



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 08:00 PM EDT

PDB ID : 3FOA  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

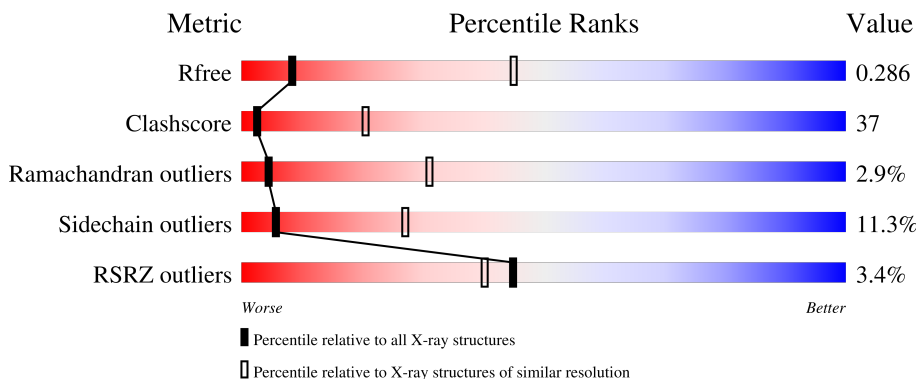
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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  $\geq 3$ , 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	
1	B	510	
1	C	510	
1	D	510	

## 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
			Total	C	N	O	S			
1	A	479	Total 3613	C 2279	N 600	O 726	S 8	0	0	0
1	B	478	Total 3605	C 2275	N 598	O 724	S 8	0	0	0
1	C	477	Total 3597	C 2271	N 596	O 722	S 8	0	0	0
1	D	476	Total 3591	C 2268	N 595	O 720	S 8	0	0	0

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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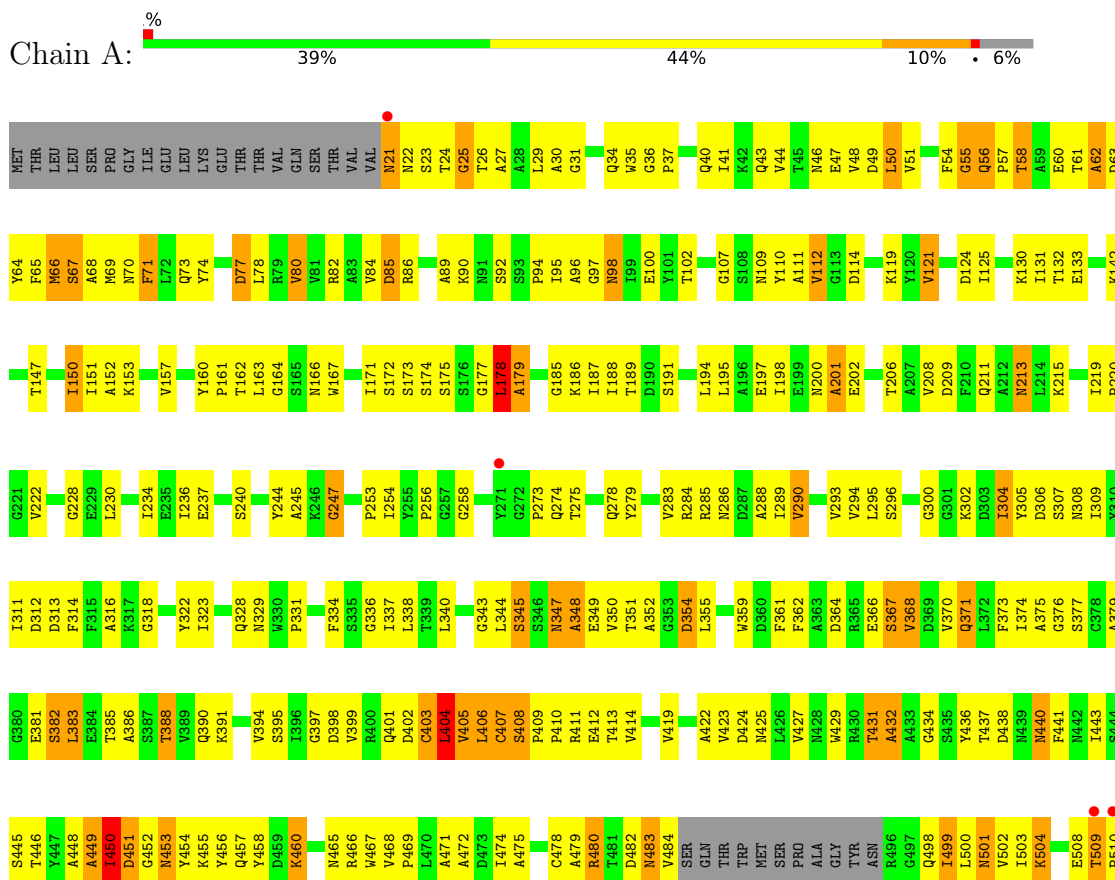
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
C	399	VAL	ALA	variant	UNP P13332
C	454	TYR	HIS	variant	UNP P13332
C	510	PRO	ARG	engineered mutation	UNP P13332
D	100	GLU	ASP	variant	UNP P13332
D	148	ALA	GLY	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

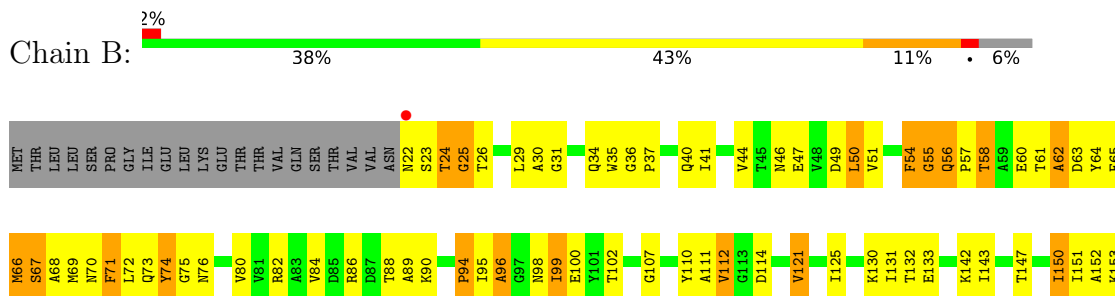
### 3 Residue-property plots i

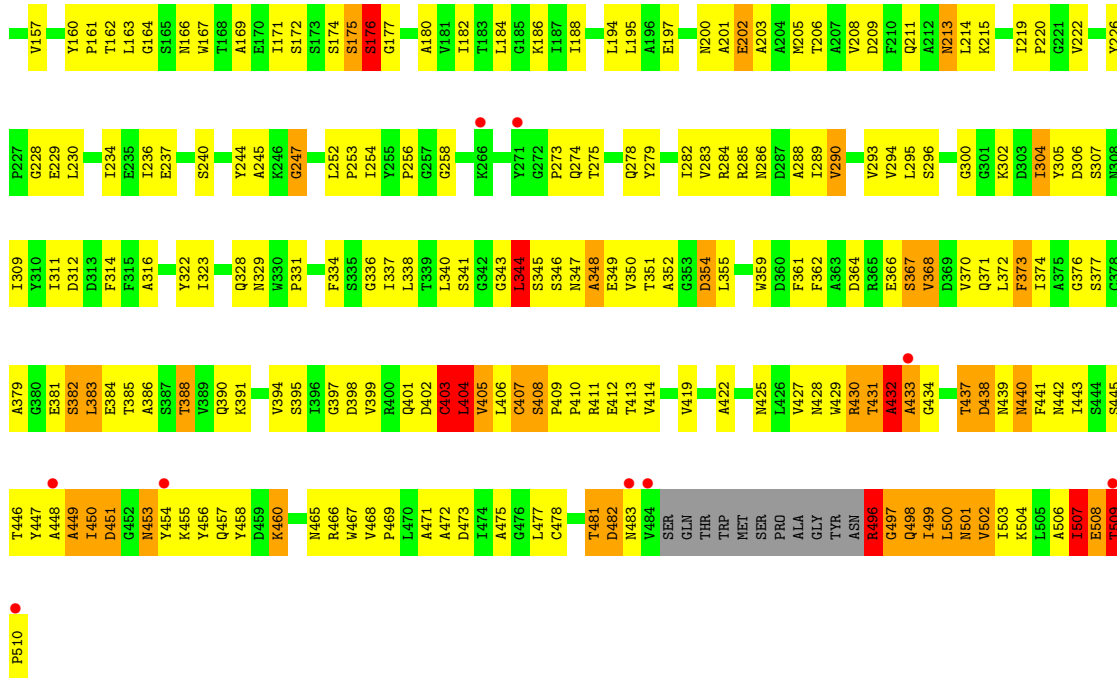
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Tail sheath protein Gp18

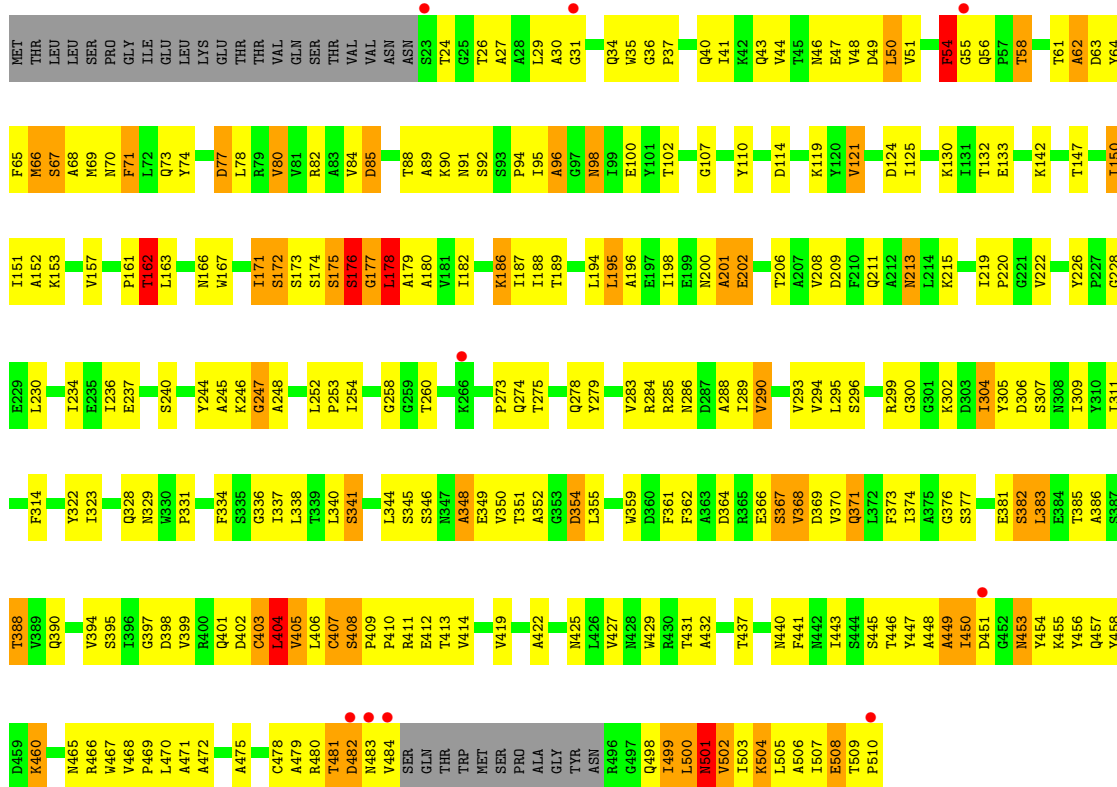


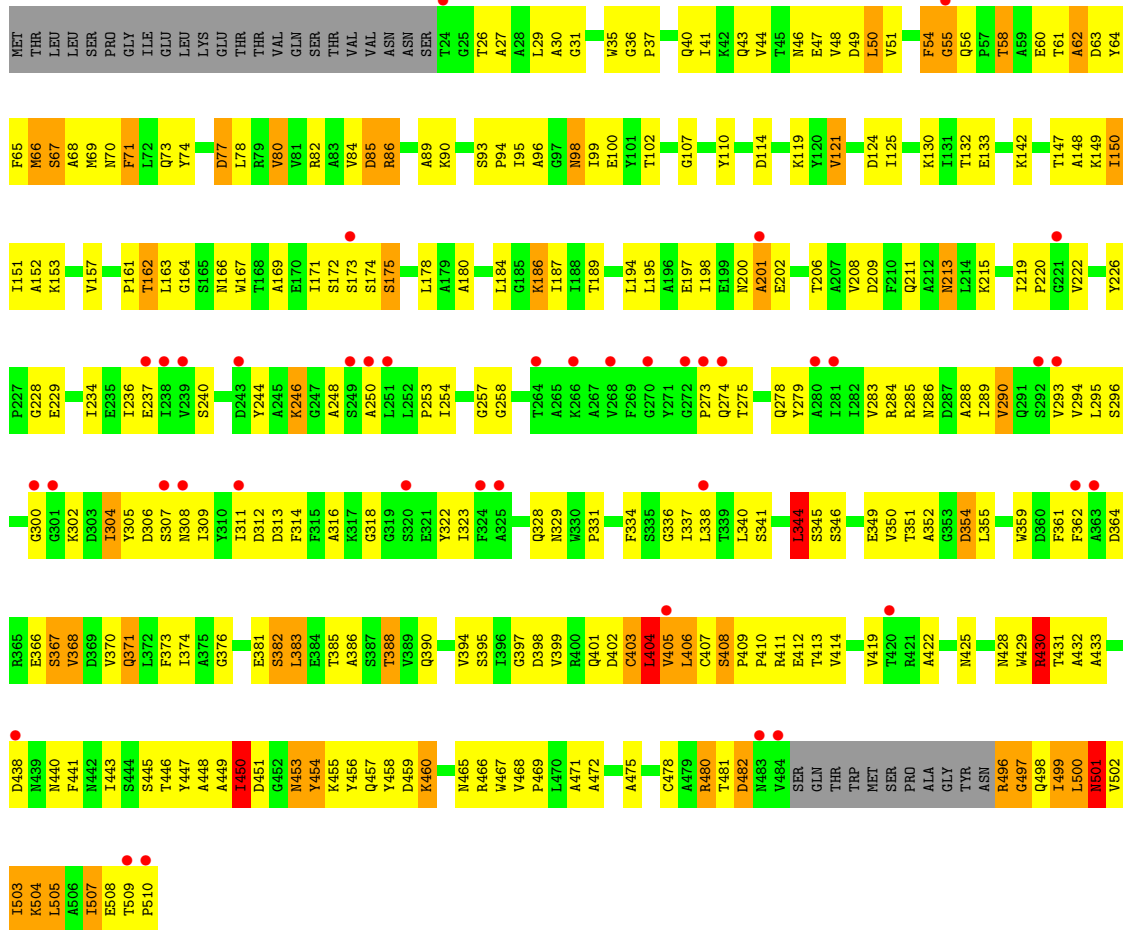
#### • Molecule 1: Tail sheath protein Gp18





• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 3.48Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.267 , 0.299 0.280 , 0.286	Depositor DCC
$R_{free}$ test set	5405 reflections (16.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtrriage
Anisotropy	0.673	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	14406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.35	0/3677	0.78	21/5001 (0.4%)
1	B	0.29	0/3669	0.91	31/4990 (0.6%)
1	C	0.30	0/3661	0.70	19/4979 (0.4%)
1	D	0.28	0/3655	0.88	27/4971 (0.5%)
All	All	0.30	0/14662	0.82	98/19941 (0.5%)

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

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ALA	N-CA-CB	-22.35	78.81	110.10
1	D	500	LEU	CB-CA-C	-18.07	75.86	110.20
1	A	55	GLY	N-CA-C	18.00	158.11	113.10
1	D	55	GLY	N-CA-C	16.20	153.61	113.10
1	B	55	GLY	N-CA-C	13.58	147.05	113.10
1	B	407	CYS	CB-CA-C	-13.07	84.26	110.40
1	D	367	SER	N-CA-CB	-12.46	91.82	110.50
1	B	403	CYS	CB-CA-C	-11.97	86.46	110.40
1	B	367	SER	N-CA-CB	-11.85	92.73	110.50
1	B	408	SER	N-CA-CB	-11.51	93.23	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ALA	CB-CA-C	-11.50	92.85	110.10
1	D	56	GLN	N-CA-CB	-11.38	90.11	110.60
1	A	56	GLN	N-CA-CB	-11.35	90.17	110.60
1	D	407	CYS	CB-CA-C	-10.81	88.78	110.40
1	B	111	ALA	CB-CA-C	10.78	126.26	110.10
1	A	367	SER	N-CA-CB	-10.63	94.55	110.50
1	B	56	GLN	N-CA-CB	-10.57	91.58	110.60
1	C	405	VAL	N-CA-C	-10.18	83.51	111.00
1	D	366	GLU	CB-CA-C	9.94	130.29	110.40
1	D	408	SER	N-CA-CB	-9.86	95.71	110.50
1	D	449	ALA	CB-CA-C	9.76	124.74	110.10
1	A	405	VAL	N-CA-C	-9.59	85.11	111.00
1	C	407	CYS	CB-CA-C	-9.58	91.25	110.40
1	D	405	VAL	N-CA-C	-9.58	85.14	111.00
1	A	111	ALA	CB-CA-C	9.56	124.45	110.10
1	A	112	VAL	N-CA-C	9.50	136.65	111.00
1	A	407	CYS	CB-CA-C	-9.49	91.42	110.40
1	B	366	GLU	CB-CA-C	9.12	128.64	110.40
1	B	180	ALA	N-CA-CB	9.07	122.80	110.10
1	D	503	ILE	CB-CA-C	8.89	129.38	111.60
1	D	85	ASP	CB-CA-C	8.86	128.12	110.40
1	A	408	SER	N-CA-CB	-8.86	97.22	110.50
1	B	201	ALA	N-CA-C	8.81	134.78	111.00
1	C	408	SER	N-CA-CB	-8.79	97.31	110.50
1	C	85	ASP	CB-CA-C	8.64	127.68	110.40
1	C	195	LEU	N-CA-C	8.60	134.23	111.00
1	C	367	SER	N-CA-CB	-8.47	97.79	110.50
1	B	404	LEU	N-CA-CB	-8.19	94.01	110.40
1	B	498	GLN	N-CA-C	-8.02	89.35	111.00
1	D	504	LYS	N-CA-CB	-8.00	96.20	110.60
1	A	112	VAL	CB-CA-C	-7.60	96.96	111.40
1	A	404	LEU	N-CA-C	-7.53	90.68	111.00
1	A	366	GLU	CB-CA-C	7.42	125.25	110.40
1	D	85	ASP	N-CA-C	-7.42	90.96	111.00
1	C	85	ASP	N-CA-C	-7.34	91.19	111.00
1	B	54	PHE	CB-CA-C	-7.29	95.83	110.40
1	D	501	ASN	N-CA-C	7.22	130.50	111.00
1	D	504	LYS	CB-CA-C	-7.09	96.22	110.40
1	C	404	LEU	N-CA-C	-7.07	91.91	111.00
1	B	372	LEU	CB-CA-C	-6.90	97.09	110.20
1	B	498	GLN	N-CA-CB	6.85	122.94	110.60
1	A	404	LEU	CB-CA-C	6.84	123.20	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	ASP	N-CA-C	-6.84	92.52	111.00
1	D	450	ILE	CB-CA-C	-6.81	97.97	111.60
1	B	497	GLY	N-CA-C	-6.81	96.08	113.10
1	D	505	LEU	CB-CA-C	-6.80	97.29	110.20
1	B	114	ASP	N-CA-C	-6.76	92.75	111.00
1	A	449	ALA	CB-CA-C	6.72	120.18	110.10
1	A	85	ASP	N-CA-C	-6.54	93.36	111.00
1	D	482	ASP	N-CA-C	-6.48	93.51	111.00
1	C	502	VAL	CB-CA-C	-6.44	99.16	111.40
1	B	449	ALA	CB-CA-C	6.42	119.73	110.10
1	D	404	LEU	N-CA-C	-6.25	94.12	111.00
1	A	406	LEU	CB-CA-C	6.17	121.92	110.20
1	B	54	PHE	N-CA-C	-6.07	94.60	111.00
1	D	498	GLN	CB-CA-C	6.05	122.50	110.40
1	B	433	ALA	N-CA-CB	-6.01	101.68	110.10
1	C	404	LEU	CB-CA-C	5.97	121.54	110.20
1	D	248	ALA	N-CA-CB	5.95	118.44	110.10
1	C	502	VAL	N-CA-C	-5.80	95.34	111.00
1	C	196	ALA	N-CA-CB	5.80	118.22	110.10
1	C	449	ALA	CB-CA-C	5.74	118.70	110.10
1	A	85	ASP	CB-CA-C	5.71	121.83	110.40
1	D	449	ALA	N-CA-C	-5.66	95.71	111.00
1	C	504	LYS	CB-CA-C	-5.61	99.18	110.40
1	B	404	LEU	CB-CA-C	5.56	120.77	110.20
1	B	405	VAL	N-CA-C	-5.56	95.99	111.00
1	D	54	PHE	CB-CA-C	-5.51	99.38	110.40
1	B	373	PHE	N-CA-C	5.44	125.69	111.00
1	B	367	SER	N-CA-C	5.38	125.52	111.00
1	D	405	VAL	CB-CA-C	5.37	121.61	111.40
1	B	112	VAL	N-CA-C	5.36	125.48	111.00
1	A	406	LEU	N-CA-C	-5.36	96.53	111.00
1	C	366	GLU	CB-CA-C	5.32	121.04	110.40
1	A	179	ALA	N-CA-C	5.25	125.16	111.00
1	C	179	ALA	N-CA-C	5.23	125.11	111.00
1	D	246	LYS	N-CA-C	-5.21	96.92	111.00
1	B	432	ALA	C-N-CA	5.21	134.73	121.70
1	B	96	ALA	N-CA-C	5.18	124.99	111.00
1	D	406	LEU	N-CA-C	-5.18	97.01	111.00
1	A	178	LEU	N-CA-CB	-5.17	100.05	110.40
1	C	196	ALA	N-CA-C	5.17	124.96	111.00
1	B	449	ALA	N-CA-C	-5.14	97.12	111.00
1	C	501	ASN	N-CA-C	-5.12	97.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	LEU	CB-CA-C	5.08	119.85	110.20
1	B	99	ILE	N-CA-CB	-5.05	99.17	110.80
1	A	21	ASN	C-N-CA	5.05	134.33	121.70
1	A	449	ALA	N-CA-C	-5.05	97.37	111.00

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
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

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	298	2
1	B	3605	0	3548	280	1
1	C	3597	0	3541	253	1
1	D	3591	0	3536	232	0
All	All	14406	0	14179	1050	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 37.

All (1050) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:24:THR:HG23	1:B:25:GLY:N	1.89	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:41:ILE:HD11	1:B:361:PHE:HB3	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:509:THR:HG22	1:B:510:PRO:C	2.03	0.77
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:24:THR:C	1:B:482:ASP:OD2	2.26	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:A:172:SER:C	1:A:174:SER:HA	2.09	0.72
1:B:200:ASN:O	1:B:203:ALA:HB3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:PRO:O	1:B:413:THR:HG22	1.90	0.72
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:24:THR:O	1:B:482:ASP:CG	2.32	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:172:SER:C	1:D:174:SER:HA	2.15	0.67
1:D:428:ASN:HB3	1:D:433:ALA:O	1.94	0.67
1:A:509:THR:OG1	1:A:510:PRO:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:24:THR:HG23	1:B:25:GLY:C	2.15	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
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: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:171:ILE:HG22	1:C:172:SER:N	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:B:50:LEU:C	1:B:50:LEU:HD12	2.21	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:HE1	1.98	0.59
1:C:213:ASN:N	1:C:213:ASN:HD22	2.00	0.59
1:A:419:VAL:HA	1:A:422:ALA:HB3	1.84	0.59
1:C:95:ILE:HG22	1:C:188:ILE:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:236:ILE:HD12	1:C:236:ILE:H	1.67	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: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: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: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:502:VAL:O	1:C:502:VAL:CG1	2.51	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:D:114:ASP:CG	1:D:175:SER:HB2	2.24	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: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:176:SER:HB3	1:C:177:GLY:C	2.26	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:B:328:GLN:HE21	1:C:299:ARG:CZ	2.19	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:23:SER:HG	1:A:483:ASN:HB3	1.68	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: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:D:73:GLN:CB	1:D:500:LEU:HD12	2.31	0.55
1:A:50:LEU:HD12	1:A:50:LEU:C	2.26	0.55
1:A:84:VAL:CG1	1:A:85:ASP:O	2.54	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:50:LEU:C	1:D:50:LEU:HD12	2.26	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:51:VAL:C	1:C:55:GLY:HA2	2.27	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:206:THR:HG22	1:A:206:THR:O	2.07	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: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:A:347:ASN:O	1:A:348:ALA:C	2.45	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:A:382:SER:O	1:A:383:LEU:C	2.45	0.54
1:C:451:ASP:OD2	1:C:470:LEU:HB3	2.06	0.54
1:D:206:THR:O	1:D:206:THR:HG22	2.07	0.54
1:A:51:VAL:HG22	1:A:65:PHE:HZ	1.73	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
1:D:236:ILE:HD12	1:D:236:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:50:LEU:HD12	1:C:50:LEU:C	2.28	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:C:382:SER:O	1:C:383:LEU:C	2.47	0.54
1:A:46:ASN:HB2	1:A:49:ASP:HB2	1.89	0.54
1:B:496:ARG:HG3	1:B:497:GLY:C	2.15	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: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:C:502:VAL:O	1:C:502:VAL:HG13	2.07	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
1:A:399:VAL:HG12	1:A:399:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:341:SER:C	1:B:343:GLY:H	2.12	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: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:D:58:THR:C	1:D:60:GLU:H	2.11	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: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:B:382:SER:O	1:B:383:LEU:C	2.47	0.52
1:A:51:VAL:HG22	1:A:65:PHE:CZ	2.45	0.52
1:A:114:ASP:CG	1:A:175:SER:HB2	2.29	0.52
1:A:275:THR:OG1	1:A:278:GLN:HG3	2.10	0.52
1:B:24:THR:HG23	1:B:26:THR:N	2.25	0.52
1:B:428:ASN:HB3	1:B:433:ALA:O	2.10	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
1:B:453:ASN:H	1:B:453:ASN:HD22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:30:ALA:HB3	1:C:359:TRP:CE2	2.46	0.51
1:D:382:SER:O	1:D:383:LEU:C	2.48	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: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
1:C:431:THR:HG23	1:C:432:ALA:N	2.26	0.51
1:C:481:THR:C	1:C:483:ASN:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:328:GLN:HG2	1:C:299:ARG:NE	2.22	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: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: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:245:ALA:C	1:A:247:GLY:H	2.15	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:C:481:THR:C	1:C:483:ASN:H	2.14	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: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
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:71:PHE:C	1:A:71:PHE:CD2	2.85	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:D:428:ASN:O	1:D:431:THR:C	2.51	0.49
1:C:304:ILE:HG13	1:C:305:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:C:71:PHE:C	1:C:71:PHE:CD2	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:71:PHE:CD2	1:B:71:PHE:C	2.87	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:B:169:ALA:HB2	1:B:184:LEU:HD11	1.95	0.47
1:D:71:PHE:C	1:D:71:PHE:CD2	2.86	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
1:C:96:ALA:HB1	1:C:341:SER:OG	2.14	0.47
1:B:362:PHE:HA	1:B:368:VAL:HG21	1.95	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:A:440:ASN:C	1:A:440:ASN:HD22	2.17	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:C:508:GLU:C	1:C:510:PRO:HD3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:HG22	1:B:294:VAL:N	2.29	0.47
1:B:501:ASN:C	1:B:502:VAL:HG12	2.27	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:245:ALA:C	1:B:247:GLY:H	2.18	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: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: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
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:B:151:ILE:HG13	1:B:152:ALA:N	2.30	0.46
1:B:410:PRO:C	1:B:454:TYR:HE1	2.18	0.46
1:C:37:PRO:HB2	1:C:40:GLN:HB2	1.97	0.46
1:A:290:VAL:HG11	1:A:322:TYR:CD1	2.50	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: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:71:PHE:C	1:C:73:GLN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:151:ILE:HG13	1:D:152:ALA:N	2.30	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: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:A:35:TRP:HB3	1:A:54:PHE:HA	1.98	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:A:411:ARG:O	1:A:412:GLU:C	2.54	0.46
1:B:71:PHE:C	1:B:73:GLN:H	2.19	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:245:ALA:C	1:C:247:GLY:H	2.19	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:B:329:ASN:CG	1:C:299:ARG:HD2	2.37	0.46
1:C:26:THR:HA	1:C:77:ASP:OD1	2.15	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: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:C:346:SER:C	1:C:348:ALA:H	2.17	0.46
1:B:385:THR:HA	1:B:388:THR:HG23	1.97	0.45
1:B:410:PRO:C	1:B:454:TYR:CE1	2.90	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:252:LEU:HA	1:C:253:PRO:HD3	1.80	0.45
1:D:71:PHE:C	1:D:73:GLN:H	2.19	0.45
1:D:293:VAL:HG22	1:D:294:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:O	1:A:132:THR:HG23	2.16	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:71:PHE:C	1:C:73:GLN:N	2.69	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:71:PHE:C	1:A:73:GLN:N	2.69	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
1:D:100:GLU:HG2	1:D:186:LYS:O	2.17	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:215:LYS:HE3	1:B:329:ASN:OD1	2.16	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:58:THR:C	1:D:60:GLU:N	2.69	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: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:151:ILE:HG13	1:C:152:ALA:N	2.31	0.45
1:A:50:LEU:HD12	1:A:51:VAL:N	2.32	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:C:478:CYS:C	1:C:480:ARG:N	2.68	0.45
1:C:34:GLN:OE1	1:C:230:LEU:HD11	2.17	0.45
1:B:347:ASN:O	1:B:348:ALA:C	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ASN:HD22	1:C:453:ASN:N	2.15	0.44
1:B:35:TRP:NE1	1:B:226:TYR:HD2	2.16	0.44
1:B:450:ILE:HG12	1:B:451:ASP:N	2.31	0.44
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:D:71:PHE:C	1:D:73:GLN:N	2.70	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:148:ALA:HB2	1:D:257:GLY:C	2.37	0.44
1:A:71:PHE:C	1:A:73:GLN:H	2.19	0.44
1:B:71:PHE:C	1:B:73:GLN:N	2.70	0.44
1:B:453:ASN:ND2	1:B:453:ASN:N	2.65	0.44
1:A:27:ALA:HB3	1:A:78:LEU:HD12	1.98	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:C:67:SER:OG	1:C:472:ALA:HB2	2.18	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: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:D:215:LYS:HE3	1:D:329:ASN:OD1	2.18	0.44
1:A:364:ASP:N	1:A:364:ASP:OD1	2.50	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:B:55:GLY:O	1:B:65:PHE:CE1	2.72	0.43
1:C:215:LYS:HE3	1:C:329:ASN:OD1	2.18	0.43
1:C:411:ARG:O	1:C:412:GLU:C	2.56	0.43
1:A:48:VAL:HG12	1:A:48:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:253:PRO:HD2	1:C:336:GLY:HA2	1.99	0.43
1:D:125:ILE:HD12	1:D:153:LYS:HG2	1.99	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: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: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:D:503:ILE:C	1:D:510:PRO:HG2	2.37	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:51:VAL:HG13	1:B:55:GLY:C	2.37	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: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
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:A:67:SER:OG	1:A:472:ALA:HB2	2.19	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:D:411:ARG:O	1:D:412:GLU:C	2.57	0.43
1:A:236:ILE:HD11	1:A:340:LEU:HD11	2.01	0.42
1:A:478:CYS:C	1:A:480:ARG:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:ASN:O	1:C:201:ALA:C	2.57	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:411:ARG:O	1:B:412:GLU:C	2.57	0.42
1:C:68:ALA:O	1:C:69:MET:C	2.58	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:C:505:LEU:O	1:C:506:ALA:C	2.57	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: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:68:ALA:O	1:D:69:MET:C	2.58	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:61:THR:O	1:C:62:ALA:C	2.57	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
1:C:70:ASN:HD22	1:C:455:LYS:HZ2	1.67	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:B:402:ASP:O	1:B:402:ASP:CG	2.58	0.42
1:C:84:VAL:HG12	1:C:85:ASP:O	2.10	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:88:THR:O	1:C:89:ALA:C	2.58	0.42
1:C:290:VAL:HG11	1:C:322:TYR:CE1	2.55	0.42
1:D:197:GLU:H	1:D:197:GLU:CD	2.22	0.42
1:D:308:ASN:HD21	1:D:313:ASP:CB	2.33	0.42
1:D:402:ASP:O	1:D:402:ASP:CG	2.57	0.42
1:A:24:THR:O	1:A:26:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:370:VAL:O	1:B:370:VAL:HG23	2.19	0.42
1:C:174:SER:O	1:C:175:SER:C	2.58	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:C:364:ASP:OD1	1:C:364:ASP:N	2.52	0.41
1:A:56:GLN:HA	1:A:57:PRO:HD3	1.81	0.41
1:A:406:LEU:HA	1:A:449:ALA:O	2.20	0.41
1:C:381:GLU:O	1:C:382:SER:C	2.58	0.41
1:C:402:ASP:CG	1:C:402:ASP:O	2.57	0.41
1:D:478:CYS:C	1:D:480:ARG:N	2.73	0.41
1:A:68:ALA:O	1:A:69:MET:C	2.58	0.41
1:B:197:GLU:H	1:B:197:GLU:CD	2.24	0.41
1:B:253:PRO:HD2	1:B:336:GLY:HA2	2.02	0.41
1:C:91:ASN:O	1:C:92:SER:C	2.57	0.41
1:D:61:THR:O	1:D:62:ALA:C	2.57	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:A:197:GLU:CD	1:A:197:GLU:H	2.23	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:51:VAL:HG13	1:C:55:GLY:C	2.40	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:61:THR:O	1:A:62:ALA:C	2.59	0.41
1:A:408:SER:OG	1:A:409:PRO:HD2	2.21	0.41
1:B:66:MET:O	1:B:67:SER:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:29:LEU:HD12	1:B:30:ALA:N	2.35	0.41
1:C:254:ILE:HB	1:C:258:GLY:O	2.21	0.41
1:D:200:ASN:O	1:D:201:ALA:C	2.59	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:D:89:ALA:O	1:D:90:LYS:HD3	2.20	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: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:500:LEU:HB3	1:D:501:ASN:OD1	2.21	0.41
1:A:46:ASN:HB2	1:A:49:ASP:CB	2.50	0.41
1:A:423:VAL:O	1:A:424:ASP:C	2.59	0.41
1:B:282:ILE:HG23	1:B:289:ILE:HG23	2.02	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: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:304:ILE:HG13	1:D:305:TYR:HE2	1.83	0.41
1:D:364:ASP:N	1:D:364:ASP:OD1	2.54	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:346:SER:C	1:C:348:ALA:N	2.73	0.41
1:D:48:VAL:O	1:D:48:VAL:HG12	2.21	0.41
1:A:200:ASN:O	1:A:201:ALA:C	2.59	0.40
1:A:215:LYS:HE3	1:A:329:ASN:CG	2.42	0.40
1:A:402:ASP:O	1:A:402:ASP:CG	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ALA:O	1:B:71:PHE:HB3	2.21	0.40
1:B:364:ASP:OD1	1:B:364:ASP:N	2.54	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:215:LYS:HE3	1:D:329:ASN:CG	2.41	0.40
1:D:370:VAL:HG23	1:D:370:VAL:O	2.20	0.40
1:D:496:ARG:HD3	1:D:497:GLY:C	2.41	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:68:ALA:O	1:B:69:MET:C	2.59	0.40
1:B:110:TYR:HE2	1:B:171:ILE:HG21	1.87	0.40
1:B:381:GLU:O	1:B:382:SER:C	2.59	0.40
1:B:502:VAL:HG13	1:B:510:PRO:HG3	2.03	0.40
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:229:GLU:CD	1:D:229:GLU:H	2.24	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: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:D:459:ASP:OD2	1:D:459:ASP:C	2.60	0.40
1:A:43:GLN:NE2	1:A:77:ASP:HB2	2.36	0.40
1:A:51:VAL:HG13	1:A:55:GLY:C	2.42	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: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: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:C:215:LYS:HE3	1:C:329:ASN:CG	2.41	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%)	3	26
1	B	474/510 (93%)	365 (77%)	94 (20%)	15 (3%)	4	29
1	C	473/510 (93%)	374 (79%)	84 (18%)	15 (3%)	4	29
1	D	472/510 (92%)	377 (80%)	87 (18%)	8 (2%)	9	42
All	All	1894/2040 (93%)	1487 (78%)	352 (19%)	55 (3%)	4	31

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/411 (93%)	340 (89%)	43 (11%)	6	27
1	B	382/411 (93%)	341 (89%)	41 (11%)	6	30
1	C	381/411 (93%)	337 (88%)	44 (12%)	5	26
1	D	380/411 (92%)	335 (88%)	45 (12%)	5	25
All	All	1526/1644 (93%)	1353 (89%)	173 (11%)	6	27

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

Mol	Chain	Res	Type
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	77	ASP
1	A	80	VAL
1	A	86	ARG
1	A	95	ILE
1	A	102	THR
1	A	150	ILE
1	A	162	THR
1	A	178	LEU
1	A	188	ILE
1	A	189	THR
1	A	202	GLU
1	A	213	ASN
1	A	290	VAL
1	A	345	SER
1	A	347	ASN
1	A	349	GLU
1	A	354	ASP
1	A	367	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	431	THR
1	A	436	TYR
1	A	437	THR
1	A	438	ASP
1	A	440	ASN
1	A	446	THR
1	A	450	ILE
1	A	453	ASN
1	A	460	LYS
1	A	483	ASN
1	A	499	ILE
1	A	501	ASN
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	86	ARG
1	B	102	THR
1	B	150	ILE
1	B	162	THR
1	B	176	SER
1	B	202	GLU
1	B	213	ASN
1	B	290	VAL
1	B	344	LEU
1	B	349	GLU
1	B	354	ASP
1	B	367	SER
1	B	368	VAL
1	B	371	GLN
1	B	382	SER
1	B	383	LEU
1	B	388	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	395	SER
1	B	404	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
1	B	450	ILE
1	B	453	ASN
1	B	460	LYS
1	B	481	THR
1	B	482	ASP
1	B	483	ASN
1	B	496	ARG
1	B	499	ILE
1	B	500	LEU
1	B	507	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	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	290	VAL
1	C	341	SER
1	C	344	LEU
1	C	349	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	354	ASP
1	C	367	SER
1	C	368	VAL
1	C	371	GLN
1	C	382	SER
1	C	383	LEU
1	C	388	THR
1	C	395	SER
1	C	404	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	481	THR
1	C	482	ASP
1	C	499	ILE
1	C	501	ASN
1	C	503	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	77	ASP
1	D	80	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	175	SER
1	D	178	LEU
1	D	186	LYS
1	D	189	THR
1	D	202	GLU
1	D	213	ASN
1	D	290	VAL
1	D	344	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	346	SER
1	D	354	ASP
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	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	480	ARG
1	D	499	ILE
1	D	501	ASN
1	D	507	ILE
1	D	509	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	43	GLN
1	A	70	ASN
1	A	213	ASN
1	A	278	GLN
1	A	329	ASN
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	213	ASN
1	B	278	GLN
1	B	328	GLN

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	390	GLN
1	B	440	ASN
1	B	453	ASN
1	B	457	GLN
1	C	43	GLN
1	C	70	ASN
1	C	213	ASN
1	C	278	GLN
1	C	390	GLN
1	C	453	ASN
1	C	457	GLN
1	C	501	ASN
1	D	43	GLN
1	D	70	ASN
1	D	213	ASN
1	D	278	GLN
1	D	329	ASN
1	D	390	GLN
1	D	440	ASN
1	D	453	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	479/510 (93%)	-0.06	4 (0%) 86 81	24, 65, 121, 227	0
1	B	478/510 (93%)	0.24	10 (2%) 63 58	20, 82, 162, 247	0
1	C	477/510 (93%)	0.12	9 (1%) 66 61	25, 80, 148, 263	0
1	D	476/510 (93%)	0.51	41 (8%) 10 11	26, 116, 254, 407	0
All	All	1910/2040 (93%)	0.20	64 (3%) 45 40	20, 84, 186, 407	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	292	SER	9.6
1	D	325	ALA	6.6
1	B	271	TYR	5.9
1	B	484	VAL	5.2
1	D	484	VAL	5.1
1	D	363	ALA	4.6
1	D	281	ILE	4.4
1	A	510	PRO	4.2
1	D	272	GLY	4.1
1	D	237	GLU	4.1
1	B	483	ASN	4.0
1	D	293	VAL	4.0
1	B	509	THR	3.9
1	B	22	ASN	3.5
1	D	509	THR	3.3
1	D	300	GLY	3.3
1	A	271	TYR	3.2
1	D	268	VAL	3.2
1	D	249	SER	3.1
1	D	308	ASN	2.9
1	D	307	SER	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	509	THR	2.7
1	D	483	ASN	2.7
1	D	264	THR	2.7
1	C	483	ASN	2.7
1	D	362	PHE	2.7
1	D	250	ALA	2.6
1	D	24	THR	2.6
1	D	274	GLN	2.6
1	D	238	ILE	2.6
1	D	243	ASP	2.6
1	D	270	GLY	2.6
1	A	21	ASN	2.6
1	D	273	PRO	2.5
1	C	510	PRO	2.5
1	C	55	GLY	2.5
1	D	280	ALA	2.5
1	D	251	LEU	2.5
1	D	510	PRO	2.5
1	B	454	TYR	2.5
1	D	338	LEU	2.5
1	D	201	ALA	2.4
1	C	482	ASP	2.4
1	D	239	VAL	2.3
1	D	420	THR	2.3
1	D	55	GLY	2.3
1	D	266	LYS	2.3
1	D	320	SER	2.3
1	C	31	GLY	2.3
1	D	301	GLY	2.3
1	C	451	ASP	2.2
1	B	448	ALA	2.2
1	C	484	VAL	2.2
1	D	405	VAL	2.2
1	D	438	ASP	2.1
1	B	266	LYS	2.1
1	B	433	ALA	2.1
1	D	221	GLY	2.1
1	D	324	PHE	2.0
1	C	266	LYS	2.0
1	B	510	PRO	2.0
1	D	173	SER	2.0
1	D	311	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	23	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.