C	2.78	0.42
1:C:377:SER:HA	1:C:469:PRO:HG3	2.01	0.42
1:C:458:TYR:CE2	1:C:460:LYS:HA	2.54	0.42
1:D:253:PRO:HD2	1:D:336:GLY:HA2	2.00	0.42
1:D:408:SER:OG	1:D:409:PRO:HD2	2.18	0.42
1:C:228:GLY:HA2	1:C:345:SER:H	1.84	0.42
1:D:312:ASP:O	1:D:316:ALA:HB2	2.20	0.42
1:A:97:GLY:O	1:A:98:ASN:O	2.37	0.42
1:B:55:GLY:O	1:B:65:PHE:HE1	2.03	0.42
1:B:56:GLN:HA	1:B:57:PRO:HD3	1.84	0.42
1:B:283:VAL:CG2	1:B:323:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LEU:HD23	1:C:194:LEU:C	2.45	0.42
1:D:43:GLN:NE2	1:D:77:ASP:HB2	2.34	0.42
1:D:344:LEU:HA	1:D:344:LEU:HD22	1.74	0.42
1:A:161:PRO:O	1:A:162:THR:C	2.63	0.42
1:B:390:GLN:O	1:B:391:LYS:C	2.62	0.42
1:C:84:VAL:HG12	1:C:85:ASP:O	2.10	0.42
1:C:211:GLN:CD	1:C:328:GLN:HG2	2.45	0.42
1:D:151:ILE:HG22	1:D:187:ILE:CD1	2.48	0.42
1:A:89:ALA:HB3	1:A:194:LEU:CD1	2.49	0.42
1:B:99:ILE:H	1:B:99:ILE:HG22	1.57	0.42
1:C:46:ASN:HB2	1:C:49:ASP:CB	2.49	0.42
1:C:290:VAL:HG11	1:C:322:TYR:CE1	2.55	0.42
1:D:308:ASN:HD21	1:D:313:ASP:CB	2.33	0.42
1:A:24:THR:O	1:A:26:THR:N	2.52	0.42
1:A:77:ASP:OD1	1:A:77:ASP:O	2.37	0.42
1:A:222:VAL:HG11	1:A:236:ILE:HG12	2.00	0.42
1:A:502:VAL:CG1	1:A:503:ILE:N	2.82	0.42
1:B:229:GLU:CD	1:B:229:GLU:H	2.27	0.42
1:B:383:LEU:O	1:B:384:GLU:C	2.62	0.42
1:C:341:SER:C	1:C:343:GLY:H	2.28	0.42
1:C:371:GLN:O	1:C:403:CYS:HA	2.20	0.42
1:C:419:VAL:HA	1:C:422:ALA:CB	2.50	0.42
1:B:88:THR:O	1:B:89:ALA:C	2.63	0.42
1:B:370:VAL:O	1:B:370:VAL:HG23	2.19	0.42
1:B:508:GLU:O	1:B:509:THR:C	2.61	0.42
1:A:312:ASP:O	1:A:316:ALA:HB2	2.19	0.42
1:C:480:ARG:O	1:C:484:VAL:HA	2.20	0.42
1:D:68:ALA:O	1:D:71:PHE:HB3	2.20	0.42
1:D:371:GLN:O	1:D:403:CYS:HA	2.19	0.42
1:A:100:GLU:HG3	1:A:186:LYS:N	2.32	0.41
1:A:304:ILE:HG13	1:A:305:TYR:HE2	1.82	0.41
1:B:194:LEU:C	1:B:194:LEU:CD2	2.93	0.41
1:B:207:ALA:O	1:B:208:VAL:C	2.63	0.41
1:C:364:ASP:OD1	1:C:364:ASP:N	2.52	0.41
1:C:459:ASP:OD2	1:C:459:ASP:C	2.63	0.41
1:A:56:GLN:HA	1:A:57:PRO:HD3	1.81	0.41
1:A:101:TYR:CD2	1:A:101:TYR:C	2.98	0.41
1:A:205:MET:HE3	1:A:205:MET:HB3	1.97	0.41
1:A:406:LEU:HA	1:A:449:ALA:O	2.20	0.41
1:C:229:GLU:H	1:C:229:GLU:CD	2.28	0.41
1:A:207:ALA:O	1:A:208:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PRO:HD2	1:B:336:GLY:HA2	2.02	0.41
1:D:86:ARG:HG3	1:D:86:ARG:HH11	1.85	0.41
1:D:162:THR:HA	1:D:186:LYS:NZ	2.36	0.41
1:D:401:GLN:HG2	1:D:447:TYR:CE1	2.55	0.41
1:A:50:LEU:HD11	1:A:65:PHE:CE1	2.56	0.41
1:B:295:LEU:HD11	1:B:314:PHE:CD2	2.55	0.41
1:C:43:GLN:NE2	1:C:77:ASP:HB2	2.35	0.41
1:C:77:ASP:OD1	1:C:77:ASP:O	2.38	0.41
1:C:222:VAL:HG11	1:C:236:ILE:HG12	2.03	0.41
1:A:341:SER:C	1:A:343:GLY:H	2.29	0.41
1:A:408:SER:OG	1:A:409:PRO:HD2	2.21	0.41
1:B:94:PRO:HD3	1:B:222:VAL:O	2.20	0.41
1:B:99:ILE:HG23	1:B:99:ILE:O	2.20	0.41
1:B:174:SER:O	1:B:175:SER:CB	2.69	0.41
1:B:379:ALA:CB	1:B:454:TYR:CZ	2.83	0.41
1:B:507:ILE:O	1:B:507:ILE:CG1	2.68	0.41
1:D:236:ILE:HD11	1:D:340:LEU:HD11	2.03	0.41
1:D:295:LEU:HD11	1:D:314:PHE:CD2	2.54	0.41
1:D:411:ARG:HG3	1:D:454:TYR:CE1	2.55	0.41
1:A:390:GLN:O	1:A:391:LYS:C	2.63	0.41
1:B:29:LEU:HD12	1:B:30:ALA:N	2.35	0.41
1:B:334:PHE:CD2	1:B:334:PHE:C	2.98	0.41
1:C:254:ILE:HB	1:C:258:GLY:O	2.21	0.41
1:D:161:PRO:O	1:D:162:THR:C	2.64	0.41
1:A:119:LYS:HE3	1:A:124:ASP:OD1	2.20	0.41
1:A:163:LEU:HB3	1:A:164:GLY:H	1.63	0.41
1:A:370:VAL:HG23	1:A:370:VAL:O	2.20	0.41
1:A:371:GLN:O	1:A:403:CYS:HA	2.20	0.41
1:C:369:ASP:OD2	1:C:369:ASP:N	2.50	0.41
1:C:370:VAL:HG23	1:C:370:VAL:O	2.21	0.41
1:C:401:GLN:HG2	1:C:447:TYR:CE1	2.55	0.41
1:C:478:CYS:C	1:C:481:THR:H	2.26	0.41
1:D:89:ALA:O	1:D:90:LYS:HD3	2.20	0.41
1:A:303:ASP:C	1:A:305:TYR:H	2.29	0.41
1:A:409:PRO:HG2	1:A:454:TYR:CE1	2.55	0.41
1:B:458:TYR:CE2	1:B:460:LYS:HA	2.56	0.41
1:C:101:TYR:CD2	1:C:101:TYR:C	2.99	0.41
1:C:283:VAL:CG2	1:C:323:ILE:HD13	2.49	0.41
1:C:295:LEU:HD11	1:C:314:PHE:CD2	2.56	0.41
1:D:334:PHE:CD2	1:D:334:PHE:C	2.98	0.41
1:D:500:LEU:HB3	1:D:501:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:HB2	1:A:49:ASP:CB	2.50	0.41
1:A:55:GLY:C	1:A:65:PHE:HE1	2.29	0.41
1:B:24:THR:CG2	1:B:25:GLY:C	2.90	0.41
1:B:282:ILE:HG23	1:B:289:ILE:HG23	2.02	0.41
1:B:451:ASP:CG	1:B:452:GLY:H	2.29	0.41
1:B:459:ASP:OD2	1:B:459:ASP:C	2.64	0.41
1:C:246:LYS:O	1:C:248:ALA:N	2.54	0.41
1:C:427:VAL:O	1:C:431:THR:HG22	2.20	0.41
1:C:480:ARG:O	1:C:484:VAL:C	2.64	0.41
1:D:51:VAL:HG13	1:D:55:GLY:C	2.44	0.41
1:D:55:GLY:C	1:D:65:PHE:HE1	2.29	0.41
1:D:67:SER:OG	1:D:472:ALA:HB2	2.21	0.41
1:D:77:ASP:OD1	1:D:77:ASP:O	2.38	0.41
1:D:149:LYS:O	1:D:152:ALA:HB3	2.21	0.41
1:D:303:ASP:C	1:D:305:TYR:H	2.29	0.41
1:D:304:ILE:HG13	1:D:305:TYR:HE2	1.83	0.41
1:A:308:ASN:HD21	1:A:313:ASP:CB	2.34	0.41
1:B:163:LEU:HD22	1:B:167:TRP:CE2	2.56	0.41
1:B:401:GLN:HG2	1:B:447:TYR:CE1	2.56	0.41
1:B:499:ILE:HG12	1:B:502:VAL:CG2	2.49	0.41
1:B:499:ILE:N	1:B:499:ILE:HD13	2.36	0.41
1:C:48:VAL:HG12	1:C:48:VAL:O	2.21	0.41
1:C:55:GLY:C	1:C:65:PHE:HE1	2.23	0.41
1:D:48:VAL:O	1:D:48:VAL:HG12	2.21	0.41
1:D:249:SER:O	1:D:250:ALA:C	2.64	0.41
1:A:383:LEU:O	1:A:384:GLU:C	2.64	0.40
1:A:410:PRO:O	1:A:411:ARG:C	2.65	0.40
1:B:68:ALA:O	1:B:71:PHE:HB3	2.21	0.40
1:B:101:TYR:CD2	1:B:101:TYR:C	2.98	0.40
1:B:364:ASP:OD1	1:B:364:ASP:N	2.54	0.40
1:C:303:ASP:C	1:C:305:TYR:H	2.29	0.40
1:C:390:GLN:NE2	1:C:407:CYS:HB3	2.36	0.40
1:C:455:LYS:HB2	1:C:470:LEU:HD13	2.03	0.40
1:C:480:ARG:O	1:C:484:VAL:CA	2.69	0.40
1:D:207:ALA:O	1:D:208:VAL:C	2.63	0.40
1:D:370:VAL:HG23	1:D:370:VAL:O	2.20	0.40
1:A:73:GLN:HB3	1:A:500:LEU:CD1	2.51	0.40
1:A:92:SER:OG	1:A:343:GLY:HA3	2.21	0.40
1:A:453:ASN:HD22	1:A:453:ASN:N	2.16	0.40
1:B:110:TYR:HE2	1:B:171:ILE:HG21	1.87	0.40
1:B:502:VAL:HG13	1:B:510:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:TYR:CD2	1:C:469:PRO:HA	2.56	0.40
1:C:498:GLN:OE1	1:C:498:GLN:HA	2.22	0.40
1:D:46:ASN:HB2	1:D:49:ASP:CB	2.50	0.40
1:D:430:ARG:NH2	1:D:443:ILE:O	2.54	0.40
1:A:160:TYR:HA	1:A:161:PRO:HA	1.82	0.40
1:A:194:LEU:C	1:A:194:LEU:CD2	2.94	0.40
1:B:303:ASP:C	1:B:305:TYR:H	2.30	0.40
1:D:110:TYR:CE1	1:D:180:ALA:HB2	2.56	0.40
1:D:454:TYR:HE2	1:D:469:PRO:CD	2.32	0.40
1:A:43:GLN:NE2	1:A:77:ASP:HB2	2.36	0.40
1:A:375:ALA:C	1:A:377:SER:N	2.79	0.40
1:A:375:ALA:C	1:A:377:SER:H	2.28	0.40
1:A:391:LYS:CE	1:A:440:ASN:ND2	2.84	0.40
1:A:460:LYS:HB3	1:A:460:LYS:HE3	1.82	0.40
1:B:62:ALA:HB1	1:B:466:ARG:HE	1.85	0.40
1:B:227:PRO:C	1:B:345:SER:HB2	2.47	0.40
1:B:377:SER:HA	1:B:469:PRO:HG3	2.04	0.40
1:C:68:ALA:O	1:C:71:PHE:HB3	2.21	0.40
1:C:173:SER:OG	1:C:176:SER:O	2.35	0.40
1:C:300:GLY:O	1:C:301:GLY:C	2.65	0.40
1:D:423:VAL:O	1:D:424:ASP:C	2.64	0.40
1:B:160:TYR:HA	1:B:161:PRO:HA	1.83	0.40
1:B:373:PHE:CB	1:B:405:VAL:HA	2.48	0.40
1:D:375:ALA:C	1:D:377:SER:H	2.30	0.40
1:D:500:LEU:HA	1:D:500:LEU:HD23	1.91	0.40

All (2) 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:A:509:THR:O	1:B:419:VAL:N[4_655]	1.92	0.28
1:A:22:ASN:ND2	1:C:260:THR:OG1[4_555]	2.00	0.20

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	475/510 (93%)	371 (78%)	87 (18%)	17 (4%)	2	22
1	B	474/510 (93%)	365 (77%)	94 (20%)	15 (3%)	3	24
1	C	473/510 (93%)	374 (79%)	84 (18%)	15 (3%)	3	24
1	D	472/510 (92%)	377 (80%)	87 (18%)	8 (2%)	7	35
All	All	1894/2040 (93%)	1487 (78%)	352 (19%)	55 (3%)	3	26

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	201	ALA
1	A	432	ALA
1	B	403	CYS
1	B	502	VAL
1	C	175	SER
1	C	201	ALA
1	C	348	ALA
1	C	500	LEU
1	D	201	ALA
1	A	403	CYS
1	A	480	ARG
1	A	504	LYS
1	B	344	LEU
1	B	508	GLU
1	C	98	ASN
1	C	311	ILE
1	A	62	ALA
1	A	311	ILE
1	A	348	ALA
1	A	482	ASP
1	B	62	ALA
1	B	311	ILE
1	B	509	THR
1	C	62	ALA
1	C	172	SER
1	C	176	SER
1	C	403	CYS
1	D	62	ALA
1	D	311	ILE

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Mol	Chain	Res	Type
1	D	403	CYS
1	B	94	PRO
1	B	348	ALA
1	A	509	THR
1	B	172	SER
1	D	497	GLY
1	A	25	GLY
1	A	304	ILE
1	B	25	GLY
1	B	304	ILE
1	C	96	ALA
1	C	162	THR
1	C	247	GLY
1	C	304	ILE
1	D	304	ILE
1	D	318	GLY
1	A	247	GLY
1	A	434	GLY
1	B	507	ILE
1	A	121	VAL
1	A	318	GLY
1	D	121	VAL
1	B	121	VAL
1	B	247	GLY
1	C	121	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/411 (93%)	335 (88%)	48 (12%)	4	22
1	B	382/411 (93%)	336 (88%)	46 (12%)	5	23
1	C	381/411 (93%)	329 (86%)	52 (14%)	3	19
1	D	380/411 (92%)	324 (85%)	56 (15%)	3	17
All	All	1526/1644 (93%)	1324 (87%)	202 (13%)	4	20

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

Mol	Chain	Res	Type
1	A	41	ILE
1	A	50	LEU
1	A	58	THR
1	A	66	MET
1	A	67	SER
1	A	71	PHE
1	A	74	TYR
1	A	80	VAL
1	A	84	VAL
1	A	86	ARG
1	A	95	ILE
1	A	102	THR
1	A	150	ILE
1	A	162	THR
1	A	188	ILE
1	A	189	THR
1	A	202	GLU
1	A	213	ASN
1	A	290	VAL
1	A	304	ILE
1	A	347	ASN
1	A	349	GLU
1	A	367	SER
1	A	368	VAL
1	A	371	GLN
1	A	382	SER
1	A	383	LEU
1	A	388	THR
1	A	395	SER
1	A	404	LEU
1	A	406	LEU
1	A	414	VAL
1	A	417	ILE
1	A	426	LEU
1	A	430	ARG
1	A	431	THR
1	A	436	TYR
1	A	438	ASP
1	A	440	ASN
1	A	446	THR
1	A	450	ILE
1	A	453	ASN

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Mol	Chain	Res	Type
1	A	460	LYS
1	A	464	VAL
1	A	483	ASN
1	A	499	ILE
1	A	501	ASN
1	A	507	ILE
1	B	41	ILE
1	B	50	LEU
1	B	58	THR
1	B	66	MET
1	B	67	SER
1	B	71	PHE
1	B	80	VAL
1	B	84	VAL
1	B	86	ARG
1	B	102	THR
1	B	150	ILE
1	B	162	THR
1	B	176	SER
1	B	213	ASN
1	B	264	THR
1	B	290	VAL
1	B	304	ILE
1	B	344	LEU
1	B	349	GLU
1	B	367	SER
1	B	368	VAL
1	B	371	GLN
1	B	382	SER
1	B	383	LEU
1	B	388	THR
1	B	395	SER
1	B	404	LEU
1	B	414	VAL
1	B	417	ILE
1	B	426	LEU
1	B	430	ARG
1	B	431	THR
1	B	437	THR
1	B	438	ASP
1	B	440	ASN
1	B	446	THR

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Mol	Chain	Res	Type
1	B	450	ILE
1	B	453	ASN
1	B	460	LYS
1	B	464	VAL
1	B	481	THR
1	B	483	ASN
1	B	499	ILE
1	B	500	LEU
1	B	507	ILE
1	B	509	THR
1	C	41	ILE
1	C	50	LEU
1	C	54	PHE
1	C	56	GLN
1	C	58	THR
1	C	66	MET
1	C	67	SER
1	C	71	PHE
1	C	74	TYR
1	C	77	ASP
1	C	80	VAL
1	C	84	VAL
1	C	98	ASN
1	C	102	THR
1	C	150	ILE
1	C	162	THR
1	C	171	ILE
1	C	178	LEU
1	C	186	LYS
1	C	189	THR
1	C	202	GLU
1	C	213	ASN
1	C	264	THR
1	C	290	VAL
1	C	304	ILE
1	C	341	SER
1	C	344	LEU
1	C	349	GLU
1	C	367	SER
1	C	368	VAL
1	C	371	GLN
1	C	382	SER

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Mol	Chain	Res	Type
1	C	383	LEU
1	C	388	THR
1	C	395	SER
1	C	404	LEU
1	C	406	LEU
1	C	414	VAL
1	C	417	ILE
1	C	426	LEU
1	C	437	THR
1	C	440	ASN
1	C	446	THR
1	C	450	ILE
1	C	453	ASN
1	C	460	LYS
1	C	464	VAL
1	C	481	THR
1	C	482	ASP
1	C	499	ILE
1	C	501	ASN
1	C	503	ILE
1	D	29	LEU
1	D	41	ILE
1	D	50	LEU
1	D	58	THR
1	D	66	MET
1	D	67	SER
1	D	71	PHE
1	D	74	TYR
1	D	80	VAL
1	D	84	VAL
1	D	86	ARG
1	D	98	ASN
1	D	99	ILE
1	D	102	THR
1	D	150	ILE
1	D	162	THR
1	D	171	ILE
1	D	175	SER
1	D	178	LEU
1	D	183	THR
1	D	186	LYS
1	D	189	THR

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Mol	Chain	Res	Type
1	D	202	GLU
1	D	213	ASN
1	D	290	VAL
1	D	304	ILE
1	D	344	LEU
1	D	346	SER
1	D	367	SER
1	D	368	VAL
1	D	371	GLN
1	D	382	SER
1	D	383	LEU
1	D	388	THR
1	D	395	SER
1	D	404	LEU
1	D	406	LEU
1	D	414	VAL
1	D	417	ILE
1	D	426	LEU
1	D	430	ARG
1	D	438	ASP
1	D	440	ASN
1	D	446	THR
1	D	450	ILE
1	D	453	ASN
1	D	454	TYR
1	D	460	LYS
1	D	464	VAL
1	D	481	THR
1	D	484	VAL
1	D	499	ILE
1	D	501	ASN
1	D	502	VAL
1	D	507	ILE
1	D	509	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	70	ASN
1	A	166	ASN
1	A	213	ASN

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	390	GLN
1	A	440	ASN
1	A	453	ASN
1	A	457	GLN
1	B	43	GLN
1	B	70	ASN
1	B	98	ASN
1	B	166	ASN
1	B	213	ASN
1	B	278	GLN
1	B	328	GLN
1	B	329	ASN
1	B	390	GLN
1	B	440	ASN
1	B	453	ASN
1	B	457	GLN
1	B	501	ASN
1	C	43	GLN
1	C	70	ASN
1	C	98	ASN
1	C	166	ASN
1	C	213	ASN
1	C	278	GLN
1	C	328	GLN
1	C	329	ASN
1	C	347	ASN
1	C	390	GLN
1	C	439	ASN
1	C	453	ASN
1	C	457	GLN
1	C	483	ASN
1	C	501	ASN
1	D	43	GLN
1	D	70	ASN
1	D	98	ASN
1	D	166	ASN
1	D	213	ASN
1	D	278	GLN
1	D	329	ASN
1	D	347	ASN
1	D	390	GLN

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Mol	Chain	Res	Type
1	D	440	ASN
1	D	457	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	479/510 (93%)	0.35	12 (2%) 58 35	24, 65, 121, 227	0
1	B	478/510 (93%)	0.66	28 (5%) 28 16	20, 82, 162, 247	0
1	C	477/510 (93%)	0.42	13 (2%) 56 33	25, 80, 148, 263	0
1	D	476/510 (93%)	0.76	31 (6%) 25 15	26, 116, 254, 407	0
All	All	1910/2040 (93%)	0.55	84 (4%) 39 21	20, 84, 186, 407	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	TYR	5.9
1	B	454	TYR	5.6
1	B	48	VAL	5.5
1	A	510	PRO	5.4
1	A	22	ASN	4.9
1	C	55	GLY	4.8
1	B	22	ASN	4.5
1	D	399	VAL	4.5
1	C	451	ASP	4.3
1	D	292	SER	4.2
1	B	55	GLY	4.2
1	C	454	TYR	4.1
1	B	271	TYR	4.1
1	A	399	VAL	4.1
1	D	325	ALA	4.1
1	A	451	ASP	3.8
1	C	510	PRO	3.7
1	B	451	ASP	3.7
1	D	55	GLY	3.6
1	D	301	GLY	3.6
1	A	23	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	454	TYR	3.5
1	D	510	PRO	3.5
1	A	21	ASN	3.4
1	D	300	GLY	3.3
1	B	424	ASP	3.3
1	C	399	VAL	3.3
1	B	509	THR	3.2
1	A	55	GLY	3.2
1	D	281	ILE	3.1
1	B	433	ALA	3.0
1	B	423	VAL	3.0
1	A	271	TYR	3.0
1	B	45	THR	2.9
1	B	436	TYR	2.9
1	D	250	ALA	2.8
1	D	272	GLY	2.8
1	B	434	GLY	2.7
1	D	509	THR	2.7
1	B	510	PRO	2.7
1	C	202	GLU	2.7
1	D	70	ASN	2.7
1	B	23	SER	2.7
1	D	246	LYS	2.6
1	B	77	ASP	2.6
1	B	427	VAL	2.6
1	B	366	GLU	2.6
1	D	405	VAL	2.5
1	D	221	GLY	2.5
1	B	399	VAL	2.5
1	D	497	GLY	2.4
1	D	427	VAL	2.4
1	D	280	ALA	2.4
1	D	307	SER	2.4
1	B	484	VAL	2.4
1	A	507	ILE	2.4
1	D	270	GLY	2.4
1	D	403	CYS	2.3
1	D	409	PRO	2.3
1	B	420	THR	2.3
1	D	420	THR	2.3
1	B	472	ALA	2.3
1	C	405	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	509	THR	2.3
1	B	351	THR	2.2
1	D	374	ILE	2.2
1	D	412	GLU	2.2
1	B	389	VAL	2.2
1	C	48	VAL	2.2
1	C	83	ALA	2.2
1	D	452	GLY	2.2
1	C	481	THR	2.2
1	C	308	ASN	2.2
1	B	386	ALA	2.2
1	B	502	VAL	2.2
1	B	182	ILE	2.2
1	D	201	ALA	2.1
1	B	100	GLU	2.1
1	A	433	ALA	2.1
1	D	394	VAL	2.1
1	D	164	GLY	2.1
1	C	133	GLU	2.1
1	C	448	ALA	2.1
1	D	449	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.