



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:49 PM UTC

PDB ID : 3IBV / pdb_00003ibv
Title : Karyopherin cytosolic state
Authors : Cook, A.G.; Fukuhara, N.; Jinek, M.; Conti, E.
Deposited on : 2009-07-17
Resolution : 3.10 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

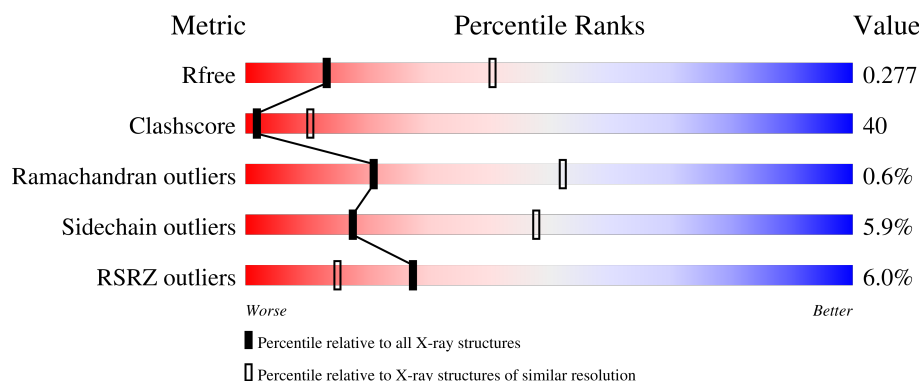
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	980	
1	B	980	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12876 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 Exportin-T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	0	0
			6515	4164	1087	1241	23			
1	B	902	Total	C	N	O	S	0	0	0
			6357	4067	1053	1212	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O94258
A	0	PRO	-	expression tag	UNP O94258
B	-1	GLY	-	expression tag	UNP O94258
B	0	PRO	-	expression tag	UNP O94258

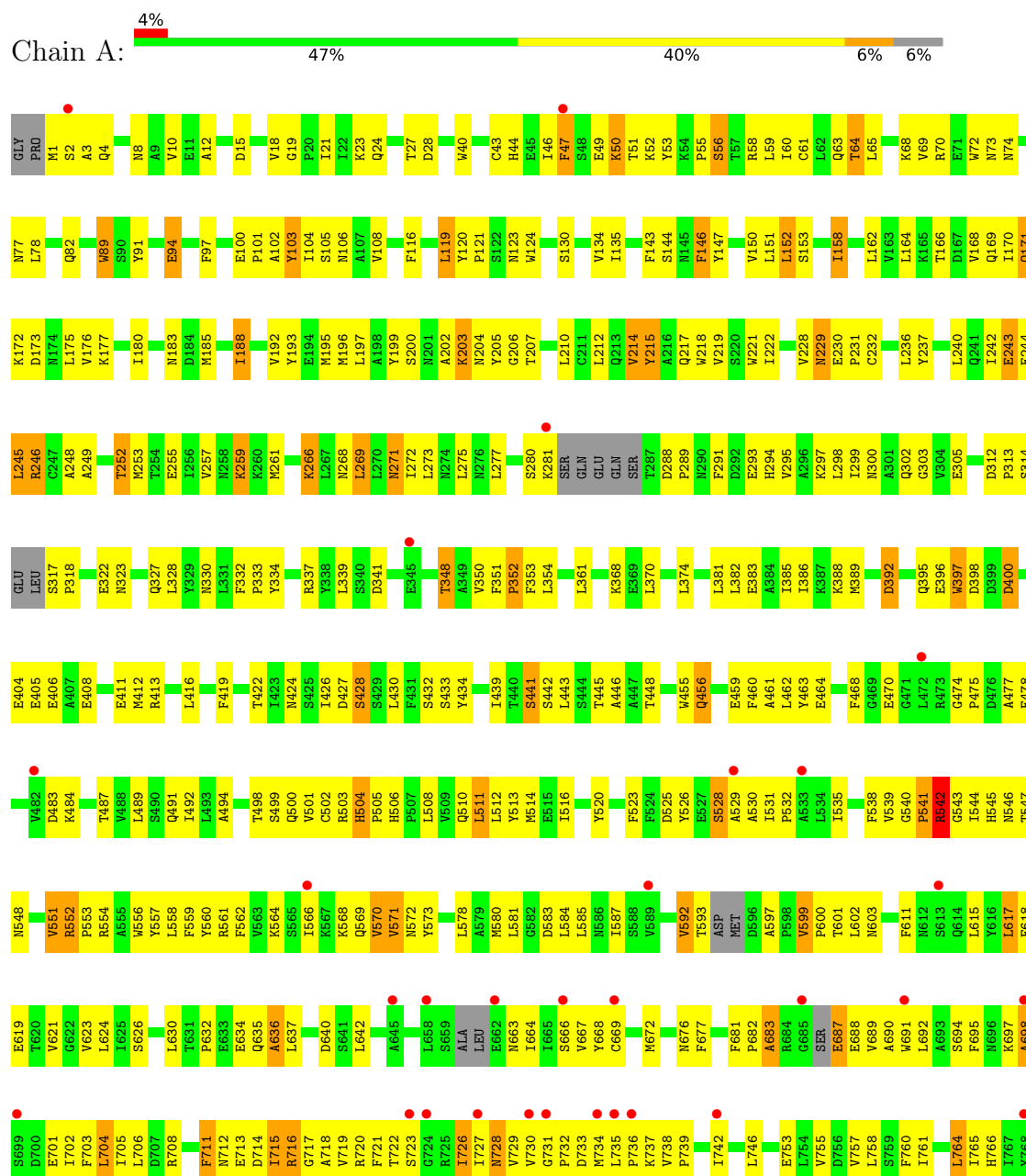
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

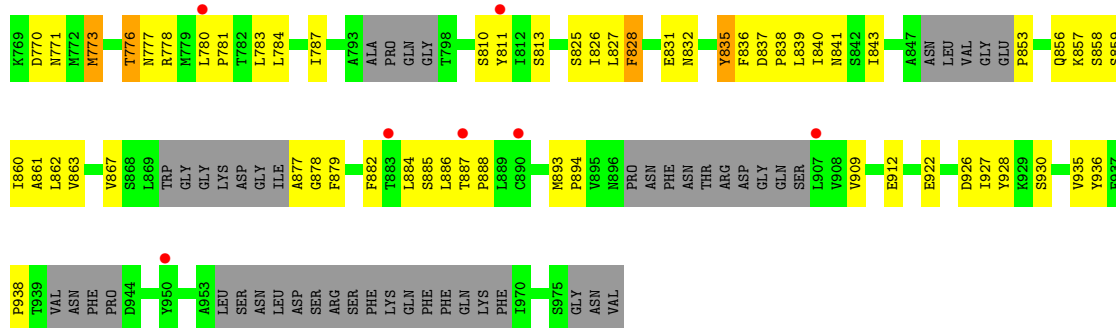
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

3 Residue-property plots

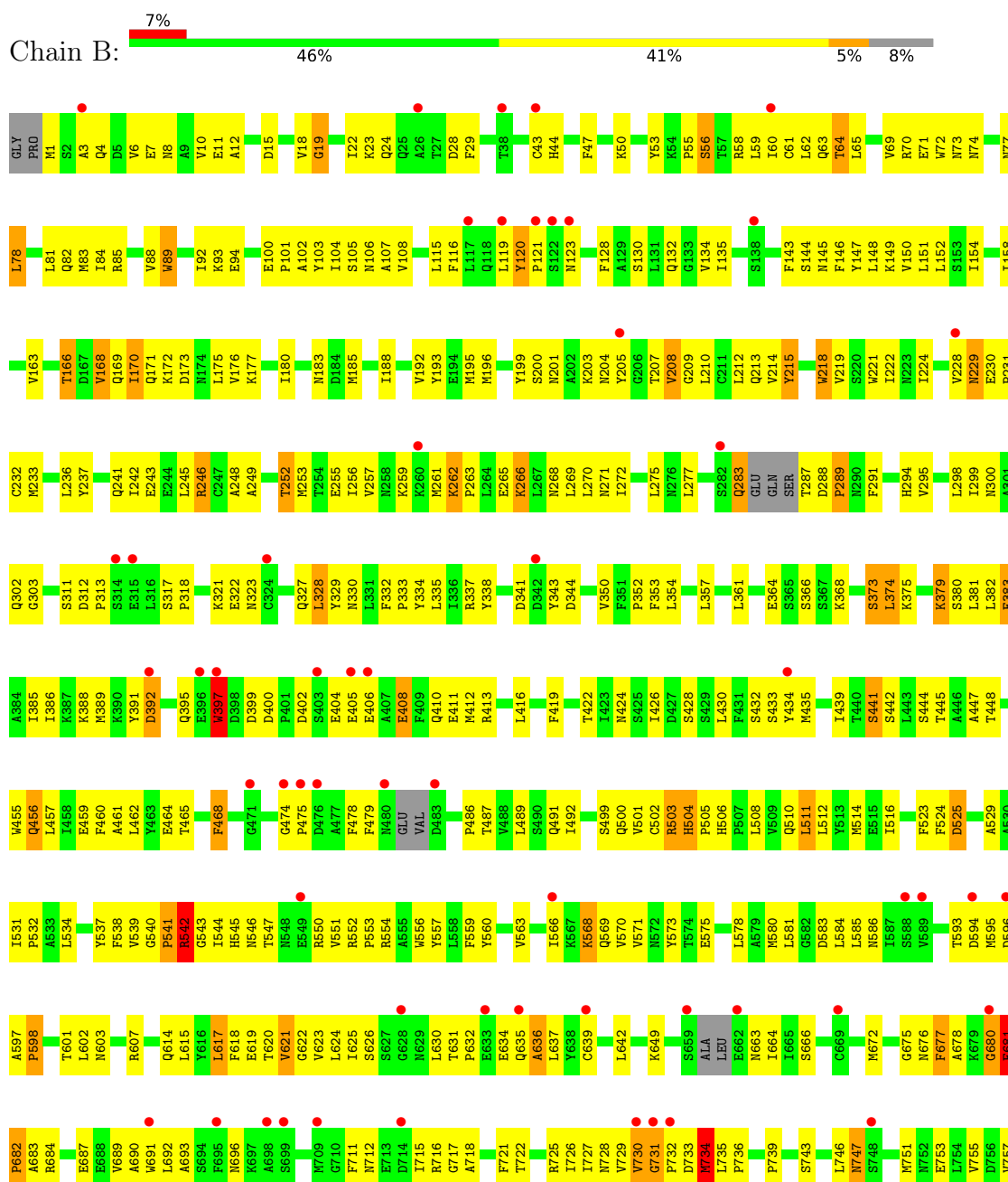
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

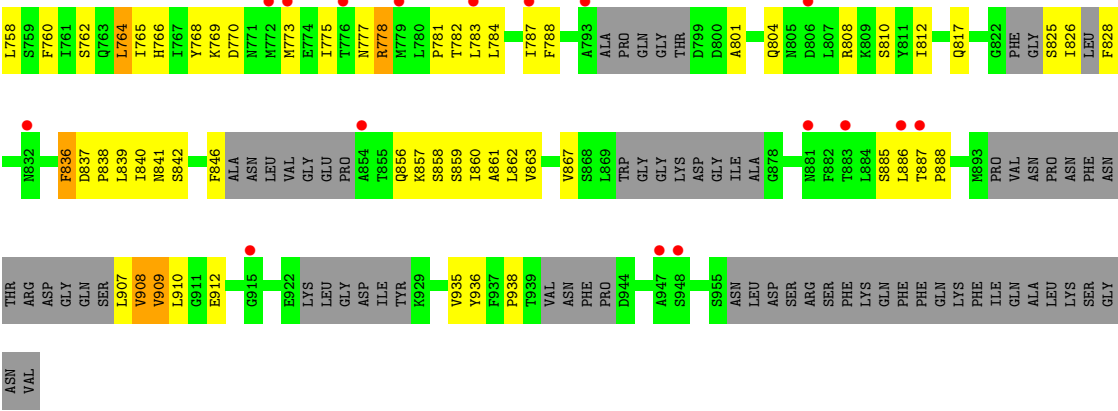
• Molecule 1: Exportin-T





• Molecule 1: Exportin-T





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.90Å 130.10Å 173.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.10 29.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.90-3.10) 97.6 (29.90-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.313 0.278 , 0.277	Depositor DCC
R_{free} test set	2496 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	88.3	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 107.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.78	6/6629 (0.1%)	1.18	72/9047 (0.8%)
1	B	0.90	16/6470 (0.2%)	1.29	76/8844 (0.9%)
All	All	0.84	22/13099 (0.2%)	1.24	148/17891 (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	6	0
1	B	8	1
All	All	14	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	681	PHE	CA-C	16.08	1.69	1.52
1	B	909	VAL	CA-C	15.67	1.73	1.52
1	A	552	ARG	NE-CZ	15.39	1.50	1.33
1	B	552	ARG	NE-CZ	15.33	1.50	1.33
1	A	542	ARG	NE-CZ	15.21	1.49	1.33
1	B	70	ARG	NE-CZ	14.55	1.49	1.33
1	A	70	ARG	NE-CZ	14.38	1.48	1.33
1	B	542	ARG	NE-CZ	14.29	1.48	1.33
1	B	681	PHE	N-CA	-12.91	1.33	1.45
1	B	681	PHE	CA-CB	11.92	1.70	1.53
1	B	910	LEU	N-CA	11.82	1.60	1.46
1	B	681	PHE	CG-CD1	-10.82	1.16	1.38
1	B	908	VAL	CA-C	-10.37	1.39	1.52
1	B	909	VAL	N-CA	-9.71	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	909	VAL	C-O	9.06	1.37	1.25
1	B	908	VAL	C-O	-8.46	1.14	1.24
1	B	734	MET	SD-CE	7.66	1.98	1.79
1	B	681	PHE	CG-CD2	6.68	1.52	1.38
1	B	218	TRP	NE1-CE2	6.34	1.44	1.37
1	A	119	LEU	CB-CG	-6.07	1.41	1.53
1	A	552	ARG	CD-NE	5.30	1.53	1.46
1	A	542	ARG	CD-NE	5.08	1.53	1.46

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	681	PHE	CB-CG-CD2	-24.24	79.50	120.70
1	B	908	VAL	CA-C-O	19.59	145.27	120.78
1	B	681	PHE	CB-CA-C	-17.18	83.34	109.97
1	B	681	PHE	CB-CG-CD1	13.54	143.72	120.70
1	A	571	VAL	N-CA-C	-11.76	102.54	113.71
1	A	704	LEU	N-CA-C	-10.94	99.43	111.36
1	A	50	LYS	N-CA-C	10.66	122.59	110.97
1	B	908	VAL	O-C-N	-10.08	109.97	122.57
1	B	770	ASP	N-CA-C	10.05	122.31	111.36
1	B	681	PHE	CA-CB-CG	-9.96	103.83	113.80
1	B	681	PHE	N-CA-CB	9.90	125.20	111.25
1	B	908	VAL	CA-C-N	-9.83	107.77	121.53
1	B	908	VAL	C-N-CA	-9.83	107.77	121.53
1	B	552	ARG	CD-NE-CZ	-9.45	111.17	124.40
1	A	630	LEU	N-CA-C	-9.43	94.76	109.76
1	B	778	ARG	N-CA-C	-9.27	101.87	113.55
1	A	698	ALA	N-CA-C	9.18	121.05	111.14
1	A	542	ARG	CD-NE-CZ	-9.12	111.64	124.40
1	B	163	VAL	N-CA-C	-8.92	100.10	112.50
1	B	542	ARG	CD-NE-CZ	-8.88	111.97	124.40
1	A	70	ARG	CD-NE-CZ	-8.76	112.14	124.40
1	B	504	HIS	CA-C-N	8.76	128.48	119.64
1	B	504	HIS	C-N-CA	8.76	128.48	119.64
1	A	552	ARG	CD-NE-CZ	-8.64	112.30	124.40
1	B	716	ARG	N-CA-C	-8.54	101.92	111.14
1	A	400	ASP	CA-C-N	8.46	130.42	119.84
1	A	400	ASP	C-N-CA	8.46	130.42	119.84
1	B	70	ARG	CD-NE-CZ	-8.37	112.69	124.40
1	B	94	GLU	N-CA-C	-8.26	95.87	108.67
1	B	936	TYR	N-CA-C	8.00	119.78	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	682	PRO	CB-CA-C	7.79	120.22	111.11
1	A	246	ARG	N-CA-C	7.76	120.63	111.71
1	B	503	ARG	N-CA-C	-7.75	103.34	114.12
1	A	312	ASP	CA-C-N	7.72	129.49	119.84
1	A	312	ASP	C-N-CA	7.72	129.49	119.84
1	A	703	PHE	N-CA-C	-7.70	102.53	112.23
1	B	769	LYS	N-CA-C	7.70	119.67	111.28
1	B	782	THR	N-CA-C	-7.67	103.89	113.55
1	B	909	VAL	CA-C-O	-7.60	110.99	119.35
1	A	455	TRP	N-CA-C	7.56	119.16	111.07
1	A	504	HIS	CA-C-N	7.55	127.27	119.64
1	A	504	HIS	C-N-CA	7.55	127.27	119.64
1	A	243	GLU	N-CA-C	7.48	119.33	111.03
1	B	909	VAL	CA-C-N	7.42	130.54	120.38
1	B	909	VAL	C-N-CA	7.42	130.54	120.38
1	B	909	VAL	N-CA-C	-7.41	106.67	113.71
1	A	728	ASN	N-CA-C	-7.39	103.25	111.82
1	B	680	GLY	CA-C-N	-7.36	109.64	122.38
1	B	680	GLY	C-N-CA	-7.36	109.64	122.38
1	B	687	GLU	N-CA-C	-7.36	100.62	110.55
1	B	598	PRO	N-CA-CB	7.07	110.68	103.25
1	B	455	TRP	N-CA-C	7.01	118.57	111.07
1	B	773	MET	N-CA-C	7.01	119.77	111.71
1	B	78	LEU	N-CA-C	6.92	118.47	111.07
1	A	773	MET	N-CA-C	6.83	122.64	111.37
1	A	541	PRO	N-CA-C	-6.77	106.07	114.20
1	A	853	PRO	N-CA-CB	6.66	110.33	103.00
1	B	468	PHE	N-CA-C	6.65	119.09	111.11
1	A	288	ASP	N-CA-C	-6.51	102.28	108.07
1	A	683	ALA	N-CA-C	6.50	121.23	113.16
1	A	636	ALA	N-CA-C	-6.47	104.43	112.90
1	A	158	ILE	N-CA-C	6.40	118.36	111.58
1	B	312	ASP	CA-C-N	6.37	126.07	119.64
1	B	312	ASP	C-N-CA	6.37	126.07	119.64
1	B	22	ILE	N-CA-C	-6.36	104.13	110.30
1	A	828	PHE	N-CA-C	-6.35	105.46	113.72
1	A	716	ARG	N-CA-C	-6.33	104.07	110.97
1	B	743	SER	N-CA-C	-6.33	104.31	111.14
1	B	938	PRO	N-CA-CB	6.31	110.21	103.52
1	B	170	ILE	N-CA-C	-6.31	104.12	111.00
1	B	568	LYS	N-CA-C	6.28	117.78	111.07
1	B	908	VAL	N-CA-C	6.27	122.37	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	TYR	N-CA-C	6.26	122.14	113.45
1	B	379	LYS	N-CA-C	-6.24	104.10	111.03
1	A	770	ASP	N-CA-C	6.21	118.13	111.36
1	A	51	THR	N-CA-C	6.16	118.80	111.71
1	A	877	ALA	CA-C-N	-6.16	112.94	122.30
1	A	877	ALA	C-N-CA	-6.16	112.94	122.30
1	A	813	SER	N-CA-C	6.11	118.02	111.36
1	B	105	SER	N-CA-C	-6.08	104.28	111.03
1	B	621	VAL	N-CA-C	-6.08	104.42	110.62
1	A	203	LYS	N-CA-C	-6.08	103.28	111.54
1	A	183	ASN	N-CA-C	6.07	120.75	112.68
1	B	474	GLY	N-CA-C	-6.04	100.02	112.34
1	A	153	SER	N-CA-C	-6.02	104.64	111.14
1	A	105	SER	N-CA-C	-6.01	103.49	111.24
1	B	541	PRO	N-CA-C	-6.00	106.64	114.03
1	B	595	MET	N-CA-C	5.91	119.81	112.24
1	B	751	MET	N-CA-C	-5.88	105.68	112.92
1	A	667	VAL	N-CA-C	-5.88	104.89	110.42
1	A	49	GLU	N-CA-C	5.88	118.79	108.56
1	A	771	ASN	N-CA-C	5.87	120.57	113.17
1	B	93	LYS	N-CA-C	-5.86	104.97	111.71
1	B	399	ASP	N-CA-C	5.86	120.44	112.88
1	A	938	PRO	N-CA-CB	5.81	109.95	103.44
1	A	269	LEU	N-CA-C	-5.80	104.86	111.07
1	B	183	ASN	N-CA-C	5.80	120.39	112.68
1	B	383	GLU	N-CA-C	-5.79	104.16	111.11
1	A	926	ASP	N-CA-C	5.77	119.42	112.38
1	B	525	ASP	N-CA-C	-5.76	106.09	113.23
1	A	726	ILE	CB-CA-C	-5.75	104.50	112.04
1	B	154	ILE	N-CA-C	-5.74	105.25	110.82
1	A	711	PHE	N-CA-C	5.72	118.73	111.69
1	A	494	ALA	N-CA-C	-5.68	104.78	110.97
1	B	636	ALA	N-CA-C	-5.63	105.53	112.90
1	B	681	PHE	CG-CD2-CE2	-5.52	111.32	120.70
1	A	587	ILE	N-CA-C	5.51	115.93	107.77
1	B	166	THR	N-CA-C	-5.51	100.68	109.23
1	A	936	TYR	N-CA-C	5.50	117.08	111.14
1	B	19	GLY	CA-C-N	5.49	125.11	119.56
1	B	19	GLY	C-N-CA	5.49	125.11	119.56
1	A	491	GLN	N-CA-C	-5.47	105.32	111.28
1	A	811	TYR	N-CA-C	-5.44	105.43	111.36
1	A	146	PHE	N-CA-C	-5.44	105.25	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	SER	N-CA-C	5.43	119.08	112.23
1	B	185	MET	N-CA-C	5.42	117.89	111.33
1	B	397	TRP	N-CA-C	5.42	118.44	110.59
1	A	861	ALA	N-CA-C	-5.42	105.46	111.36
1	A	525	ASP	N-CA-C	-5.41	106.68	113.28
1	B	262	LYS	N-CA-C	5.41	116.70	109.83
1	A	188	ILE	N-CA-C	-5.41	104.61	110.23
1	B	731	GLY	CA-C-N	5.41	125.08	119.56
1	B	731	GLY	C-N-CA	5.41	125.08	119.56
1	A	474	GLY	CA-C-N	5.30	125.62	119.47
1	A	474	GLY	C-N-CA	5.30	125.62	119.47
1	B	935	VAL	N-CA-C	5.30	120.36	109.34
1	A	271	ASN	N-CA-C	-5.29	105.97	112.90
1	B	836	PHE	N-CA-C	5.27	117.44	111.11
1	A	697	LYS	N-CA-C	-5.25	105.98	112.38
1	A	664	ILE	N-CA-C	-5.24	104.78	110.23
1	B	801	ALA	N-CA-C	5.23	117.38	111.11
1	B	391	TYR	N-CA-C	-5.22	103.64	110.53
1	A	245	LEU	N-CA-C	5.21	118.80	112.23
1	A	935	VAL	N-CA-C	5.21	120.17	109.34
1	B	677	PHE	N-CA-C	-5.19	105.80	111.82
1	A	19	GLY	CA-C-N	5.19	124.69	119.19
1	A	19	GLY	C-N-CA	5.19	124.69	119.19
1	A	339	LEU	N-CA-C	-5.18	105.71	111.36
1	A	688	GLU	N-CA-C	5.18	117.22	110.43
1	B	747	ASN	N-CA-C	-5.17	105.08	111.33
1	A	843	ILE	N-CA-C	-5.15	105.52	110.72
1	B	168	VAL	N-CA-C	5.15	115.82	110.82
1	A	922	GLU	N-CA-C	5.15	116.58	111.07
1	A	196	MET	N-CA-C	-5.14	105.57	111.07
1	A	214	VAL	CB-CA-C	-5.12	105.41	111.81
1	A	599	VAL	N-CA-C	5.12	119.93	108.88
1	A	879	PHE	N-CA-C	5.04	116.47	111.07
1	B	402	ASP	N-CA-C	5.04	119.42	113.12

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	46	ILE	CB
1	A	158	ILE	CB
1	A	674	ILE	CB
1	A	761	ILE	CB

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Mol	Chain	Res	Type	Atom
1	A	767	ILE	CB
1	A	840	ILE	CB
1	B	46	ILE	CB
1	B	158	ILE	CB
1	B	674	ILE	CB
1	B	726	ILE	CB
1	B	727	ILE	CB
1	B	761	ILE	CB
1	B	787	ILE	CB
1	B	840	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	681	PHE	Sidechain

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	6515	0	5799	485	0
1	B	6357	0	5573	485	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	12876	0	11372	958	1

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 (958) 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:101:PRO:HB2	1:A:103:TYR:CE2	1.58	1.36
1:B:683:ALA:HB1	1:B:728:ASN:C	1.52	1.32
1:A:101:PRO:CB	1:A:103:TYR:HE2	1.47	1.27
1:A:204:ASN:HD22	1:B:204:ASN:CB	1.45	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASN:ND2	1:B:204:ASN:HB3	1.50	1.26
1:A:716:ARG:O	1:A:720:ARG:HG3	1.43	1.18
1:A:101:PRO:CB	1:A:103:TYR:CE2	2.24	1.16
1:B:205:TYR:HE2	1:B:242:ILE:HD13	1.03	1.16
1:B:229:ASN:C	1:B:229:ASN:HD22	1.50	1.16
1:B:683:ALA:CB	1:B:729:VAL:HA	1.77	1.14
1:A:248:ALA:O	1:A:252:THR:HG22	1.46	1.13
1:B:683:ALA:CA	1:B:729:VAL:HA	1.77	1.13
1:A:370:LEU:HD22	1:A:374:LEU:HD23	1.22	1.12
1:B:856:GLN:CG	1:B:909:VAL:HG11	1.80	1.12
1:A:229:ASN:C	1:A:229:ASN:HD22	1.52	1.10
1:A:716:ARG:HB2	1:A:720:ARG:HH21	1.03	1.10
1:B:683:ALA:HB1	1:B:729:VAL:N	1.65	1.09
1:A:672:MET:HA	1:A:672:MET:HE2	1.34	1.09
1:A:511:LEU:HG	1:A:551:VAL:HG13	1.31	1.09
1:A:59:LEU:HD22	1:A:103:TYR:HD1	1.10	1.07
1:B:78:LEU:HG	1:B:82:GLN:NE2	1.69	1.07
1:A:568:LYS:H	1:A:568:LYS:HD2	1.11	1.06
1:B:692:LEU:HD22	1:B:730:VAL:HG22	1.35	1.06
1:A:59:LEU:HD22	1:A:103:TYR:CD1	1.91	1.06
1:B:78:LEU:HG	1:B:82:GLN:HE21	1.15	1.06
1:A:78:LEU:HG	1:A:82:GLN:HE21	1.20	1.04
1:B:683:ALA:HA	1:B:729:VAL:HA	1.35	1.03
1:B:205:TYR:CE2	1:B:242:ILE:HD13	1.94	1.02
1:B:783:LEU:O	1:B:787:ILE:HG23	1.58	1.02
1:B:229:ASN:HD21	1:B:232:CYS:H	1.04	1.02
1:A:370:LEU:CD2	1:A:374:LEU:HD23	1.89	1.01
1:A:632:PRO:HA	1:A:635:GLN:HG2	1.42	1.01
1:B:692:LEU:HD22	1:B:730:VAL:CG2	1.91	1.01
1:A:742:ILE:O	1:A:746:LEU:HG	1.62	0.99
1:A:716:ARG:HB2	1:A:720:ARG:NH2	1.76	0.98
1:A:204:ASN:HD22	1:B:204:ASN:HB3	0.86	0.98
1:A:300:ASN:HD22	1:A:350:VAL:HA	1.29	0.98
1:B:152:LEU:HD13	1:B:214:VAL:HG22	1.43	0.97
1:A:101:PRO:HB2	1:A:103:TYR:CD2	1.99	0.97
1:A:716:ARG:C	1:A:720:ARG:HE	1.72	0.97
1:A:389:MET:HE2	1:A:413:ARG:HG2	1.45	0.97
1:A:593:THR:HG21	1:A:597:ALA:O	1.64	0.97
1:A:244:GLU:HB3	1:B:203:LYS:HZ2	1.28	0.96
1:A:73:ASN:H	1:A:77:ASN:HD22	1.05	0.96
1:A:405:GLU:O	1:A:408:GLU:HG2	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:GLY:O	1:A:882:PHE:CG	2.19	0.96
1:A:368:LYS:O	1:A:368:LYS:HD3	1.65	0.96
1:B:856:GLN:CG	1:B:909:VAL:CG1	2.42	0.96
1:B:300:ASN:HD22	1:B:350:VAL:HA	1.30	0.96
1:A:783:LEU:O	1:A:787:ILE:HG13	1.65	0.95
1:B:837:ASP:HB3	1:B:841:ASN:HD21	1.31	0.95
1:A:758:LEU:HD12	1:A:810:SER:OG	1.65	0.95
1:B:784:LEU:HD22	1:B:839:LEU:HD21	1.49	0.94
1:A:538:PHE:O	1:A:544:ILE:HG13	1.66	0.94
1:A:293:GLU:HG2	1:A:297:LYS:HE3	1.46	0.94
1:B:60:ILE:O	1:B:64:THR:HG22	1.68	0.93
1:B:639:CYS:HG	1:B:681:PHE:HZ	1.06	0.93
1:B:318:PRO:HA	1:B:321:LYS:HB3	1.50	0.93
1:A:229:ASN:HD21	1:A:232:CYS:H	1.01	0.93
1:B:368:LYS:O	1:B:368:LYS:HD3	1.68	0.93
1:A:68:LYS:HA	1:A:68:LYS:HE2	1.49	0.92
1:B:777:ASN:HD21	1:B:826:ILE:CB	1.83	0.92
1:A:78:LEU:HG	1:A:82:GLN:NE2	1.82	0.92
1:B:683:ALA:CB	1:B:729:VAL:CA	2.48	0.91
1:B:683:ALA:HB1	1:B:729:VAL:CA	2.00	0.91
1:A:204:ASN:ND2	1:B:204:ASN:CB	2.20	0.91
1:B:73:ASN:H	1:B:77:ASN:ND2	1.70	0.90
1:B:683:ALA:HB1	1:B:728:ASN:O	1.71	0.90
1:B:248:ALA:O	1:B:252:THR:HG22	1.70	0.90
1:B:257:VAL:O	1:B:266:LYS:HE2	1.73	0.89
1:B:538:PHE:O	1:B:544:ILE:HG13	1.72	0.88
1:B:104:ILE:O	1:B:108:VAL:HG23	1.72	0.88
1:B:405:GLU:O	1:B:408:GLU:HG3	1.72	0.88
1:B:73:ASN:H	1:B:77:ASN:HD22	0.90	0.88
1:A:299:ILE:HD13	1:A:334:TYR:HB3	1.55	0.88
1:A:568:LYS:H	1:A:568:LYS:CD	1.83	0.88
1:A:784:LEU:HD23	1:A:787:ILE:HD12	1.54	0.88
1:A:60:ILE:O	1:A:64:THR:HG22	1.73	0.87
1:B:229:ASN:C	1:B:229:ASN:ND2	2.28	0.87
1:A:504:HIS:HD2	1:A:506:HIS:H	1.22	0.87
1:A:55:PRO:HB2	1:A:103:TYR:OH	1.74	0.87
1:A:152:LEU:HD13	1:A:214:VAL:HG22	1.57	0.86
1:A:229:ASN:C	1:A:229:ASN:ND2	2.30	0.86
1:B:241:GLN:HE21	1:B:283:GLN:NE2	1.73	0.86
1:B:299:ILE:HD13	1:B:334:TYR:HB3	1.57	0.86
1:A:204:ASN:HA	1:B:204:ASN:HA	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:SER:HB2	1:B:318:PRO:HD2	1.56	0.86
1:B:375:LYS:HE2	1:B:379:LYS:NZ	1.90	0.86
1:A:74:ASN:O	1:A:78:LEU:HB2	1.76	0.85
1:B:683:ALA:CB	1:B:728:ASN:C	2.45	0.85
1:B:739:PRO:HD3	1:B:775:ILE:HD13	1.58	0.85
1:A:3:ALA:HB1	1:A:53:TYR:HE2	1.42	0.85
1:B:389:MET:HE2	1:B:413:ARG:HG2	1.58	0.84
1:B:241:GLN:NE2	1:B:283:GLN:NE2	2.24	0.84
1:B:288:ASP:OD1	1:B:289:PRO:HD2	1.77	0.84
1:B:199:TYR:CD1	1:B:207:THR:HG21	2.12	0.84
1:A:689:VAL:HG13	1:A:691:TRP:CE3	2.13	0.84
1:A:863:VAL:O	1:A:867:VAL:HG23	1.78	0.84
1:B:683:ALA:CB	1:B:729:VAL:N	2.41	0.83
1:B:416:LEU:HA	1:B:419:PHE:HD1	1.42	0.83
1:A:760:PHE:O	1:A:764:LEU:HB2	1.77	0.83
1:B:504:HIS:HD2	1:B:506:HIS:H	1.27	0.83
1:A:47:PHE:HA	1:A:58:ARG:HG2	1.58	0.83
1:B:836:PHE:O	1:B:840:ILE:HG23	1.79	0.83
1:A:416:LEU:HA	1:A:419:PHE:HD1	1.44	0.83
1:B:199:TYR:CE1	1:B:207:THR:HG21	2.14	0.83
1:A:244:GLU:HB3	1:B:203:LYS:NZ	1.92	0.82
1:B:205:TYR:CE2	1:B:242:ILE:HG21	2.14	0.82
1:A:738:VAL:N	1:A:739:PRO:HD2	1.94	0.82
1:A:737:LYS:C	1:A:739:PRO:HD2	2.05	0.82
1:A:100:GLU:HB3	1:A:101:PRO:HD2	1.62	0.81
1:A:1:MET:HG3	1:A:4:GLN:H	1.44	0.81
1:A:24:GLN:O	1:A:27:THR:HG22	1.80	0.81
1:A:566:ILE:CG2	1:A:569:GLN:HB2	2.10	0.81
1:A:528:SER:O	1:A:531:ILE:HG13	1.81	0.81
1:B:65:LEU:O	1:B:69:VAL:HG23	1.81	0.81
1:A:101:PRO:CG	1:A:103:TYR:HE2	1.94	0.81
1:A:229:ASN:ND2	1:A:232:CYS:H	1.79	0.80
1:A:104:ILE:O	1:A:108:VAL:HG23	1.80	0.80
1:A:713:GLU:HA	1:A:716:ARG:HG3	1.63	0.80
1:A:215:TYR:O	1:A:219:VAL:HG23	1.81	0.80
1:B:59:LEU:HD22	1:B:103:TYR:CD1	2.16	0.80
1:A:640:ASP:OD1	1:A:694:SER:HB3	1.81	0.80
1:B:570:VAL:HG12	1:B:570:VAL:O	1.80	0.80
1:B:375:LYS:HG2	1:B:379:LYS:HE3	1.62	0.80
1:A:885:SER:C	1:A:888:PRO:HD2	2.08	0.79
1:A:171:GLN:O	1:A:175:LEU:HG	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:HB3	1:B:261:MET:HE3	1.65	0.79
1:B:681:PHE:HB3	1:B:682:PRO:HD2	1.65	0.79
1:A:859:SER:HA	1:A:862:LEU:HD12	1.65	0.78
1:A:831:GLU:O	1:A:835:TYR:CE1	2.36	0.78
1:B:683:ALA:HB1	1:B:729:VAL:HA	1.57	0.78
1:A:370:LEU:HD22	1:A:374:LEU:CD2	2.09	0.78
1:B:44:HIS:HE1	1:B:83:MET:HG2	1.48	0.78
1:B:166:THR:HG22	1:B:168:VAL:H	1.48	0.78
1:A:411:GLU:CG	1:A:412:MET:N	2.47	0.77
1:A:836:PHE:O	1:A:840:ILE:HG23	1.84	0.77
1:B:837:ASP:HB3	1:B:841:ASN:ND2	1.99	0.77
1:A:43:CYS:SG	1:A:64:THR:HG21	2.25	0.77
1:B:3:ALA:HB1	1:B:53:TYR:HE2	1.49	0.77
1:A:722:THR:HG22	1:A:726:ILE:HD12	1.67	0.77
1:A:716:ARG:O	1:A:720:ARG:CG	2.31	0.77
1:B:784:LEU:CD2	1:B:839:LEU:HD21	2.15	0.77
1:A:55:PRO:HB3	1:A:104:ILE:HD11	1.66	0.76
1:A:704:LEU:O	1:A:708:ARG:CG	2.33	0.76
1:A:55:PRO:CB	1:A:103:TYR:OH	2.34	0.76
1:A:593:THR:HG23	1:A:599:VAL:O	1.86	0.76
1:B:734:MET:HA	1:B:734:MET:HE2	1.66	0.76
1:A:120:TYR:HA	1:A:124:TRP:HB3	1.66	0.76
1:B:500:GLN:H	1:B:500:GLN:CD	1.92	0.76
1:A:856:GLN:O	1:A:860:ILE:HG23	1.86	0.76
1:A:733:ASP:O	1:A:736:PRO:HD2	1.87	0.75
1:B:246:ARG:HD3	1:B:291:PHE:CD1	2.21	0.75
1:A:570:VAL:HG12	1:A:570:VAL:O	1.87	0.75
1:B:300:ASN:HD21	1:B:352:PRO:HD2	1.52	0.75
1:A:539:VAL:HG12	1:A:539:VAL:O	1.84	0.75
1:B:271:ASN:HA	1:B:327:GLN:NE2	2.02	0.74
1:B:539:VAL:HG12	1:B:539:VAL:O	1.86	0.74
1:B:229:ASN:ND2	1:B:232:CYS:H	1.82	0.74
1:B:299:ILE:CD1	1:B:334:TYR:HB3	2.18	0.74
1:A:672:MET:HE2	1:A:672:MET:CA	2.16	0.74
1:A:778:ARG:O	1:A:781:PRO:HD2	1.86	0.74
1:A:731:GLY:N	1:A:732:PRO:HD2	2.01	0.74
1:B:130:SER:O	1:B:134:VAL:HG23	1.86	0.74
1:A:632:PRO:HA	1:A:635:GLN:CG	2.17	0.74
1:A:689:VAL:HG22	1:A:691:TRP:CH2	2.23	0.74
1:B:625:ILE:HG21	1:B:639:CYS:SG	2.28	0.74
1:B:727:ILE:HG22	1:B:734:MET:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:H	1:A:77:ASN:ND2	1.83	0.74
1:A:229:ASN:HD21	1:A:232:CYS:N	1.84	0.73
1:B:73:ASN:N	1:B:77:ASN:HD22	1.76	0.73
1:A:230:GLU:N	1:A:231:PRO:HD2	2.02	0.73
1:B:171:GLN:O	1:B:175:LEU:HG	1.89	0.73
1:B:636:ALA:HB2	1:B:690:ALA:HB1	1.69	0.73
1:A:777:ASN:HD21	1:A:826:ILE:CB	2.01	0.73
1:B:722:THR:O	1:B:726:ILE:HG23	1.88	0.73
1:A:566:ILE:HG22	1:A:569:GLN:HB2	1.70	0.72
1:B:58:ARG:NH1	1:B:100:GLU:OE1	2.21	0.72
1:B:329:TYR:CE1	1:B:373:SER:OG	2.41	0.72
1:B:672:MET:HE2	1:B:672:MET:HA	1.69	0.72
1:B:860:ILE:CD1	1:B:912:GLU:CB	2.68	0.72
1:B:762:SER:HA	1:B:817:GLN:HE22	1.54	0.72
1:B:860:ILE:HD11	1:B:912:GLU:CB	2.20	0.71
1:B:61:CYS:O	1:B:64:THR:HG23	1.90	0.71
1:A:257:VAL:O	1:A:266:LYS:HE2	1.91	0.71
1:B:568:LYS:O	1:B:571:VAL:HG23	1.90	0.71
1:B:626:SER:HB2	1:B:682:PRO:CD	2.21	0.71
1:B:236:LEU:HB2	1:B:253:MET:HE3	1.73	0.71
1:B:683:ALA:O	1:B:684:ARG:C	2.30	0.71
1:B:50:LYS:HA	1:B:58:ARG:NH2	2.06	0.71
1:B:544:ILE:HG23	1:B:556:TRP:CD1	2.26	0.71
1:A:173:ASP:O	1:A:177:LYS:HG3	1.92	0.70
1:B:329:TYR:HE1	1:B:373:SER:HG	1.39	0.70
1:A:386:ILE:HG23	1:A:460:PHE:CZ	2.26	0.70
1:A:511:LEU:HG	1:A:551:VAL:CG1	2.17	0.70
1:A:169:GLN:NE2	1:A:173:ASP:OD2	2.25	0.70
1:B:259:LYS:HB3	1:B:261:MET:CE	2.22	0.70
1:A:682:PRO:O	1:A:729:VAL:HG22	1.92	0.70
1:B:257:VAL:O	1:B:266:LYS:CE	2.39	0.69
1:A:702:ILE:O	1:A:706:LEU:N	2.25	0.69
1:B:50:LYS:O	1:B:58:ARG:NH2	2.25	0.69
1:B:715:ILE:HA	1:B:718:ALA:HB3	1.73	0.69
1:B:886:LEU:C	1:B:888:PRO:HD2	2.17	0.69
1:B:885:SER:O	1:B:888:PRO:HD2	1.92	0.69
1:A:59:LEU:O	1:A:63:GLN:HG3	1.92	0.69
1:A:130:SER:O	1:A:134:VAL:HG23	1.93	0.68
1:A:271:ASN:HA	1:A:327:GLN:NE2	2.07	0.68
1:A:546:ASN:HD22	1:A:547:THR:N	1.91	0.68
1:A:717:GLY:N	1:A:720:ARG:HE	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LYS:HE2	1:B:379:LYS:HZ1	1.57	0.68
1:B:731:GLY:N	1:B:732:PRO:HD2	2.08	0.68
1:A:727:ILE:HG23	1:A:734:MET:CB	2.23	0.68
1:A:58:ARG:HH12	1:A:100:GLU:CD	2.02	0.68
1:A:177:LYS:HE2	1:A:221:TRP:HB3	1.76	0.68
1:A:293:GLU:O	1:A:297:LYS:HG3	1.93	0.68
1:A:3:ALA:HB1	1:A:53:TYR:CE2	2.28	0.68
1:A:503:ARG:HA	1:A:542:ARG:CZ	2.22	0.68
1:B:299:ILE:HD13	1:B:334:TYR:CB	2.24	0.67
1:B:546:ASN:HD22	1:B:547:THR:N	1.92	0.67
1:B:836:PHE:CE2	1:B:840:ILE:HG21	2.29	0.67
1:B:215:TYR:O	1:B:219:VAL:HG23	1.94	0.67
1:A:504:HIS:CD2	1:A:506:HIS:H	2.11	0.67
1:A:104:ILE:O	1:A:104:ILE:HG22	1.94	0.67
1:A:389:MET:CE	1:A:413:ARG:HG2	2.21	0.67
1:A:1:MET:HB3	1:A:4:GLN:HB2	1.76	0.66
1:A:300:ASN:HD21	1:A:352:PRO:HD2	1.60	0.66
1:A:44:HIS:CD2	1:A:44:HIS:O	2.48	0.66
1:A:102:ALA:O	1:A:106:ASN:ND2	2.28	0.66
1:B:188:ILE:O	1:B:192:VAL:HG23	1.94	0.66
1:A:101:PRO:HB3	1:A:103:TYR:CE2	2.27	0.66
1:A:299:ILE:CD1	1:A:334:TYR:HB3	2.24	0.66
1:B:177:LYS:HE2	1:B:221:TRP:HB3	1.77	0.66
1:B:731:GLY:HA3	1:B:768:TYR:CE2	2.30	0.66
1:A:405:GLU:HB2	1:A:408:GLU:OE2	1.96	0.66
1:B:885:SER:O	1:B:888:PRO:CD	2.44	0.66
1:A:689:VAL:HG13	1:A:691:TRP:CD2	2.31	0.66
1:A:119:LEU:HB3	1:A:123:ASN:HB2	1.78	0.65
1:B:506:HIS:O	1:B:510:GLN:HG3	1.96	0.65
1:A:68:LYS:HE2	1:A:68:LYS:CA	2.24	0.65
1:A:672:MET:HE3	1:A:718:ALA:HB1	1.78	0.65
1:A:713:GLU:CA	1:A:716:ARG:HG3	2.26	0.65
1:A:831:GLU:O	1:A:835:TYR:HE1	1.78	0.65
1:A:615:LEU:HD22	1:A:676:ASN:HD22	1.60	0.65
1:B:44:HIS:O	1:B:44:HIS:CD2	2.49	0.65
1:B:411:GLU:CG	1:B:412:MET:N	2.59	0.65
1:A:408:GLU:O	1:A:411:GLU:CG	2.44	0.65
1:A:683:ALA:HB1	1:A:728:ASN:OD1	1.97	0.65
1:A:753:GLU:O	1:A:757:VAL:HG23	1.97	0.65
1:B:836:PHE:CZ	1:B:840:ILE:HG21	2.31	0.65
1:B:229:ASN:HD21	1:B:232:CYS:N	1.85	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:LEU:HD12	1:A:810:SER:CB	2.27	0.64
1:A:773:MET:HE2	1:A:773:MET:HA	1.79	0.64
1:B:230:GLU:N	1:B:231:PRO:HD2	2.12	0.64
1:B:288:ASP:OD1	1:B:289:PRO:CD	2.46	0.64
1:A:44:HIS:O	1:A:44:HIS:HD2	1.79	0.64
1:A:204:ASN:HD22	1:B:204:ASN:HB2	1.53	0.64
1:A:687:GLU:N	1:A:687:GLU:CD	2.56	0.64
1:B:50:LYS:HA	1:B:58:ARG:CZ	2.27	0.64
1:B:566:ILE:HG22	1:B:569:GLN:HG3	1.79	0.64
1:A:237:TYR:OH	1:A:277:LEU:HD23	1.98	0.64
1:A:611:PHE:CZ	1:A:669:CYS:HB2	2.32	0.64
1:A:689:VAL:CG1	1:A:691:TRP:CD2	2.80	0.64
1:B:408:GLU:O	1:B:411:GLU:CG	2.46	0.64
1:A:695:PHE:O	1:A:698:ALA:HB3	1.98	0.64
1:B:856:GLN:HB3	1:B:909:VAL:HG21	1.80	0.64
1:A:299:ILE:HD13	1:A:334:TYR:CB	2.27	0.63
1:B:218:TRP:O	1:B:222:ILE:HG13	1.98	0.63
1:A:825:SER:HA	1:A:828:PHE:CD1	2.33	0.63
1:B:74:ASN:O	1:B:78:LEU:HB2	1.98	0.63
1:B:758:LEU:HD12	1:B:810:SER:CB	2.28	0.63
1:A:400:ASP:HB3	1:A:404:GLU:HB2	1.81	0.63
1:B:100:GLU:HB3	1:B:101:PRO:HD2	1.79	0.63
1:B:311:SER:O	1:B:313:PRO:HD3	1.98	0.63
1:A:204:ASN:ND2	1:B:204:ASN:HB2	2.11	0.63
1:A:780:LEU:HB2	1:A:781:PRO:HD3	1.80	0.63
1:A:780:LEU:O	1:A:784:LEU:HG	1.97	0.63
1:A:672:MET:HE3	1:A:718:ALA:CB	2.28	0.63
1:B:152:LEU:HD13	1:B:214:VAL:CG2	2.25	0.63
1:A:294:HIS:HA	1:A:297:LYS:HD2	1.80	0.63
1:A:687:GLU:N	1:A:687:GLU:OE1	2.32	0.63
1:B:173:ASP:O	1:B:177:LYS:HG3	1.98	0.63
1:B:784:LEU:O	1:B:788:PHE:HD1	1.82	0.63
1:B:784:LEU:HB3	1:B:788:PHE:HE1	1.62	0.63
1:A:47:PHE:O	1:A:58:ARG:HD3	1.98	0.62
1:B:300:ASN:ND2	1:B:352:PRO:HD2	2.14	0.62
1:B:44:HIS:O	1:B:44:HIS:HD2	1.80	0.62
1:B:837:ASP:HB2	1:B:838:PRO:CD	2.28	0.62
1:B:43:CYS:SG	1:B:64:THR:HG21	2.40	0.62
1:B:681:PHE:HB3	1:B:682:PRO:CD	2.28	0.62
1:A:528:SER:HB2	1:A:531:ILE:HD11	1.80	0.62
1:A:566:ILE:HG22	1:A:566:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:THR:HG22	1:A:726:ILE:CD1	2.29	0.62
1:B:734:MET:HA	1:B:734:MET:CE	2.30	0.62
1:A:385:ILE:HG23	1:A:416:LEU:HD22	1.82	0.62
1:A:601:THR:HG22	1:A:602:LEU:N	2.15	0.62
1:B:784:LEU:O	1:B:788:PHE:CD1	2.53	0.62
1:A:101:PRO:CB	1:A:103:TYR:CD2	2.70	0.62
1:A:570:VAL:HG22	1:A:573:TYR:HB2	1.81	0.62
1:A:742:ILE:O	1:A:746:LEU:CG	2.42	0.62
1:A:544:ILE:HG23	1:A:556:TRP:CD1	2.35	0.62
1:A:689:VAL:CG1	1:A:690:ALA:N	2.63	0.62
1:B:241:GLN:HE21	1:B:283:GLN:HE21	1.48	0.62
1:B:570:VAL:HA	1:B:573:TYR:HD1	1.64	0.62
1:B:566:ILE:HG21	1:B:569:GLN:CD	2.24	0.62
1:B:783:LEU:C	1:B:787:ILE:HG23	2.25	0.62
1:A:177:LYS:HE2	1:A:221:TRP:CB	2.30	0.61
1:A:119:LEU:CB	1:A:123:ASN:HB2	2.31	0.61
1:A:546:ASN:HD22	1:A:547:THR:H	1.47	0.61
1:B:762:SER:HA	1:B:817:GLN:NE2	2.16	0.61
1:A:370:LEU:CD2	1:A:374:LEU:CD2	2.74	0.61
1:A:568:LYS:HD2	1:A:568:LYS:N	1.97	0.61
1:B:3:ALA:HB1	1:B:53:TYR:CE2	2.34	0.61
1:A:52:LYS:HD2	1:A:53:TYR:HE1	1.65	0.61
1:A:411:GLU:CG	1:A:412:MET:H	2.14	0.60
1:A:500:GLN:HB2	1:A:503:ARG:HE	1.66	0.60
1:B:566:ILE:CG2	1:B:569:GLN:HG3	2.31	0.60
1:B:632:PRO:HA	1:B:635:GLN:HG2	1.82	0.60
1:A:778:ARG:C	1:A:781:PRO:HD2	2.26	0.60
1:B:753:GLU:O	1:B:757:VAL:HG23	2.01	0.60
1:A:636:ALA:HB2	1:A:690:ALA:HB1	1.83	0.60
1:B:777:ASN:ND2	1:B:826:ILE:CB	2.61	0.60
1:A:50:LYS:HA	1:A:58:ARG:NH2	2.17	0.60
1:A:204:ASN:HA	1:B:204:ASN:CA	2.28	0.60
1:A:689:VAL:HG12	1:A:692:LEU:H	1.67	0.60
1:B:241:GLN:NE2	1:B:283:GLN:HE21	1.99	0.60
1:A:386:ILE:HD12	1:A:434:TYR:HE2	1.66	0.60
1:A:681:PHE:HB3	1:A:682:PRO:HD2	1.84	0.60
1:B:406:GLU:O	1:B:410:GLN:HG2	2.01	0.60
1:B:730:VAL:HG12	1:B:730:VAL:O	2.00	0.60
1:A:100:GLU:HB3	1:A:101:PRO:CD	2.30	0.60
1:A:738:VAL:N	1:A:739:PRO:CD	2.65	0.60
1:B:400:ASP:O	1:B:404:GLU:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:ASP:O	1:B:841:ASN:N	2.30	0.60
1:A:68:LYS:HA	1:A:68:LYS:CE	2.28	0.59
1:A:602:LEU:HD22	1:A:714:ASP:OD2	2.02	0.59
1:A:784:LEU:HA	1:A:787:ILE:HD12	1.84	0.59
1:A:835:TYR:O	1:A:838:PRO:HG2	2.02	0.59
1:A:499:SER:HB2	1:A:501:VAL:HG23	1.83	0.59
1:B:546:ASN:HD22	1:B:547:THR:H	1.49	0.59
1:A:27:THR:HG23	1:A:28:ASP:N	2.16	0.59
1:A:229:ASN:HD22	1:A:230:GLU:N	2.00	0.59
1:B:649:LYS:HE2	1:B:666:SER:OG	2.02	0.59
1:B:271:ASN:CA	1:B:327:GLN:NE2	2.66	0.59
1:B:622:GLY:C	1:B:680:GLY:O	2.46	0.59
1:B:147:TYR:CZ	1:B:151:LEU:HD11	2.38	0.59
1:A:61:CYS:O	1:A:64:THR:HG23	2.03	0.59
1:B:731:GLY:HA3	1:B:768:TYR:CZ	2.38	0.58
1:A:592:VAL:HG12	1:A:593:THR:N	2.18	0.58
1:A:176:VAL:O	1:A:180:ILE:HG13	2.03	0.58
1:B:570:VAL:O	1:B:570:VAL:CG1	2.49	0.58
1:A:506:HIS:O	1:A:510:GLN:HG3	2.03	0.58
1:B:689:VAL:HG12	1:B:691:TRP:H	1.67	0.58
1:A:249:ALA:O	1:A:253:MET:HG3	2.03	0.58
1:B:15:ASP:HB3	1:B:18:VAL:HG23	1.85	0.58
1:A:249:ALA:O	1:A:252:THR:HG23	2.04	0.58
1:A:837:ASP:O	1:A:841:ASN:ND2	2.36	0.58
1:A:397:TRP:HE3	1:A:406:GLU:OE2	1.85	0.58
1:B:199:TYR:CD1	1:B:207:THR:CG2	2.86	0.58
1:B:462:LEU:HD11	1:B:501:VAL:CG1	2.33	0.58
1:B:575:GLU:CG	1:B:630:LEU:HD21	2.33	0.58
1:B:615:LEU:HD22	1:B:676:ASN:HD22	1.68	0.58
1:A:727:ILE:O	1:A:731:GLY:HA2	2.04	0.58
1:B:158:ILE:CG1	1:B:177:LYS:HG2	2.34	0.58
1:B:860:ILE:HD12	1:B:912:GLU:CB	2.34	0.58
1:A:236:LEU:HB2	1:A:253:MET:HE3	1.86	0.57
1:B:489:LEU:O	1:B:492:ILE:HB	2.04	0.57
1:A:689:VAL:HG12	1:A:690:ALA:N	2.18	0.57
1:A:701:GLU:O	1:A:705:ILE:N	2.37	0.57
1:B:361:LEU:HB3	1:B:426:ILE:HD13	1.85	0.57
1:A:640:ASP:OD1	1:A:694:SER:CB	2.51	0.57
1:B:636:ALA:HB2	1:B:690:ALA:CB	2.35	0.57
1:A:857:LYS:O	1:A:860:ILE:HG12	2.04	0.57
1:B:456:GLN:H	1:B:456:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HD2	1:A:337:ARG:O	2.03	0.57
1:A:514:MET:HE1	1:A:543:GLY:HA2	1.86	0.57
1:A:592:VAL:HG12	1:A:593:THR:H	1.68	0.57
1:A:731:GLY:N	1:A:732:PRO:CD	2.68	0.57
1:A:734:MET:C	1:A:736:PRO:HD2	2.29	0.57
1:B:825:SER:HA	1:B:828:PHE:CD1	2.38	0.57
1:A:300:ASN:ND2	1:A:350:VAL:HA	2.10	0.57
1:A:317:SER:HB2	1:A:318:PRO:HD2	1.87	0.57
1:B:120:TYR:OH	1:B:180:ILE:HA	2.05	0.57
1:A:103:TYR:H	1:A:103:TYR:HD2	1.53	0.57
1:A:277:LEU:HD11	1:A:302:GLN:HE22	1.69	0.57
1:A:884:LEU:O	1:A:887:THR:HB	2.04	0.57
1:B:177:LYS:HE2	1:B:221:TRP:CB	2.34	0.57
1:B:385:ILE:HG23	1:B:416:LEU:HD22	1.87	0.56
1:A:212:LEU:HD22	1:A:252:THR:HG21	1.86	0.56
1:A:884:LEU:O	1:A:888:PRO:HD3	2.04	0.56
1:A:885:SER:O	1:A:888:PRO:HD2	2.04	0.56
1:B:504:HIS:CD2	1:B:506:HIS:H	2.15	0.56
1:A:735:LEU:N	1:A:736:PRO:CD	2.68	0.56
1:B:193:TYR:C	1:B:193:TYR:CD2	2.83	0.56
1:B:424:ASN:HD22	1:B:428:SER:HA	1.71	0.56
1:B:499:SER:HB3	1:B:501:VAL:HG23	1.87	0.56
1:B:683:ALA:HA	1:B:729:VAL:CA	2.24	0.56
1:A:734:MET:C	1:A:736:PRO:CD	2.78	0.56
1:B:329:TYR:HE1	1:B:373:SER:OG	1.83	0.56
1:B:544:ILE:HG23	1:B:556:TRP:HD1	1.70	0.56
1:A:271:ASN:CA	1:A:327:GLN:NE2	2.69	0.56
1:A:619:GLU:O	1:A:623:VAL:HG23	2.05	0.56
1:B:619:GLU:O	1:B:623:VAL:HG23	2.05	0.56
1:A:416:LEU:HA	1:A:419:PHE:CD1	2.34	0.56
1:A:784:LEU:HD13	1:A:839:LEU:HD11	1.88	0.56
1:B:145:ASN:O	1:B:149:LYS:HG3	2.05	0.56
1:A:120:TYR:N	1:A:121:PRO:HD2	2.20	0.56
1:A:835:TYR:O	1:A:839:LEU:HG	2.06	0.56
1:A:835:TYR:CD1	1:A:835:TYR:N	2.74	0.56
1:A:634:GLU:O	1:A:637:LEU:N	2.38	0.56
1:A:727:ILE:O	1:A:731:GLY:CA	2.54	0.56
1:B:559:PHE:O	1:B:563:VAL:HG23	2.06	0.56
1:A:361:LEU:HB3	1:A:426:ILE:HD13	1.87	0.56
1:B:405:GLU:O	1:B:408:GLU:CG	2.52	0.56
1:B:601:THR:HG22	1:B:603:ASN:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:SER:CA	1:B:817:GLN:HE22	2.19	0.56
1:A:230:GLU:H	1:A:231:PRO:HD2	1.70	0.55
1:B:58:ARG:HH12	1:B:100:GLU:CD	2.14	0.55
1:B:856:GLN:HB3	1:B:909:VAL:CG2	2.35	0.55
1:A:193:TYR:C	1:A:193:TYR:CD2	2.84	0.55
1:A:717:GLY:N	1:A:720:ARG:NE	2.54	0.55
1:B:241:GLN:NE2	1:B:283:GLN:HE22	2.04	0.55
1:B:462:LEU:HD11	1:B:501:VAL:HG11	1.87	0.55
1:A:566:ILE:HG23	1:A:569:GLN:HB2	1.89	0.55
1:A:672:MET:CE	1:A:718:ALA:HA	2.36	0.55
1:B:195:MET:CE	1:B:199:TYR:HE1	2.19	0.55
1:B:219:VAL:O	1:B:259:LYS:HE2	2.06	0.55
1:B:241:GLN:HE21	1:B:283:GLN:HE22	1.53	0.55
1:B:856:GLN:CG	1:B:909:VAL:HG13	2.31	0.55
1:B:424:ASN:ND2	1:B:428:SER:HA	2.22	0.55
1:A:269:LEU:HA	1:A:272:ILE:HD12	1.89	0.55
1:A:636:ALA:O	1:A:640:ASP:CG	2.50	0.55
1:B:195:MET:HE3	1:B:199:TYR:HE1	1.71	0.55
1:B:283:GLN:CD	1:B:283:GLN:C	2.74	0.55
1:A:430:LEU:O	1:A:430:LEU:HD12	2.07	0.55
1:B:295:VAL:HG11	1:B:338:TYR:OH	2.07	0.55
1:B:330:ASN:HD22	1:B:330:ASN:N	2.05	0.55
1:A:511:LEU:HD21	1:A:554:ARG:HG2	1.89	0.55
1:A:293:GLU:HG2	1:A:297:LYS:CE	2.28	0.55
1:A:672:MET:HA	1:A:672:MET:CE	2.20	0.55
1:B:335:LEU:HD12	1:B:350:VAL:HG11	1.88	0.55
1:B:634:GLU:O	1:B:637:LEU:N	2.39	0.55
1:A:498:THR:O	1:A:498:THR:HG22	2.06	0.54
1:B:334:TYR:N	1:B:334:TYR:CD1	2.75	0.54
1:B:812:ILE:CB	1:B:862:LEU:HD11	2.37	0.54
1:A:398:ASP:OD2	1:A:404:GLU:CD	2.50	0.54
1:B:55:PRO:HB3	1:B:104:ILE:HD11	1.89	0.54
1:A:578:LEU:HD21	1:A:624:LEU:HB2	1.90	0.54
1:A:412:MET:HG2	1:A:412:MET:O	2.06	0.54
1:A:445:THR:O	1:A:448:THR:HB	2.08	0.54
1:A:887:THR:N	1:A:888:PRO:HD2	2.23	0.54
1:B:511:LEU:HD21	1:B:554:ARG:HG2	1.89	0.54
1:A:158:ILE:CG1	1:A:177:LYS:HG2	2.38	0.54
1:A:218:TRP:O	1:A:222:ILE:HG13	2.08	0.54
1:B:539:VAL:O	1:B:539:VAL:CG1	2.55	0.54
1:B:541:PRO:O	1:B:546:ASN:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASN:N	1:A:330:ASN:HD22	2.05	0.54
1:B:416:LEU:HA	1:B:419:PHE:CD1	2.32	0.54
1:A:172:LYS:O	1:A:176:VAL:HG23	2.07	0.54
1:A:716:ARG:C	1:A:720:ARG:NE	2.56	0.54
1:A:737:LYS:C	1:A:739:PRO:CD	2.78	0.54
1:B:55:PRO:O	1:B:56:SER:C	2.51	0.54
1:B:626:SER:CB	1:B:682:PRO:HD3	2.38	0.54
1:B:50:LYS:CA	1:B:58:ARG:NH2	2.71	0.54
1:B:271:ASN:CA	1:B:327:GLN:HE22	2.21	0.54
1:B:525:ASP:OD1	1:B:566:ILE:HG12	2.07	0.54
1:B:626:SER:CB	1:B:682:PRO:CD	2.85	0.54
1:A:94:GLU:OE1	1:A:94:GLU:HA	2.08	0.53
1:B:727:ILE:O	1:B:731:GLY:N	2.41	0.53
1:A:570:VAL:O	1:A:570:VAL:CG1	2.54	0.53
1:B:88:VAL:O	1:B:92:ILE:HG13	2.09	0.53
1:B:158:ILE:CG1	1:B:177:LYS:HE3	2.37	0.53
1:A:261:MET:HE3	1:A:266:LYS:HD3	1.91	0.53
1:B:541:PRO:HA	1:B:545:HIS:HB2	1.91	0.53
1:B:858:SER:O	1:B:861:ALA:HB3	2.08	0.53
1:B:116:PHE:CE1	1:B:120:TYR:CD1	2.97	0.53
1:B:503:ARG:HA	1:B:542:ARG:CZ	2.38	0.53
1:B:531:ILE:HD12	1:B:569:GLN:OE1	2.09	0.53
1:B:804:GLN:O	1:B:808:ARG:N	2.39	0.53
1:B:255:GLU:HA	1:B:255:GLU:OE1	2.08	0.53
1:A:58:ARG:NH1	1:A:100:GLU:OE1	2.39	0.53
1:A:197:LEU:O	1:A:200:SER:HB3	2.09	0.53
1:A:271:ASN:CA	1:A:327:GLN:HE22	2.22	0.53
1:A:300:ASN:ND2	1:A:352:PRO:HD2	2.21	0.53
1:A:557:TYR:O	1:A:560:TYR:HB3	2.09	0.53
1:B:837:ASP:C	1:B:841:ASN:HD22	2.16	0.53
1:B:859:SER:HA	1:B:862:LEU:HD12	1.91	0.53
1:A:237:TYR:O	1:A:240:LEU:HB2	2.09	0.53
1:A:773:MET:O	1:A:776:THR:HB	2.09	0.53
1:A:593:THR:CG2	1:A:597:ALA:O	2.48	0.53
1:B:102:ALA:O	1:B:106:ASN:ND2	2.42	0.53
1:B:837:ASP:C	1:B:841:ASN:ND2	2.67	0.53
1:A:477:ALA:O	1:A:487:THR:OG1	2.27	0.52
1:A:499:SER:CB	1:A:501:VAL:HG23	2.38	0.52
1:B:412:MET:O	1:B:412:MET:HG2	2.08	0.52
1:B:479:PHE:HA	1:B:486:PRO:HA	1.91	0.52
1:B:514:MET:HE1	1:B:543:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:THR:HG22	1:B:448:THR:O	2.09	0.52
1:A:689:VAL:HG12	1:A:691:TRP:N	2.25	0.52
1:B:135:ILE:HG12	1:B:143:PHE:HD2	1.75	0.52
1:B:229:ASN:HD22	1:B:230:GLU:N	2.02	0.52
1:B:243:GLU:CD	1:B:243:GLU:C	2.77	0.52
1:B:386:ILE:HD12	1:B:434:TYR:HE2	1.74	0.52
1:B:386:ILE:HG23	1:B:460:PHE:CZ	2.44	0.52
1:A:219:VAL:O	1:A:259:LYS:HE2	2.09	0.52
1:A:860:ILE:HD11	1:A:912:GLU:CB	2.39	0.52
1:B:172:LYS:O	1:B:176:VAL:HG23	2.10	0.52
1:B:392:ASP:O	1:B:395:GLN:O	2.28	0.52
1:B:846:PHE:CG	1:B:846:PHE:O	2.61	0.52
1:A:24:GLN:O	1:A:27:THR:CG2	2.55	0.52
1:A:242:ILE:O	1:A:246:ARG:HB3	2.09	0.52
1:A:489:LEU:O	1:A:492:ILE:HB	2.10	0.52
1:B:887:THR:N	1:B:888:PRO:CD	2.73	0.52
1:A:65:LEU:O	1:A:69:VAL:HG23	2.08	0.52
1:A:478:PHE:CE2	1:A:523:PHE:HB2	2.44	0.52
1:A:672:MET:HE1	1:A:721:PHE:CD2	2.44	0.52
1:B:578:LEU:HD21	1:B:624:LEU:HB2	1.92	0.52
1:B:783:LEU:O	1:B:787:ILE:CG2	2.45	0.52
1:B:249:ALA:O	1:B:252:THR:HG23	2.09	0.52
1:B:593:THR:HG22	1:B:594:ASP:N	2.25	0.52
1:A:101:PRO:HG2	1:A:103:TYR:HE2	1.73	0.52
1:A:162:LEU:HG	1:A:164:LEU:H	1.75	0.52
1:A:716:ARG:CB	1:A:720:ARG:NH2	2.63	0.52
1:B:712:ASN:CB	1:B:715:ILE:HD12	2.40	0.52
1:A:544:ILE:CG2	1:A:584:LEU:HD13	2.40	0.51
1:A:712:ASN:O	1:A:716:ARG:HG3	2.10	0.51
1:B:422:THR:O	1:B:426:ILE:HG13	2.09	0.51
1:B:445:THR:O	1:B:448:THR:HB	2.10	0.51
1:A:341:ASP:O	1:A:388:LYS:HE3	2.11	0.51
1:A:398:ASP:OD2	1:A:404:GLU:OE2	2.29	0.51
1:B:50:LYS:C	1:B:58:ARG:NH2	2.68	0.51
1:B:69:VAL:HG11	1:B:115:LEU:HD23	1.92	0.51
1:A:15:ASP:HB3	1:A:18:VAL:HG23	1.93	0.51
1:B:119:LEU:HB3	1:B:123:ASN:HB2	1.93	0.51
1:B:166:THR:O	1:B:170:ILE:HG13	2.11	0.51
1:A:146:PHE:O	1:A:150:VAL:HG23	2.11	0.51
1:B:570:VAL:HA	1:B:573:TYR:CD1	2.46	0.51
1:B:731:GLY:N	1:B:732:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:ARG:O	1:B:553:PRO:HD2	2.11	0.51
1:B:838:PRO:O	1:B:842:SER:CB	2.59	0.51
1:A:147:TYR:CZ	1:A:151:LEU:HD11	2.45	0.51
1:B:72:TRP:HE3	1:B:81:LEU:HD23	1.76	0.51
1:B:176:VAL:O	1:B:180:ILE:HG13	2.11	0.51
1:A:825:SER:HA	1:A:828:PHE:HD1	1.73	0.50
1:B:147:TYR:CE2	1:B:151:LEU:HD11	2.47	0.50
1:B:514:MET:CE	1:B:543:GLY:HA2	2.41	0.50
1:A:689:VAL:CG1	1:A:691:TRP:H	2.25	0.50
1:A:188:ILE:O	1:A:192:VAL:HG23	2.10	0.50
1:A:514:MET:CE	1:A:543:GLY:HA2	2.40	0.50
1:A:615:LEU:HD13	1:A:676:ASN:HD21	1.76	0.50
1:B:462:LEU:O	1:B:516:ILE:HD11	2.11	0.50
1:A:55:PRO:O	1:A:56:SER:C	2.55	0.50
1:A:268:ASN:O	1:A:272:ILE:HG13	2.11	0.50
1:A:413:ARG:NH2	1:A:459:GLU:OE1	2.43	0.50
1:A:886:LEU:C	1:A:888:PRO:HD2	2.37	0.50
1:A:531:ILE:O	1:A:535:ILE:HD12	2.12	0.50
1:B:350:VAL:HG12	1:B:350:VAL:O	2.11	0.50
1:B:857:LYS:HA	1:B:860:ILE:HD11	1.92	0.50
1:A:230:GLU:N	1:A:231:PRO:CD	2.74	0.50
1:A:334:TYR:CD1	1:A:334:TYR:N	2.79	0.50
1:A:689:VAL:HG11	1:A:691:TRP:CD2	2.44	0.50
1:B:233:MET:HE1	1:B:256:ILE:CD1	2.42	0.50
1:B:546:ASN:OD1	1:B:551:VAL:HG11	2.12	0.50
1:B:663:ASN:HA	1:B:666:SER:HB3	1.93	0.50
1:A:441:SER:O	1:A:442:SER:C	2.54	0.50
1:A:4:GLN:O	1:A:8:ASN:ND2	2.45	0.50
1:B:116:PHE:CD1	1:B:120:TYR:HB2	2.47	0.50
1:A:382:LEU:O	1:A:383:GLU:C	2.54	0.50
1:A:475:PRO:HB3	1:A:526:TYR:OH	2.11	0.50
1:B:733:ASP:O	1:B:734:MET:HE2	2.10	0.50
1:A:626:SER:HB3	1:A:681:PHE:CD2	2.46	0.49
1:B:277:LEU:CD1	1:B:302:GLN:HE22	2.25	0.49
1:B:300:ASN:HD22	1:B:350:VAL:CA	2.14	0.49
1:A:462:LEU:O	1:A:516:ILE:HD11	2.12	0.49
1:A:539:VAL:HG11	1:A:580:MET:HG3	1.93	0.49
1:A:827:LEU:O	1:A:832:ASN:CB	2.60	0.49
1:A:89:TRP:CE3	1:A:89:TRP:HA	2.48	0.49
1:A:456:GLN:H	1:A:456:GLN:NE2	2.10	0.49
1:B:249:ALA:O	1:B:253:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:ARG:HD2	1:B:728:ASN:ND2	2.26	0.49
1:B:212:LEU:HD22	1:B:252:THR:HG21	1.93	0.49
1:B:626:SER:OG	1:B:682:PRO:HD3	2.12	0.49
1:A:205:TYR:CD2	1:A:245:LEU:HD11	2.47	0.49
1:A:539:VAL:O	1:A:539:VAL:CG1	2.54	0.49
1:B:544:ILE:CG2	1:B:584:LEU:HD13	2.43	0.49
1:A:733:ASP:O	1:A:736:PRO:CD	2.58	0.49
1:B:210:LEU:O	1:B:214:VAL:HG23	2.13	0.49
1:B:389:MET:CE	1:B:413:ARG:HG2	2.37	0.49
1:B:837:ASP:HB2	1:B:838:PRO:HD3	1.93	0.49
1:A:611:PHE:CE1	1:A:669:CYS:HB2	2.48	0.49
1:B:341:ASP:O	1:B:388:LYS:HE3	2.12	0.49
1:B:585:LEU:HD22	1:B:618:PHE:CD2	2.47	0.49
1:B:237:TYR:OH	1:B:277:LEU:HD23	2.13	0.48
1:B:886:LEU:C	1:B:888:PRO:CD	2.86	0.48
1:A:511:LEU:O	1:A:512:LEU:C	2.56	0.48
1:A:777:ASN:ND2	1:A:826:ILE:CB	2.75	0.48
1:B:89:TRP:HH2	1:B:134:VAL:HG21	1.77	0.48
1:B:397:TRP:CH2	1:B:508:LEU:HD13	2.48	0.48
1:B:626:SER:HB2	1:B:682:PRO:HD3	1.95	0.48
1:A:448:THR:HG22	1:A:448:THR:O	2.13	0.48
1:A:506:HIS:CD2	1:A:508:LEU:HB2	2.49	0.48
1:A:599:VAL:HG13	1:A:600:PRO:HD2	1.94	0.48
1:B:318:PRO:HA	1:B:321:LYS:CB	2.34	0.48
1:A:135:ILE:HG12	1:A:143:PHE:HD2	1.79	0.48
1:A:642:LEU:HD23	1:A:677:PHE:CD2	2.48	0.48
1:B:100:GLU:HB3	1:B:101:PRO:CD	2.42	0.48
1:B:343:TYR:O	1:B:344:ASP:C	2.56	0.48
1:A:40:TRP:CB	1:A:68:LYS:HG3	2.43	0.48
1:A:253:MET:HE2	1:A:273:LEU:HD21	1.95	0.48
1:B:631:THR:CG2	1:B:632:PRO:HD2	2.44	0.48
1:B:725:ARG:HA	1:B:728:ASN:ND2	2.28	0.48
1:A:24:GLN:C	1:A:27:THR:HG22	2.38	0.48
1:A:229:ASN:ND2	1:A:231:PRO:HG2	2.28	0.48
1:A:541:PRO:HA	1:A:545:HIS:HB2	1.96	0.48
1:A:761:ILE:O	1:A:765:ILE:N	2.44	0.48
1:B:649:LYS:CE	1:B:666:SER:OG	2.62	0.48
1:A:592:VAL:O	1:A:593:THR:OG1	2.31	0.48
1:B:152:LEU:CD1	1:B:214:VAL:HG22	2.29	0.48
1:A:27:THR:CG2	1:A:28:ASP:N	2.76	0.48
1:A:777:ASN:O	1:A:781:PRO:CD	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:CD	1:B:243:GLU:O	2.57	0.48
1:A:887:THR:N	1:A:888:PRO:CD	2.77	0.47
1:B:145:ASN:ND2	1:B:210:LEU:HD12	2.29	0.47
1:B:413:ARG:HH22	1:B:459:GLU:CD	2.21	0.47
1:B:689:VAL:HG12	1:B:690:ALA:N	2.28	0.47
1:A:152:LEU:HD12	1:A:217:GLN:OE1	2.14	0.47
1:B:116:PHE:CE1	1:B:120:TYR:HB2	2.49	0.47
1:B:825:SER:HA	1:B:828:PHE:HD1	1.78	0.47
1:A:348:THR:HA	1:A:351:PHE:CD1	2.49	0.47
1:B:663:ASN:O	1:B:664:ILE:C	2.56	0.47
1:B:693:ALA:O	1:B:696:ASN:HB2	2.13	0.47
1:A:116:PHE:CE1	1:A:120:TYR:CG	3.03	0.47
1:B:44:HIS:ND1	1:B:83:MET:HE3	2.30	0.47
1:A:40:TRP:HB2	1:A:68:LYS:HG3	1.97	0.47
1:A:500:GLN:CD	1:A:500:GLN:H	2.23	0.47
1:A:10:VAL:CG2	1:A:60:ILE:HD12	2.44	0.47
1:B:631:THR:HG23	1:B:632:PRO:HD2	1.95	0.47
1:A:413:ARG:HH22	1:A:459:GLU:CD	2.22	0.47
1:A:755:VAL:HG13	1:A:810:SER:HB2	1.97	0.47
1:B:432:SER:O	1:B:433:SER:C	2.56	0.47
1:B:435:MET:O	1:B:439:ILE:HG13	2.15	0.47
1:B:836:PHE:O	1:B:840:ILE:CG2	2.58	0.47
1:B:856:GLN:O	1:B:860:ILE:HG23	2.15	0.47
1:B:332:PHE:N	1:B:333:PRO:CD	2.78	0.47
1:B:375:LYS:HE2	1:B:379:LYS:HZ3	1.76	0.47
1:B:441:SER:O	1:B:442:SER:C	2.58	0.47
1:B:681:PHE:CD2	1:B:682:PRO:HD2	2.50	0.47
1:B:169:GLN:O	1:B:173:ASP:CG	2.58	0.47
1:A:199:TYR:CE1	1:A:207:THR:HG21	2.49	0.47
1:A:462:LEU:HD11	1:A:501:VAL:CG1	2.45	0.47
1:A:718:ALA:O	1:A:722:THR:OG1	2.32	0.47
1:B:411:GLU:CG	1:B:412:MET:H	2.28	0.47
1:B:626:SER:HB2	1:B:682:PRO:HD2	1.97	0.47
1:A:89:TRP:HH2	1:A:134:VAL:HG21	1.79	0.46
1:A:104:ILE:O	1:A:104:ILE:CG2	2.62	0.46
1:A:776:THR:O	1:A:780:LEU:HG	2.15	0.46
1:B:295:VAL:O	1:B:298:LEU:HB3	2.15	0.46
1:A:332:PHE:N	1:A:333:PRO:CD	2.78	0.46
1:A:464:GLU:OE1	1:A:464:GLU:HA	2.16	0.46
1:B:736:PRO:HA	1:B:775:ILE:HD11	1.96	0.46
1:A:529:ALA:O	1:A:532:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TRP:HA	1:B:89:TRP:CE3	2.50	0.46
1:B:169:GLN:O	1:B:173:ASP:HB2	2.14	0.46
1:B:681:PHE:CB	1:B:682:PRO:CD	2.93	0.46
1:B:838:PRO:O	1:B:842:SER:HB3	2.15	0.46
1:A:120:TYR:CD2	1:A:121:PRO:N	2.83	0.46
1:A:544:ILE:HG22	1:A:584:LEU:HD13	1.96	0.46
1:B:762:SER:C	1:B:817:GLN:HE22	2.23	0.46
1:A:24:GLN:HG3	1:A:28:ASP:OD2	2.15	0.46
1:A:116:PHE:CE1	1:A:120:TYR:CD1	3.04	0.46
1:A:350:VAL:HG12	1:A:350:VAL:O	2.15	0.46
1:B:277:LEU:HD11	1:B:302:GLN:HE22	1.80	0.46
1:B:544:ILE:HG22	1:B:584:LEU:HD13	1.98	0.46
1:B:857:LYS:HA	1:B:860:ILE:CD1	2.46	0.46
1:A:166:THR:O	1:A:170:ILE:HG13	2.16	0.46
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.71	0.46
1:A:392:ASP:HB2	1:A:395:GLN:CB	2.46	0.46
1:A:581:LEU:O	1:A:585:LEU:HG	2.15	0.46
1:B:15:ASP:O	1:B:23:LYS:NZ	2.36	0.46
1:B:89:TRP:HA	1:B:89:TRP:HE3	1.81	0.46
1:B:560:TYR:HB2	1:B:620:THR:OG1	2.15	0.46
1:B:642:LEU:HD23	1:B:677:PHE:CD2	2.51	0.46
1:B:778:ARG:O	1:B:781:PRO:HD2	2.15	0.46
1:A:89:TRP:HA	1:A:89:TRP:HE3	1.79	0.46
1:A:468:PHE:O	1:A:468:PHE:CD2	2.68	0.46
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.76	0.46
1:A:611:PHE:CZ	1:A:615:LEU:HD21	2.51	0.46
1:A:672:MET:HE1	1:A:718:ALA:HA	1.97	0.46
1:B:224:ILE:HD13	1:B:261:MET:CB	2.45	0.46
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.76	0.46
1:A:672:MET:CA	1:A:672:MET:CE	2.90	0.46
1:A:858:SER:O	1:A:862:LEU:HG	2.16	0.46
1:B:762:SER:HA	1:B:817:GLN:OE1	2.16	0.46
1:A:636:ALA:O	1:A:640:ASP:OD2	2.33	0.46
1:B:71:GLU:O	1:B:71:GLU:CG	2.63	0.46
1:B:328:LEU:HD22	1:B:332:PHE:HE1	1.81	0.46
1:B:329:TYR:CZ	1:B:373:SER:OG	2.63	0.46
1:B:540:GLY:C	1:B:542:ARG:H	2.23	0.46
1:B:837:ASP:CB	1:B:841:ASN:ND2	2.74	0.46
1:A:295:VAL:O	1:A:298:LEU:HB3	2.16	0.45
1:A:663:ASN:HA	1:A:666:SER:HB3	1.97	0.45
1:B:539:VAL:HG11	1:B:580:MET:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:LEU:HD13	1:B:676:ASN:HD21	1.81	0.45
1:A:53:TYR:N	1:A:53:TYR:CD1	2.84	0.45
1:A:271:ASN:CB	1:A:327:GLN:NE2	2.80	0.45
1:A:632:PRO:CA	1:A:635:GLN:HG2	2.30	0.45
1:B:334:TYR:HD1	1:B:334:TYR:H	1.64	0.45
1:B:715:ILE:O	1:B:715:ILE:HG22	2.15	0.45
1:B:717:GLY:O	1:B:721:PHE:HB3	2.17	0.45
1:B:837:ASP:O	1:B:838:PRO:C	2.59	0.45
1:A:280:SER:O	1:A:281:LYS:C	2.58	0.45
1:B:10:VAL:HG22	1:B:60:ILE:CD1	2.47	0.45
1:B:268:ASN:O	1:B:272:ILE:HG13	2.17	0.45
1:B:232:CYS:O	1:B:236:LEU:HG	2.16	0.45
1:A:333:PRO:O	1:A:337:ARG:HB3	2.16	0.45
1:B:195:MET:HE3	1:B:199:TYR:CE1	2.52	0.45
1:B:672:MET:HE2	1:B:672:MET:CA	2.42	0.45
1:B:762:SER:CB	1:B:817:GLN:OE1	2.64	0.45
1:B:907:LEU:C	1:B:909:VAL:H	2.24	0.45
1:A:361:LEU:HB3	1:A:426:ILE:CD1	2.47	0.45
1:A:510:GLN:NE2	1:A:542:ARG:HB3	2.31	0.45
1:A:730:VAL:C	1:A:732:PRO:HD2	2.42	0.45
1:B:196:MET:HG3	1:B:208:VAL:CG1	2.46	0.45
1:A:10:VAL:HG22	1:A:60:ILE:CD1	2.46	0.45
1:A:243:GLU:C	1:A:243:GLU:CD	2.85	0.45
1:A:548:ASN:HB3	1:A:551:VAL:HG23	1.99	0.45
1:B:683:ALA:CB	1:B:728:ASN:O	2.55	0.45
1:A:228:VAL:O	1:A:229:ASN:C	2.60	0.45
1:B:411:GLU:C	1:B:413:ARG:N	2.74	0.45
1:B:457:LEU:O	1:B:460:PHE:HB3	2.17	0.45
1:B:556:TRP:CZ2	1:B:584:LEU:HD22	2.51	0.45
1:B:593:THR:CG2	1:B:594:ASP:N	2.80	0.45
1:A:411:GLU:C	1:A:413:ARG:N	2.75	0.45
1:A:424:ASN:O	1:A:424:ASN:ND2	2.49	0.45
1:A:424:ASN:ND2	1:A:428:SER:HA	2.32	0.45
1:A:689:VAL:CG2	1:A:691:TRP:CH2	2.97	0.45
1:A:715:ILE:O	1:A:719:VAL:HG23	2.17	0.45
1:B:478:PHE:CE2	1:B:523:PHE:HB2	2.51	0.45
1:B:566:ILE:HG22	1:B:566:ILE:O	2.17	0.45
1:B:788:PHE:HZ	1:B:839:LEU:CD2	2.29	0.45
1:B:120:TYR:CD2	1:B:120:TYR:C	2.93	0.45
1:B:135:ILE:HD11	1:B:147:TYR:CB	2.47	0.45
1:B:375:LYS:HE2	1:B:379:LYS:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ILE:HG22	1:A:584:LEU:CD1	2.46	0.44
1:B:246:ARG:HD3	1:B:291:PHE:CE1	2.50	0.44
1:A:483:ASP:O	1:A:484:LYS:CB	2.65	0.44
1:B:53:TYR:N	1:B:53:TYR:CD1	2.85	0.44
1:B:439:ILE:HG23	1:B:461:ALA:HB1	1.99	0.44
1:B:464:GLU:HA	1:B:464:GLU:OE1	2.17	0.44
1:A:10:VAL:HG22	1:A:60:ILE:HD12	1.98	0.44
1:A:52:LYS:HD2	1:A:53:TYR:CE1	2.48	0.44
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.81	0.44
1:A:512:LEU:O	1:A:513:TYR:C	2.60	0.44
1:A:520:TYR:O	1:A:523:PHE:HB3	2.18	0.44
1:A:601:THR:CG2	1:A:602:LEU:N	2.78	0.44
1:A:119:LEU:C	1:A:121:PRO:HD2	2.43	0.44
1:A:166:THR:HG22	1:A:168:VAL:H	1.83	0.44
1:A:462:LEU:HD11	1:A:501:VAL:HG11	1.99	0.44
1:B:397:TRP:CD1	1:B:397:TRP:C	2.93	0.44
1:B:444:SER:O	1:B:447:ALA:HB3	2.17	0.44
1:B:907:LEU:C	1:B:909:VAL:N	2.76	0.44
1:A:313:PRO:O	1:A:314:SER:CB	2.66	0.44
1:A:500:GLN:CB	1:A:503:ARG:HH21	2.30	0.44
1:B:617:LEU:O	1:B:621:VAL:HG23	2.17	0.44
1:B:727:ILE:O	1:B:731:GLY:CA	2.65	0.44
1:A:52:LYS:HB2	1:A:53:TYR:CD1	2.53	0.44
1:A:424:ASN:HD22	1:A:428:SER:HA	1.82	0.44
1:A:689:VAL:HG21	1:A:691:TRP:CZ2	2.53	0.44
1:B:524:PHE:CE2	1:B:534:LEU:HD11	2.53	0.44
1:A:91:TYR:CZ	1:A:97:PHE:HB3	2.53	0.44
1:A:432:SER:O	1:A:433:SER:C	2.60	0.44
1:A:558:LEU:O	1:A:559:PHE:C	2.61	0.44
1:A:702:ILE:HA	1:A:705:ILE:CB	2.48	0.44
1:A:885:SER:C	1:A:888:PRO:CD	2.87	0.44
1:B:230:GLU:H	1:B:231:PRO:HD2	1.78	0.44
1:A:422:THR:O	1:A:426:ILE:HG13	2.18	0.44
1:A:552:ARG:N	1:A:553:PRO:CD	2.81	0.44
1:B:672:MET:CE	1:B:718:ALA:HA	2.48	0.44
1:A:50:LYS:HA	1:A:58:ARG:HH21	1.81	0.43
1:B:61:CYS:O	1:B:64:THR:CG2	2.64	0.43
1:B:784:LEU:HB3	1:B:788:PHE:CE1	2.48	0.43
1:A:572:ASN:N	1:A:572:ASN:HD22	2.14	0.43
1:A:689:VAL:CG1	1:A:691:TRP:N	2.82	0.43
1:A:722:THR:CG2	1:A:726:ILE:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:PHE:CE2	1:A:764:LEU:HD12	2.53	0.43
1:B:4:GLN:O	1:B:8:ASN:ND2	2.51	0.43
1:B:430:LEU:HD12	1:B:430:LEU:O	2.17	0.43
1:B:53:TYR:O	1:B:58:ARG:NH2	2.51	0.43
1:B:540:GLY:C	1:B:542:ARG:N	2.74	0.43
1:A:302:GLN:O	1:A:303:GLY:C	2.62	0.43
1:A:439:ILE:HG23	1:A:461:ALA:HB1	2.00	0.43
1:A:568:LYS:O	1:A:571:VAL:HG23	2.17	0.43
1:B:1:MET:CB	1:B:4:GLN:HB2	2.48	0.43
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.79	0.43
1:B:601:THR:HG22	1:B:602:LEU:N	2.34	0.43
1:B:856:GLN:CB	1:B:909:VAL:HG21	2.47	0.43
1:B:100:GLU:OE1	1:B:104:ILE:HD13	2.19	0.43
1:B:585:LEU:HD22	1:B:618:PHE:CE2	2.54	0.43
1:A:556:TRP:CZ2	1:A:584:LEU:HD22	2.53	0.43
1:A:556:TRP:O	1:A:557:TYR:C	2.61	0.43
1:A:885:SER:O	1:A:888:PRO:HG2	2.18	0.43
1:B:169:GLN:O	1:B:173:ASP:CB	2.66	0.43
1:B:735:LEU:O	1:B:775:ILE:CD1	2.66	0.43
1:B:788:PHE:CZ	1:B:839:LEU:HD23	2.53	0.43
1:A:727:ILE:HG12	1:A:734:MET:CB	2.49	0.43
1:B:464:GLU:O	1:B:468:PHE:HB2	2.19	0.43
1:A:291:PHE:O	1:A:294:HIS:HB2	2.18	0.43
1:B:353:PHE:O	1:B:354:LEU:C	2.60	0.43
1:A:255:GLU:OE1	1:A:255:GLU:HA	2.18	0.43
1:B:6:VAL:HA	1:B:29:PHE:HE2	1.84	0.43
1:B:196:MET:HG3	1:B:208:VAL:HG13	2.00	0.43
1:B:291:PHE:O	1:B:294:HIS:HB2	2.19	0.43
1:A:443:LEU:O	1:A:446:ALA:HB3	2.19	0.43
1:B:413:ARG:NH2	1:B:459:GLU:OE1	2.50	0.43
1:A:169:GLN:OE1	1:A:172:LYS:HE2	2.18	0.42
1:A:210:LEU:O	1:A:214:VAL:HG23	2.19	0.42
1:A:735:LEU:N	1:A:736:PRO:HD3	2.33	0.42
1:B:116:PHE:HE1	1:B:120:TYR:CD1	2.35	0.42
1:A:206:GLY:N	1:B:203:LYS:O	2.52	0.42
1:A:277:LEU:CD1	1:A:302:GLN:HE22	2.31	0.42
1:A:427:ASP:C	1:A:427:ASP:OD1	2.61	0.42
1:B:10:VAL:CG2	1:B:60:ILE:HD12	2.49	0.42
1:B:205:TYR:HD2	1:B:245:LEU:CD1	2.32	0.42
1:B:302:GLN:O	1:B:303:GLY:C	2.60	0.42
1:B:381:LEU:O	1:B:385:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLN:O	1:B:511:LEU:C	2.60	0.42
1:B:512:LEU:HD12	1:B:512:LEU:HA	1.78	0.42
1:B:675:GLY:O	1:B:678:ALA:HB3	2.19	0.42
1:A:202:ALA:O	1:A:203:LYS:C	2.61	0.42
1:A:672:MET:HE3	1:A:718:ALA:CA	2.48	0.42
1:B:116:PHE:CE1	1:B:120:TYR:CG	3.08	0.42
1:B:275:LEU:HA	1:B:275:LEU:HD12	1.72	0.42
1:B:762:SER:HA	1:B:817:GLN:CD	2.44	0.42
1:A:299:ILE:O	1:A:300:ASN:C	2.60	0.42
1:A:599:VAL:CG1	1:A:600:PRO:N	2.82	0.42
1:B:228:VAL:O	1:B:229:ASN:C	2.62	0.42
1:B:300:ASN:ND2	1:B:350:VAL:HA	2.14	0.42
1:A:585:LEU:HD22	1:A:618:PHE:CE2	2.55	0.42
1:A:689:VAL:CG2	1:A:691:TRP:CZ2	3.02	0.42
1:B:146:PHE:O	1:B:150:VAL:HG23	2.19	0.42
1:B:230:GLU:O	1:B:233:MET:N	2.53	0.42
1:B:382:LEU:O	1:B:383:GLU:C	2.60	0.42
1:B:857:LYS:O	1:B:860:ILE:HG12	2.19	0.42
1:B:859:SER:O	1:B:862:LEU:HB2	2.19	0.42
1:A:147:TYR:CE2	1:A:151:LEU:HD11	2.55	0.42
1:A:271:ASN:CB	1:A:327:GLN:HE22	2.33	0.42
1:A:302:GLN:O	1:A:305:GLU:HB2	2.20	0.42
1:A:562:PHE:CZ	1:A:566:ILE:HD12	2.54	0.42
1:B:84:ILE:O	1:B:85:ARG:C	2.62	0.42
1:B:89:TRP:CH2	1:B:134:VAL:HG21	2.53	0.42
1:B:214:VAL:O	1:B:215:TYR:C	2.63	0.42
1:B:257:VAL:HG13	1:B:270:LEU:HD21	2.01	0.42
1:B:642:LEU:HD23	1:B:677:PHE:CE2	2.55	0.42
1:A:544:ILE:CG2	1:A:584:LEU:CD1	2.97	0.42
1:A:780:LEU:O	1:A:784:LEU:CG	2.68	0.42
1:B:24:GLN:HG3	1:B:28:ASP:OD2	2.20	0.42
1:B:199:TYR:CB	1:B:208:VAL:HG22	2.50	0.42
1:B:672:MET:HE3	1:B:718:ALA:HA	2.02	0.42
1:A:144:SER:HB3	1:A:195:MET:CE	2.50	0.42
1:B:10:VAL:HG22	1:B:60:ILE:HD13	2.01	0.42
1:B:271:ASN:CB	1:B:327:GLN:NE2	2.83	0.42
1:B:746:LEU:O	1:B:747:ASN:C	2.62	0.42
1:A:144:SER:HB3	1:A:195:MET:HE1	2.02	0.42
1:A:504:HIS:CD2	1:A:505:PRO:HD2	2.55	0.42
1:A:760:PHE:CD2	1:A:760:PHE:C	2.97	0.42
1:A:837:ASP:N	1:A:838:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:CYS:HB2	1:B:537:TYR:CD1	2.55	0.42
1:A:757:VAL:O	1:A:761:ILE:HG23	2.20	0.42
1:A:835:TYR:O	1:A:838:PRO:HD2	2.20	0.42
1:B:59:LEU:O	1:B:63:GLN:HG3	2.19	0.42
1:B:364:GLU:O	1:B:366:SER:N	2.47	0.42
1:B:379:LYS:O	1:B:380:SER:C	2.63	0.42
1:B:765:ILE:CB	1:B:817:GLN:NE2	2.83	0.42
1:B:508:LEU:HD12	1:B:508:LEU:HA	1.82	0.41
1:B:511:LEU:O	1:B:512:LEU:C	2.63	0.41
1:A:101:PRO:HG2	1:A:103:TYR:CE2	2.54	0.41
1:B:344:ASP:OD1	1:B:388:LYS:NZ	2.53	0.41
1:B:557:TYR:O	1:B:560:TYR:HB3	2.20	0.41
1:B:581:LEU:HD22	1:B:617:LEU:HD21	2.03	0.41
1:A:351:PHE:N	1:A:352:PRO:CD	2.83	0.41
1:A:546:ASN:O	1:A:552:ARG:HG3	2.21	0.41
1:A:835:TYR:C	1:A:838:PRO:HD2	2.45	0.41
1:B:201:ASN:C	1:B:203:LYS:H	2.28	0.41
1:B:209:GLY:O	1:B:213:GLN:HG2	2.20	0.41
1:A:540:GLY:C	1:A:542:ARG:H	2.28	0.41
1:A:578:LEU:HD21	1:A:624:LEU:CB	2.51	0.41
1:B:148:LEU:HD13	1:B:210:LEU:HB3	2.03	0.41
1:B:224:ILE:HD13	1:B:261:MET:HB3	2.02	0.41
1:B:500:GLN:CB	1:B:503:ARG:HH21	2.34	0.41
1:B:755:VAL:HG13	1:B:810:SER:CB	2.50	0.41
1:A:180:ILE:HG22	1:A:185:MET:HE2	2.01	0.41
1:B:271:ASN:O	1:B:275:LEU:HB2	2.20	0.41
1:B:504:HIS:CD2	1:B:505:PRO:HD2	2.54	0.41
1:A:322:GLU:O	1:A:323:ASN:C	2.62	0.41
1:B:381:LEU:HD12	1:B:381:LEU:HA	1.90	0.41
1:B:62:LEU:HA	1:B:62:LEU:HD23	1.78	0.41
1:A:12:ALA:O	1:A:23:LYS:HE3	2.21	0.41
1:A:689:VAL:HG12	1:A:692:LEU:N	2.32	0.41
1:B:120:TYR:CE1	1:B:128:PHE:CE1	3.08	0.41
1:B:120:TYR:CE1	1:B:128:PHE:HE1	2.38	0.41
1:B:132:GLN:HE22	1:B:188:ILE:HA	1.85	0.41
1:B:262:LYS:O	1:B:265:GLU:N	2.51	0.41
1:B:322:GLU:O	1:B:323:ASN:C	2.62	0.41
1:B:762:SER:O	1:B:817:GLN:NE2	2.50	0.41
1:A:24:GLN:HA	1:A:27:THR:HG22	2.03	0.41
1:A:103:TYR:CD2	1:A:103:TYR:N	2.88	0.41
1:A:353:PHE:O	1:A:354:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:TYR:CA	1:A:512:LEU:HD21	2.51	0.41
1:A:581:LEU:HD12	1:A:621:VAL:HG22	2.03	0.41
1:A:668:TYR:O	1:A:672:MET:HG2	2.21	0.41
1:A:672:MET:HE3	1:A:718:ALA:HA	2.03	0.41
1:B:7:GLU:O	1:B:11:GLU:HB2	2.21	0.41
1:B:12:ALA:O	1:B:23:LYS:HE3	2.21	0.41
1:B:119:LEU:HD22	1:B:123:ASN:ND2	2.36	0.41
1:B:135:ILE:HD13	1:B:144:SER:HA	2.02	0.41
1:B:205:TYR:CD2	1:B:242:ILE:HG21	2.53	0.41
1:B:357:LEU:O	1:B:361:LEU:HD13	2.21	0.41
1:B:863:VAL:O	1:B:867:VAL:HG23	2.21	0.41
1:A:514:MET:HE1	1:A:543:GLY:CA	2.51	0.41
1:B:103:TYR:O	1:B:107:ALA:HB2	2.21	0.41
1:B:287:THR:O	1:B:288:ASP:HB2	2.21	0.41
1:B:909:VAL:O	1:B:909:VAL:HG12	2.21	0.41
1:A:300:ASN:HD22	1:A:350:VAL:CA	2.15	0.40
1:A:470:GLU:HG2	1:A:470:GLU:O	2.21	0.40
1:B:69:VAL:CG1	1:B:115:LEU:HD23	2.51	0.40
1:B:120:TYR:N	1:B:121:PRO:CD	2.83	0.40
1:B:269:LEU:HA	1:B:272:ILE:HD12	2.03	0.40
1:B:531:ILE:CD1	1:B:569:GLN:OE1	2.69	0.40
1:B:553:PRO:HD2	1:B:554:ARG:H	1.86	0.40
1:B:586:ASN:O	1:B:614:GLN:NE2	2.48	0.40
1:B:681:PHE:HD2	1:B:682:PRO:HD2	1.86	0.40
1:A:72:TRP:HB3	1:A:77:ASN:HB2	2.03	0.40
1:A:530:ALA:O	1:A:531:ILE:C	2.64	0.40
1:A:560:TYR:CZ	1:A:564:LYS:HD2	2.56	0.40
1:A:615:LEU:HD13	1:A:676:ASN:ND2	2.36	0.40
1:A:884:LEU:O	1:A:888:PRO:CD	2.69	0.40
1:A:927:ILE:O	1:A:930:SER:N	2.54	0.40
1:B:19:GLY:O	1:B:23:LYS:HB2	2.22	0.40
1:A:100:GLU:OE2	1:A:104:ILE:HD13	2.21	0.40
1:A:244:GLU:CB	1:B:203:LYS:NZ	2.73	0.40
1:A:397:TRP:CH2	1:A:508:LEU:HD13	2.57	0.40
1:A:617:LEU:O	1:A:621:VAL:HG23	2.21	0.40
1:A:856:GLN:CG	1:A:909:VAL:CG2	2.99	0.40
1:B:424:ASN:ND2	1:B:424:ASN:O	2.54	0.40
1:B:487:THR:O	1:B:491:GLN:HG3	2.22	0.40
1:B:529:ALA:O	1:B:532:PRO:HD2	2.21	0.40
1:A:21:ILE:O	1:A:24:GLN:HB3	2.20	0.40
1:A:510:GLN:O	1:A:514:MET:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLY:C	1:A:542:ARG:N	2.79	0.40
1:A:927:ILE:O	1:A:928:TYR:C	2.64	0.40
1:B:578:LEU:HD21	1:B:624:LEU:CB	2.52	0.40
1:B:760:PHE:O	1:B:764:LEU:HB2	2.21	0.40
1:A:89:TRP:CH2	1:A:134:VAL:HG21	2.55	0.40
1:A:116:PHE:CD2	1:A:116:PHE:C	3.00	0.40
1:A:341:ASP:O	1:A:388:LYS:CE	2.70	0.40
1:A:514:MET:HE2	1:A:538:PHE:CD2	2.57	0.40
1:A:758:LEU:CD1	1:A:810:SER:OG	2.53	0.40
1:A:893:MET:N	1:A:894:PRO:HD2	2.36	0.40
1:B:233:MET:HE1	1:B:256:ILE:HD13	2.02	0.40

All (1) 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:B:596:ASP:O	1:B:607:ARG:NH2[2_655]	2.17	0.03

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	893/980 (91%)	813 (91%)	76 (8%)	4 (0%)	30 61
1	B	878/980 (90%)	800 (91%)	71 (8%)	7 (1%)	16 47
All	All	1771/1960 (90%)	1613 (91%)	147 (8%)	11 (1%)	21 52

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	598	PRO
1	A	289	PRO

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Mol	Chain	Res	Type
1	A	592	VAL
1	B	289	PRO
1	B	730	VAL
1	B	263	PRO
1	B	597	ALA
1	B	908	VAL
1	A	46	ILE
1	A	352	PRO
1	B	475	PRO

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	592/880 (67%)	553 (93%)	39 (7%)	15	43
1	B	569/880 (65%)	539 (95%)	30 (5%)	20	51
All	All	1161/1760 (66%)	1092 (94%)	69 (6%)	18	48

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	47	PHE
1	A	56	SER
1	A	64	THR
1	A	89	TRP
1	A	94	GLU
1	A	103	TYR
1	A	152	LEU
1	A	171	GLN
1	A	215	TYR
1	A	229	ASN
1	A	252	THR
1	A	259	LYS
1	A	266	LYS

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	348	THR
1	A	392	ASP
1	A	396	GLU
1	A	397	TRP
1	A	441	SER
1	A	456	GLN
1	A	502	CYS
1	A	511	LEU
1	A	528	SER
1	A	542	ARG
1	A	551	VAL
1	A	561	ARG
1	A	570	VAL
1	A	583	ASP
1	A	603	ASN
1	A	617	LEU
1	A	687	GLU
1	A	711	PHE
1	A	715	ILE
1	A	723	SER
1	A	764	LEU
1	A	766	HIS
1	A	776	THR
1	A	835	TYR
1	B	47	PHE
1	B	56	SER
1	B	64	THR
1	B	89	TRP
1	B	200	SER
1	B	208	VAL
1	B	215	TYR
1	B	229	ASN
1	B	246	ARG
1	B	252	THR
1	B	266	LYS
1	B	283	GLN
1	B	328	LEU
1	B	337	ARG
1	B	373	SER
1	B	374	LEU
1	B	392	ASP

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Mol	Chain	Res	Type
1	B	397	TRP
1	B	408	GLU
1	B	441	SER
1	B	456	GLN
1	B	465	THR
1	B	511	LEU
1	B	542	ARG
1	B	583	ASP
1	B	617	LEU
1	B	711	PHE
1	B	734	MET
1	B	764	LEU
1	B	766	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	63	GLN
1	A	74	ASN
1	A	77	ASN
1	A	82	GLN
1	A	106	ASN
1	A	109	GLN
1	A	118	GLN
1	A	183	ASN
1	A	204	ASN
1	A	223	ASN
1	A	229	ASN
1	A	258	ASN
1	A	271	ASN
1	A	300	ASN
1	A	302	GLN
1	A	327	GLN
1	A	330	ASN
1	A	420	GLN
1	A	424	ASN
1	A	456	GLN
1	A	504	HIS
1	A	506	HIS
1	A	545	HIS
1	A	546	ASN

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Mol	Chain	Res	Type
1	A	572	ASN
1	A	603	ASN
1	A	676	ASN
1	A	777	ASN
1	A	841	ASN
1	B	4	GLN
1	B	8	ASN
1	B	74	ASN
1	B	77	ASN
1	B	82	GLN
1	B	106	ASN
1	B	109	GLN
1	B	123	ASN
1	B	145	ASN
1	B	183	ASN
1	B	223	ASN
1	B	229	ASN
1	B	271	ASN
1	B	283	GLN
1	B	300	ASN
1	B	302	GLN
1	B	327	GLN
1	B	330	ASN
1	B	420	GLN
1	B	424	ASN
1	B	456	GLN
1	B	491	GLN
1	B	504	HIS
1	B	506	HIS
1	B	545	HIS
1	B	546	ASN
1	B	603	ASN
1	B	676	ASN
1	B	696	ASN
1	B	728	ASN
1	B	777	ASN
1	B	841	ASN

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	917/980 (93%)	0.24	37 (4%)	42	23	47, 117, 195, 201	0
1	B	902/980 (92%)	0.45	73 (8%)	18	10	56, 120, 195, 201	0
All	All	1819/1960 (92%)	0.34	110 (6%)	27	15	47, 118, 195, 201	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	776	THR	5.2
1	B	434	TYR	4.5
1	B	396	GLU	4.5
1	A	669	CYS	4.2
1	B	947	ALA	4.2
1	B	43	CYS	4.1
1	A	950	TYR	4.0
1	A	662	GLU	4.0
1	B	589	VAL	4.0
1	A	723	SER	4.0
1	A	698	ALA	3.7
1	B	772	MET	3.7
1	B	698	ALA	3.4
1	B	669	CYS	3.4
1	B	476	ASP	3.4
1	B	730	VAL	3.3
1	B	324	CYS	3.3
1	B	680	GLY	3.3
1	B	480	ASN	3.3
1	B	883	THR	3.3
1	B	886	LEU	3.2
1	B	26	ALA	3.1
1	B	779	MET	3.1
1	B	228	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	731	GLY	3.0
1	A	734	MET	3.0
1	B	119	LEU	2.9
1	B	635	GLN	2.9
1	A	780	LEU	2.9
1	A	731	GLY	2.9
1	A	907	LEU	2.9
1	B	787	ILE	2.9
1	B	406	GLU	2.9
1	B	832	ASN	2.9
1	B	783	LEU	2.8
1	A	730	VAL	2.8
1	A	613	SER	2.8
1	B	122	SER	2.8
1	A	2	SER	2.8
1	B	38	THR	2.8
1	B	714	ASP	2.7
1	B	205	TYR	2.7
1	B	260	LYS	2.7
1	B	633	GLU	2.7
1	B	915	GLY	2.7
1	A	736	PRO	2.7
1	B	691	TRP	2.7
1	A	345	GLU	2.7
1	B	403	SER	2.7
1	A	666	SER	2.7
1	B	123	ASN	2.7
1	B	475	PRO	2.6
1	A	281	LYS	2.6
1	A	887	THR	2.6
1	B	138	SER	2.6
1	A	724	GLY	2.6
1	A	685	GLY	2.5
1	A	533	ALA	2.5
1	B	397	TRP	2.5
1	A	768	TYR	2.5
1	A	890	CYS	2.5
1	B	773	MET	2.5
1	B	483	ASP	2.5
1	A	811	TYR	2.5
1	A	699	SER	2.4
1	B	639	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	735	LEU	2.4
1	B	117	LEU	2.4
1	A	589	VAL	2.4
1	B	392	ASP	2.4
1	B	594	ASP	2.4
1	A	472	LEU	2.4
1	B	699	SER	2.4
1	B	887	THR	2.3
1	B	748	SER	2.3
1	B	121	PRO	2.3
1	A	691	TRP	2.3
1	B	60	ILE	2.3
1	B	471	GLY	2.2
1	B	315	GLU	2.2
1	B	596	ASP	2.2
1	B	806	ASP	2.2
1	B	474	GLY	2.2
1	B	282	SER	2.2
1	A	727	ILE	2.2
1	B	405	GLU	2.2
1	A	883	THR	2.2
1	A	566	ILE	2.2
1	A	742	ILE	2.2
1	A	645	ALA	2.2
1	A	47	PHE	2.2
1	B	659	SER	2.2
1	B	3	ALA	2.2
1	B	588	SER	2.1
1	B	566	ILE	2.1
1	B	342	ASP	2.1
1	A	658	LEU	2.1
1	B	628	GLY	2.1
1	B	709	MET	2.1
1	B	314	SER	2.1
1	B	881	ASN	2.1
1	B	549	GLU	2.1
1	A	529	ALA	2.0
1	B	732	PRO	2.0
1	A	482	VAL	2.0
1	B	948	SER	2.0
1	B	793	ALA	2.0
1	B	854	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	695	PHE	2.0
1	B	662	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	2001	1/1	0.97	0.05	53,53,53,53	0
2	CA	A	2002	1/1	0.97	0.12	52,52,52,52	0
2	CA	B	2001	1/1	0.97	0.04	53,53,53,53	0
2	CA	B	2002	1/1	0.98	0.15	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.