



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:50 AM UTC

PDB ID : 2IUB / pdb_00002iub
Title : Crystal structure of a divalent metal ion transporter CorA at 2.9 Å resolution.
Authors : Eshaghi, S.; Niegowski, D.; Kohl, A.; Martinez Molina, D.; Lesley, S.A.; Nordlund, P.
Deposited on : 2006-06-01
Resolution : 2.90 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

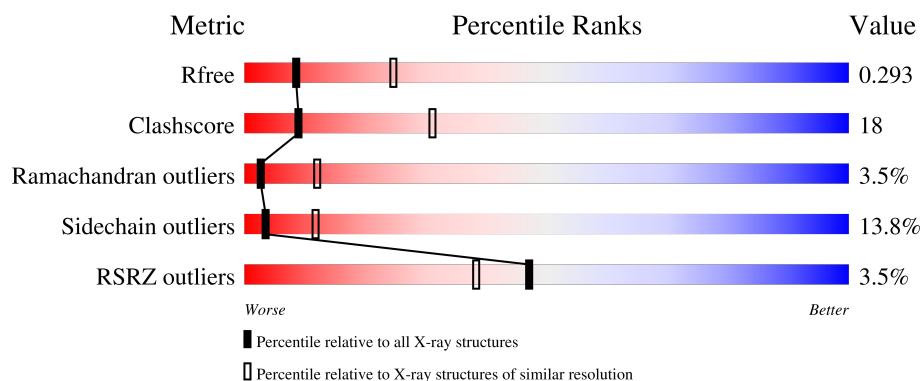
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	363	3% 52% 33% 9%
1	B	363	5% 51% 32% 7% 9%
1	C	363	2% 53% 31% 6% 9%
1	D	363	4% 55% 30% 5% 9%
1	E	363	2% 55% 28% 6% 9%

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Mol	Chain	Length	Quality of chain
1	F	363	
1	G	363	
1	H	363	
1	I	363	
1	J	363	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27580 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 DIVALENT CATION TRANSPORT-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2736	1780	447	501	8			
1	B	331	Total	C	N	O	S	0	0	0
			2728	1775	444	501	8			
1	C	331	Total	C	N	O	S	0	0	0
			2726	1773	444	501	8			
1	D	331	Total	C	N	O	S	0	0	0
			2730	1777	444	501	8			
1	E	331	Total	C	N	O	S	0	0	0
			2730	1777	444	501	8			
1	F	342	Total	C	N	O	S	0	0	0
			2793	1814	458	512	9			
1	G	342	Total	C	N	O	S	0	0	0
			2790	1812	458	512	8			
1	H	338	Total	C	N	O	S	0	0	0
			2767	1799	451	508	9			
1	I	340	Total	C	N	O	S	0	0	0
			2776	1804	453	510	9			
1	J	336	Total	C	N	O	S	0	0	0
			2763	1796	452	506	9			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	D	2	Total	Cl	0	0
			2	2		
2	F	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Cl	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	D	5	Total	Mg	0	0
			5	5		
3	E	1	Total	Mg	0	0
			1	1		
3	F	3	Total	Mg	0	0
			3	3		
3	G	3	Total	Mg	0	0
			3	3		
3	H	1	Total	Mg	0	0
			1	1		
3	J	3	Total	Mg	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		

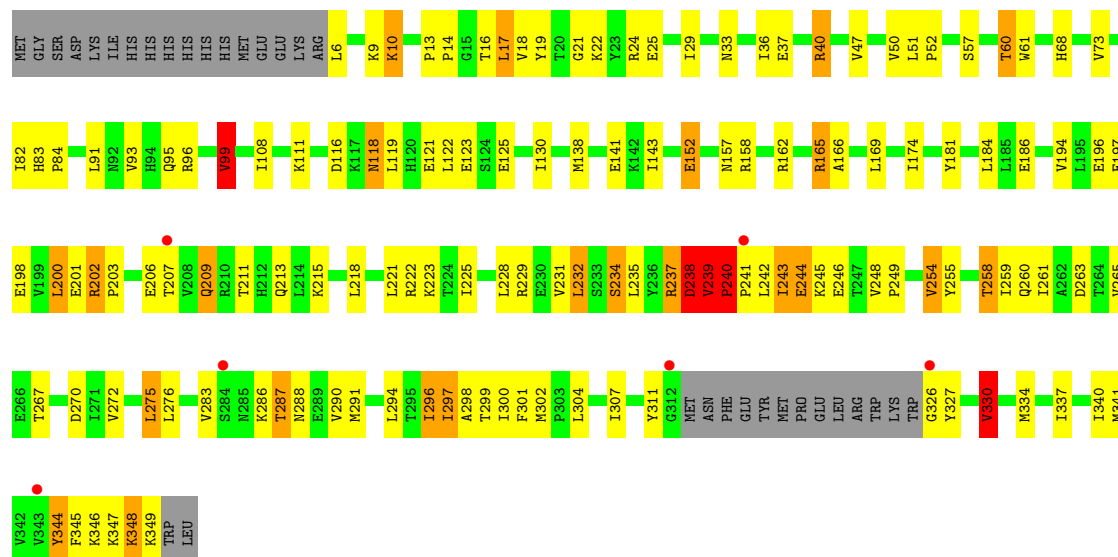
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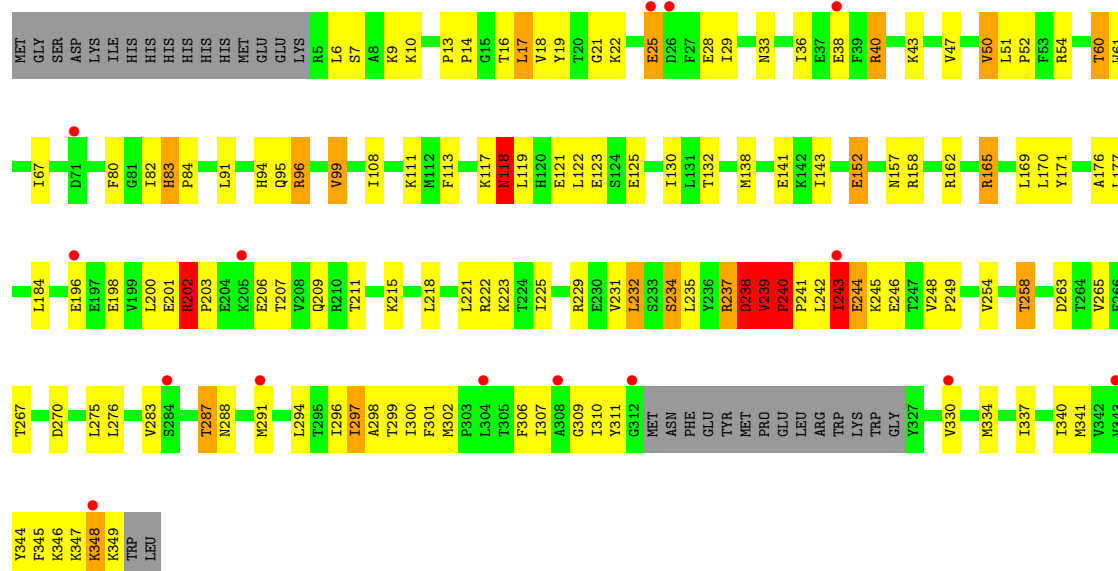
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	2	Total	O	0	0
			2	2		



• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

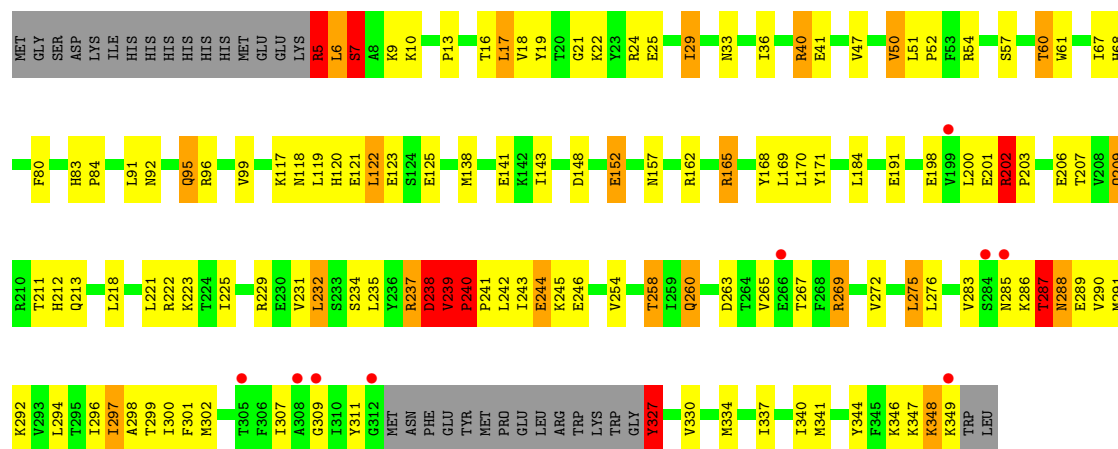


• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

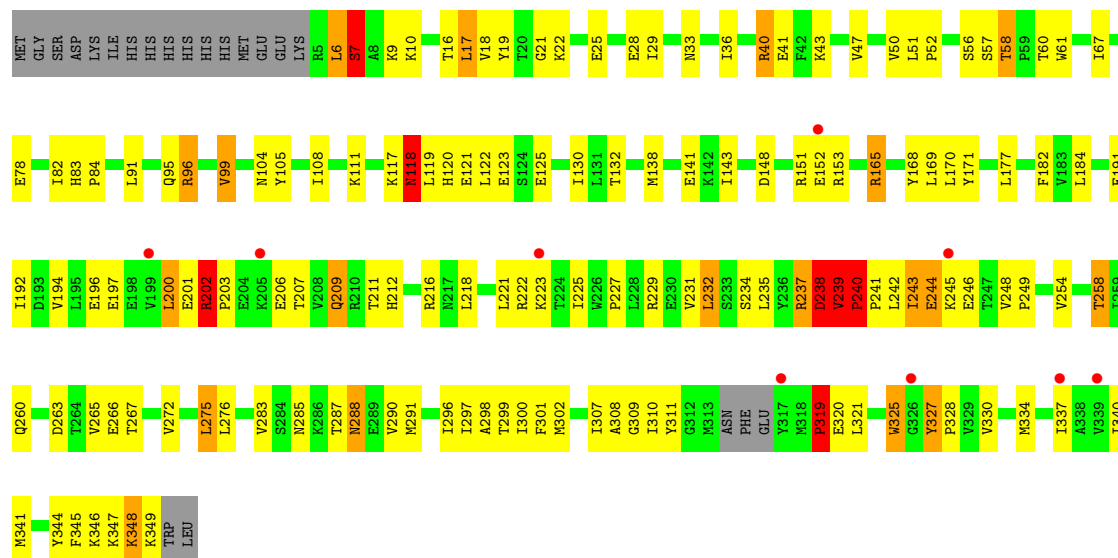


• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

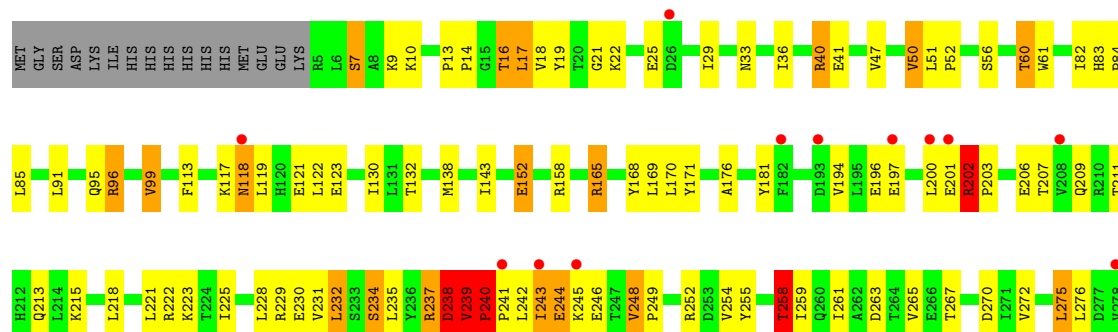


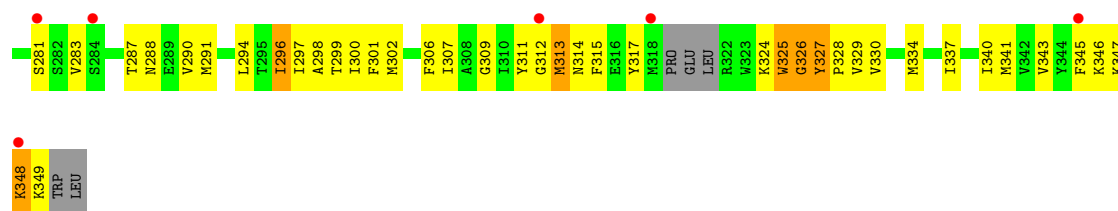


• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN



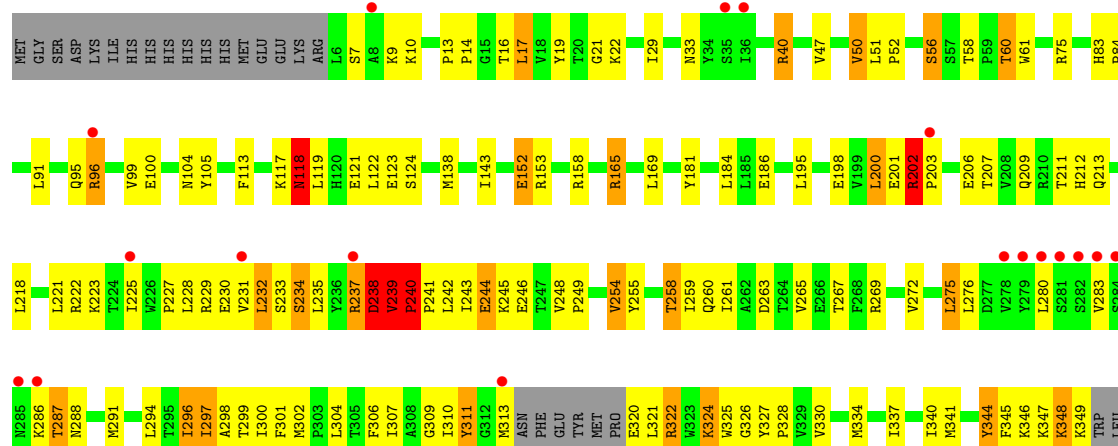
• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN





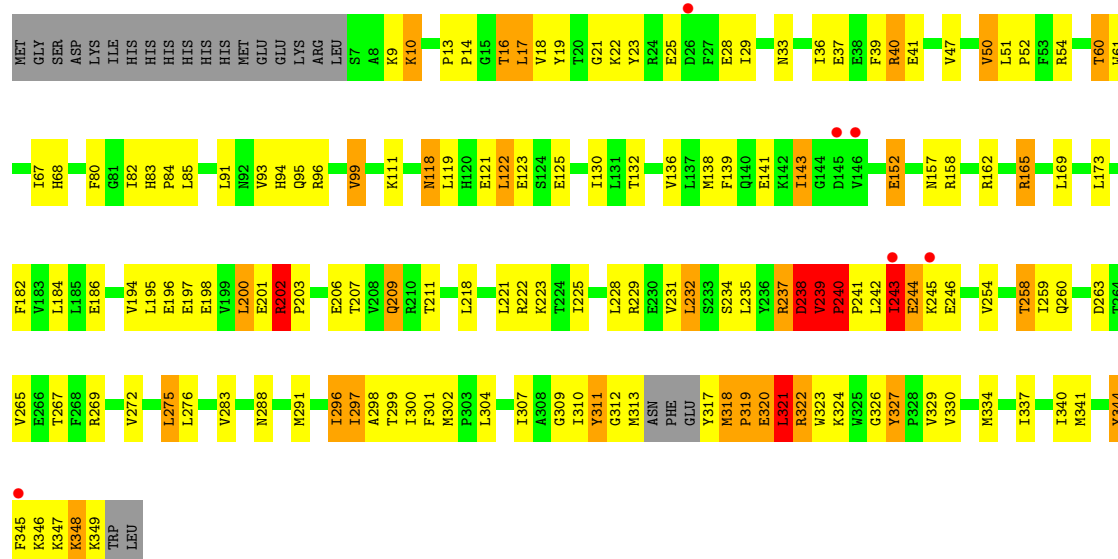
• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

Chain H: 5% 55% 31% 7% 7%



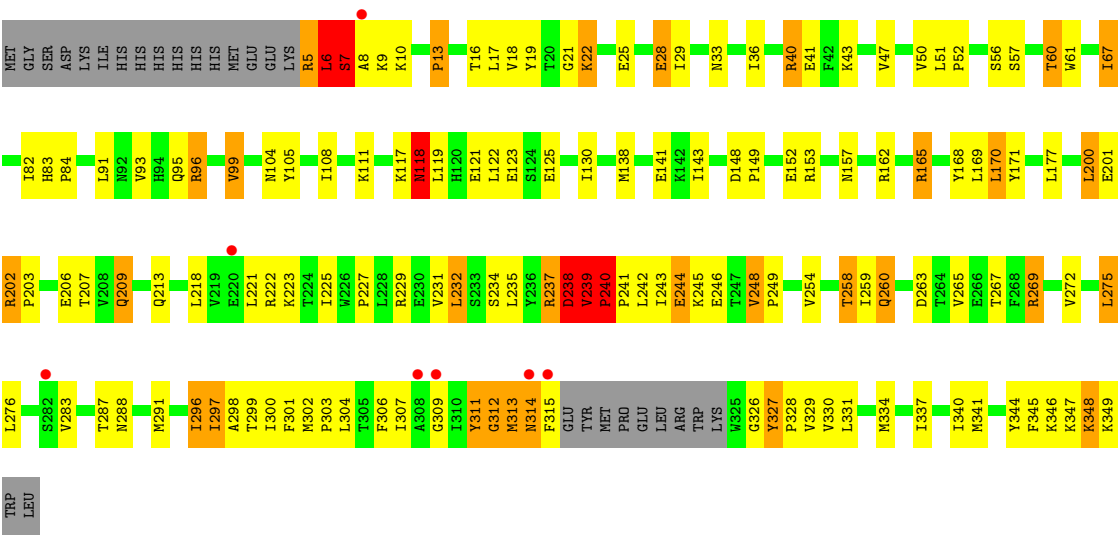
• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

Chain I: 2% 53% 31% 8% 6%



• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

Chain J: 2% 53% 30% 8% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.23Å 151.46Å 143.32Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.90) 90.2 (30.00-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.260 , 0.291 0.261 , 0.293	Depositor DCC
R_{free} test set	4921 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27580	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	4/2792 (0.1%)	1.08	7/3783 (0.2%)
1	B	1.04	6/2784 (0.2%)	1.07	5/3773 (0.1%)
1	C	1.02	5/2782 (0.2%)	1.10	6/3770 (0.2%)
1	D	1.07	4/2786 (0.1%)	1.10	5/3776 (0.1%)
1	E	1.04	2/2786 (0.1%)	1.11	14/3776 (0.4%)
1	F	1.02	2/2849 (0.1%)	1.12	10/3861 (0.3%)
1	G	1.08	4/2846 (0.1%)	1.12	11/3858 (0.3%)
1	H	1.11	8/2823 (0.3%)	1.16	11/3826 (0.3%)
1	I	1.02	3/2833 (0.1%)	1.15	15/3841 (0.4%)
1	J	1.05	6/2819 (0.2%)	1.16	19/3819 (0.5%)
All	All	1.05	44/28100 (0.2%)	1.12	103/38083 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	F	0	3
1	G	0	1
1	I	0	3
All	All	0	9

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	287	THR	N-CA	8.98	1.56	1.46
1	D	240	PRO	CA-C	8.69	1.60	1.52
1	E	13	PRO	CA-C	8.08	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	13	PRO	CA-C	7.45	1.55	1.51
1	J	240	PRO	CA-C	7.36	1.59	1.52
1	I	240	PRO	CA-C	7.08	1.58	1.52
1	J	239	VAL	CA-CB	7.04	1.63	1.54
1	G	240	PRO	CA-C	7.00	1.58	1.52
1	B	240	PRO	CA-C	6.99	1.58	1.52
1	B	239	VAL	CA-CB	6.88	1.63	1.54
1	H	240	PRO	CA-C	6.84	1.58	1.52
1	G	243	ILE	CA-CB	6.80	1.63	1.54
1	B	243	ILE	CA-CB	6.68	1.63	1.54
1	D	243	ILE	CA-CB	6.47	1.63	1.54
1	D	176	ALA	CA-CB	-6.45	1.43	1.53
1	B	92	ASN	CA-C	-6.43	1.45	1.52
1	J	13	PRO	CA-C	6.38	1.55	1.51
1	H	287	THR	CA-CB	6.27	1.63	1.53
1	D	13	PRO	C-O	-6.27	1.19	1.24
1	H	286	LYS	C-N	6.23	1.41	1.33
1	J	248	VAL	CA-CB	6.21	1.57	1.54
1	F	243	ILE	CA-CB	6.09	1.62	1.54
1	G	176	ALA	CA-CB	-6.07	1.43	1.53
1	B	226	TRP	CA-C	5.88	1.59	1.52
1	H	239	VAL	CA-CB	5.76	1.61	1.54
1	I	239	VAL	CA-CB	5.70	1.61	1.54
1	C	240	PRO	CA-C	5.60	1.57	1.52
1	F	240	PRO	CA-C	5.57	1.57	1.52
1	C	243	ILE	CA-CB	5.48	1.61	1.54
1	J	313	MET	N-CA	5.44	1.53	1.46
1	C	239	VAL	CA-CB	5.43	1.61	1.54
1	E	240	PRO	CA-C	5.42	1.57	1.52
1	I	243	ILE	CA-CB	5.38	1.61	1.54
1	C	174	ILE	CA-CB	-5.36	1.47	1.54
1	J	7	SER	N-CA	5.36	1.52	1.46
1	G	248	VAL	CA-CB	-5.31	1.51	1.54
1	H	286	LYS	CA-C	5.30	1.59	1.52
1	H	16	THR	CA-CB	5.25	1.60	1.53
1	A	174	ILE	CA-CB	-5.22	1.48	1.54
1	B	98	LYS	C-O	-5.21	1.18	1.23
1	A	240	PRO	CA-C	5.14	1.56	1.52
1	A	94	HIS	CA-C	-5.07	1.46	1.52
1	C	296	ILE	CA-CB	5.03	1.60	1.54
1	A	239	VAL	CA-CB	5.00	1.60	1.54

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	318	MET	CA-C-N	9.79	132.08	119.84
1	I	318	MET	C-N-CA	9.79	132.08	119.84
1	J	239	VAL	CA-C-N	8.21	128.84	120.38
1	J	239	VAL	C-N-CA	8.21	128.84	120.38
1	E	269	ARG	NE-CZ-NH2	-8.20	111.82	119.20
1	D	239	VAL	CA-C-N	7.91	128.52	120.38
1	D	239	VAL	C-N-CA	7.91	128.52	120.38
1	J	269	ARG	NE-CZ-NH2	-7.85	112.13	119.20
1	A	239	VAL	CA-C-N	7.81	128.42	120.38
1	A	239	VAL	C-N-CA	7.81	128.42	120.38
1	H	239	VAL	CA-C-N	7.71	128.32	120.38
1	H	239	VAL	C-N-CA	7.71	128.32	120.38
1	J	170	LEU	N-CA-C	-7.33	102.98	110.97
1	J	269	ARG	CD-NE-CZ	7.31	134.63	124.40
1	F	239	VAL	CA-C-N	7.29	127.89	120.38
1	F	239	VAL	C-N-CA	7.29	127.89	120.38
1	E	5	ARG	CA-C-N	7.28	134.80	121.70
1	E	5	ARG	C-N-CA	7.28	134.80	121.70
1	I	322	ARG	N-CA-C	-7.27	101.16	111.56
1	F	319	PRO	N-CA-CB	7.25	110.86	103.25
1	C	239	VAL	CA-C-N	7.23	127.83	120.38
1	C	239	VAL	C-N-CA	7.23	127.83	120.38
1	J	269	ARG	NE-CZ-NH1	7.12	128.62	121.50
1	G	239	VAL	CA-C-N	7.10	127.69	120.38
1	G	239	VAL	C-N-CA	7.10	127.69	120.38
1	C	330	VAL	N-CA-CB	7.08	119.63	110.57
1	H	311	TYR	N-CA-C	7.02	119.85	108.41
1	E	239	VAL	CA-C-N	6.87	127.46	120.38
1	E	239	VAL	C-N-CA	6.87	127.46	120.38
1	H	286	LYS	CA-C-N	6.86	129.96	120.63
1	H	286	LYS	C-N-CA	6.86	129.96	120.63
1	I	346	LYS	N-CA-C	-6.68	103.52	112.94
1	E	269	ARG	CD-NE-CZ	6.67	133.74	124.40
1	G	325	TRP	N-CA-C	-6.66	96.62	110.80
1	J	313	MET	CA-C-N	6.60	133.59	121.70
1	J	313	MET	C-N-CA	6.60	133.59	121.70
1	G	113	PHE	N-CA-C	6.55	120.21	110.52
1	H	325	TRP	CA-C-N	6.50	133.39	121.70
1	H	325	TRP	C-N-CA	6.50	133.39	121.70
1	J	5	ARG	CA-C-N	6.49	133.39	121.70
1	J	5	ARG	C-N-CA	6.49	133.39	121.70
1	J	313	MET	N-CA-C	6.46	124.56	110.80
1	G	324	LYS	N-CA-C	6.45	124.54	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	I	239	VAL	CA-C-N	6.38	126.95	120.38
1	I	239	VAL	C-N-CA	6.38	126.95	120.38
1	I	99	VAL	CB-CA-C	-6.33	100.75	110.50
1	I	312	GLY	N-CA-C	-6.27	98.32	113.18
1	B	57	SER	N-CA-C	-6.17	105.79	113.38
1	F	346	LYS	N-CA-C	-6.00	104.49	112.94
1	H	346	LYS	N-CA-C	-5.98	104.51	112.94
1	I	16	THR	N-CA-C	5.86	118.21	109.25
1	E	346	LYS	N-CA-C	-5.85	104.69	112.94
1	F	99	VAL	CB-CA-C	-5.76	100.74	110.71
1	F	57	SER	N-CA-C	-5.72	105.97	113.17
1	B	93	VAL	N-CA-C	5.69	117.64	112.29
1	G	16	THR	N-CA-C	5.68	117.95	109.25
1	I	318	MET	N-CA-C	-5.67	98.32	108.47
1	A	57	SER	N-CA-C	-5.63	106.41	113.28
1	D	113	PHE	N-CA-C	5.63	118.85	110.52
1	E	122	LEU	N-CA-C	5.63	117.57	108.34
1	G	324	LYS	CA-C-N	5.62	132.28	121.54
1	G	324	LYS	C-N-CA	5.62	132.28	121.54
1	D	346	LYS	N-CA-C	-5.62	105.02	112.94
1	J	93	VAL	N-CA-C	5.61	117.50	112.17
1	B	239	VAL	CA-C-N	5.56	126.11	120.38
1	B	239	VAL	C-N-CA	5.56	126.11	120.38
1	I	321	LEU	CA-C-N	5.55	130.52	122.36
1	I	321	LEU	C-N-CA	5.55	130.52	122.36
1	A	99	VAL	CB-CA-C	-5.52	102.28	110.33
1	J	57	SER	N-CA-C	-5.48	106.27	113.17
1	H	324	LYS	N-CA-C	5.45	122.42	110.80
1	G	346	LYS	N-CA-C	-5.44	105.34	112.41
1	J	346	LYS	N-CA-C	-5.44	105.27	112.94
1	B	83	HIS	N-CA-C	5.43	116.25	109.57
1	E	57	SER	N-CA-C	-5.43	106.43	113.16
1	J	312	GLY	N-CA-C	5.41	126.00	113.18
1	I	122	LEU	N-CA-C	5.37	117.14	108.34
1	G	258	THR	N-CA-C	-5.37	105.34	111.14
1	I	68	HIS	N-CA-C	-5.30	105.92	112.38
1	A	346	LYS	N-CA-C	-5.30	105.47	112.94
1	F	58	THR	CA-C-N	5.27	125.56	119.93
1	F	58	THR	C-N-CA	5.27	125.56	119.93
1	J	311	TYR	N-CA-C	5.26	117.99	107.62
1	J	6	LEU	CA-CB-CG	5.26	134.70	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	99	VAL	CB-CA-C	-5.25	102.42	110.50
1	J	67	ILE	N-CA-C	-5.21	106.81	112.80
1	H	286	LYS	CA-C-O	-5.19	114.24	120.10
1	A	327	TYR	CA-C-N	-5.17	114.72	120.45
1	A	327	TYR	C-N-CA	-5.17	114.72	120.45
1	E	29	ILE	N-CA-C	-5.15	100.95	108.99
1	C	346	LYS	N-CA-C	-5.14	106.25	112.88
1	D	83	HIS	N-CA-C	5.14	115.89	109.57
1	C	57	SER	N-CA-C	-5.10	107.11	113.38
1	E	7	SER	N-CA-C	5.09	121.64	110.80
1	I	269	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	C	99	VAL	CB-CA-C	-5.06	102.28	110.28
1	E	327	TYR	CA-C-N	-5.06	114.83	120.45
1	E	327	TYR	C-N-CA	-5.06	114.83	120.45
1	F	325	TRP	CA-C-N	5.03	130.75	121.70
1	F	325	TRP	C-N-CA	5.03	130.75	121.70
1	H	287	THR	N-CA-CB	5.03	117.27	109.98
1	G	99	VAL	CB-CA-C	-5.01	102.78	110.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	326	GLY	Peptide
1	E	5	ARG	Peptide
1	F	319	PRO	Peptide
1	F	325	TRP	Peptide
1	F	7	SER	Peptide
1	G	326	GLY	Peptide
1	I	311	TYR	Peptide
1	I	317	TYR	Peptide
1	I	321	LEU	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	2736	0	2797	111	0
1	B	2728	0	2779	122	0
1	C	2726	0	2778	115	2
1	D	2730	0	2786	101	1
1	E	2730	0	2786	111	2
1	F	2793	0	2826	121	2
1	G	2790	0	2820	114	0
1	H	2767	0	2808	117	2
1	I	2776	0	2808	132	1
1	J	2763	0	2815	123	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	F	1	0	0	1	0
2	G	2	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	5	0	0	0	0
3	E	1	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
3	J	3	0	0	0	0
4	A	2	0	0	3	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
All	All	27580	0	28003	1025	5

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 18.

All (1025) 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:F:311:TYR:CD2	1:I:313:MET:HE2	1.72	1.24
1:I:320:GLU:CB	1:I:321:LEU:HA	1.72	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:OE1	1:B:6:LEU:HG	1.45	1.16
1:E:165:ARG:HH12	1:E:243:ILE:HD13	1.01	1.16
1:H:165:ARG:HH12	1:H:243:ILE:HD13	0.99	1.13
1:A:165:ARG:HH12	1:A:243:ILE:HD13	0.98	1.11
1:J:165:ARG:HH12	1:J:243:ILE:HD13	0.98	1.10
1:G:165:ARG:NH1	1:G:243:ILE:HD13	1.68	1.08
1:I:165:ARG:HH12	1:I:243:ILE:HD13	0.91	1.07
1:D:165:ARG:HH12	1:D:243:ILE:HD13	0.95	1.07
1:E:240:PRO:HB2	1:E:241:PRO:CD	1.86	1.06
1:C:165:ARG:NH1	1:C:243:ILE:HD13	1.69	1.06
1:F:311:TYR:HD2	1:I:313:MET:HE2	0.91	1.06
1:B:165:ARG:NH1	1:B:243:ILE:HD13	1.70	1.06
1:F:165:ARG:HH12	1:F:243:ILE:HD13	0.91	1.06
1:I:165:ARG:NH1	1:I:243:ILE:HD13	1.72	1.04
1:F:165:ARG:NH1	1:F:243:ILE:HD13	1.72	1.03
1:C:165:ARG:HH12	1:C:243:ILE:HD13	0.87	1.03
1:I:307:ILE:HD11	1:I:334:MET:HG2	1.39	1.02
1:A:240:PRO:HB2	1:A:241:PRO:CD	1.89	1.01
1:G:165:ARG:HH12	1:G:243:ILE:HD13	0.88	1.01
1:H:321:LEU:HA	1:H:322:ARG:CB	1.89	1.01
1:A:302:MET:HE2	1:B:298:ALA:HA	1.42	1.01
1:B:165:ARG:HH12	1:B:243:ILE:HD13	0.88	1.00
1:B:240:PRO:HB2	1:B:241:PRO:CD	1.91	1.00
1:J:240:PRO:HB2	1:J:241:PRO:CD	1.90	1.00
1:H:240:PRO:HB2	1:H:241:PRO:CD	1.92	0.99
1:F:240:PRO:HB2	1:F:241:PRO:CD	1.93	0.99
1:D:165:ARG:NH1	1:D:243:ILE:HD13	1.77	0.98
1:C:240:PRO:HB2	1:C:241:PRO:CD	1.93	0.98
1:F:300:ILE:HG22	1:F:341:MET:HG3	1.46	0.97
1:D:240:PRO:HB2	1:D:241:PRO:CD	1.95	0.97
1:G:313:MET:CB	1:H:311:TYR:HB3	1.96	0.96
1:E:237:ARG:NH2	1:E:237:ARG:HB2	1.79	0.95
1:G:240:PRO:HB2	1:G:241:PRO:CD	1.96	0.95
1:A:165:ARG:NH1	1:A:243:ILE:HD13	1.81	0.95
1:J:165:ARG:NH1	1:J:243:ILE:HD13	1.82	0.95
1:H:165:ARG:NH1	1:H:243:ILE:HD13	1.82	0.95
1:E:244:GLU:O	1:E:246:GLU:N	2.00	0.94
1:I:240:PRO:HB2	1:I:241:PRO:CD	1.97	0.94
1:A:298:ALA:HA	1:D:302:MET:HE2	1.48	0.94
1:G:165:ARG:HH12	1:G:243:ILE:CD1	1.79	0.94
1:G:299:THR:HG21	1:G:345:PHE:CZ	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:GLU:O	1:I:246:GLU:N	2.00	0.94
1:G:244:GLU:O	1:G:246:GLU:N	2.00	0.94
1:A:237:ARG:NH2	1:A:237:ARG:HB2	1.83	0.93
1:J:83:HIS:ND1	1:J:84:PRO:HD2	1.83	0.93
1:H:237:ARG:NH2	1:H:237:ARG:HB2	1.84	0.92
1:H:244:GLU:O	1:H:246:GLU:N	2.01	0.92
1:E:165:ARG:NH1	1:E:243:ILE:HD13	1.83	0.92
1:J:244:GLU:O	1:J:246:GLU:N	2.02	0.92
1:F:244:GLU:O	1:F:246:GLU:N	2.01	0.92
1:B:237:ARG:HB2	1:B:237:ARG:NH2	1.83	0.92
1:E:240:PRO:HB2	1:E:241:PRO:HD2	1.50	0.92
1:C:307:ILE:HD11	1:C:334:MET:HG2	1.52	0.92
1:F:237:ARG:NH2	1:F:237:ARG:HB2	1.84	0.91
1:J:237:ARG:NH2	1:J:237:ARG:HB2	1.84	0.91
1:C:165:ARG:HH12	1:C:243:ILE:CD1	1.80	0.91
1:I:165:ARG:HH12	1:I:243:ILE:CD1	1.83	0.90
1:B:307:ILE:HD11	1:B:334:MET:HG2	1.52	0.90
1:J:240:PRO:HB2	1:J:241:PRO:HD2	1.50	0.90
1:A:240:PRO:HB2	1:A:241:PRO:HD2	1.54	0.90
1:B:165:ARG:HH12	1:B:243:ILE:CD1	1.81	0.89
1:A:307:ILE:HD11	1:A:334:MET:HG2	1.52	0.89
1:E:19:TYR:CZ	1:E:21:GLY:HA3	2.08	0.89
1:B:83:HIS:ND1	1:B:84:PRO:HD2	1.89	0.88
1:D:237:ARG:HB2	1:D:237:ARG:NH2	1.89	0.88
1:I:237:ARG:HB2	1:I:237:ARG:NH2	1.89	0.87
1:A:244:GLU:O	1:A:246:GLU:N	2.07	0.87
1:I:298:ALA:HA	1:J:302:MET:HE2	1.53	0.87
1:C:244:GLU:O	1:C:246:GLU:N	2.07	0.87
1:F:99:VAL:HG22	1:F:231:VAL:HG13	1.57	0.87
1:C:237:ARG:NH2	1:C:237:ARG:HB2	1.89	0.86
1:D:99:VAL:HG22	1:D:231:VAL:HG13	1.55	0.86
1:G:240:PRO:HB2	1:G:241:PRO:HD2	1.55	0.86
1:G:299:THR:HG21	1:G:345:PHE:HZ	1.39	0.86
1:B:244:GLU:O	1:B:246:GLU:N	2.09	0.86
1:D:240:PRO:HB2	1:D:241:PRO:HD2	1.56	0.86
1:G:237:ARG:HB2	1:G:237:ARG:NH2	1.89	0.86
1:D:244:GLU:O	1:D:246:GLU:N	2.09	0.85
1:H:302:MET:HE2	1:J:298:ALA:HA	1.58	0.85
1:G:302:MET:HE2	1:H:298:ALA:HA	1.57	0.85
1:F:240:PRO:HB2	1:F:241:PRO:HD2	1.57	0.85
1:D:165:ARG:HH12	1:D:243:ILE:CD1	1.87	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:307:ILE:HD11	1:H:334:MET:HG2	1.59	0.85
1:G:19:TYR:CZ	1:G:21:GLY:HA3	2.12	0.84
1:F:165:ARG:HH12	1:F:243:ILE:CD1	1.84	0.84
1:A:83:HIS:ND1	1:A:84:PRO:HD2	1.93	0.83
1:J:6:LEU:HD23	1:J:8:ALA:H	1.41	0.83
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.61	0.83
1:A:348:LYS:HE2	1:A:349:LYS:H	1.43	0.83
1:D:348:LYS:HE2	1:D:349:LYS:H	1.39	0.83
1:A:299:THR:HG21	1:A:345:PHE:CZ	2.13	0.83
1:F:19:TYR:CZ	1:F:21:GLY:HA3	2.14	0.82
1:C:19:TYR:CZ	1:C:21:GLY:HA3	2.14	0.82
1:C:348:LYS:HE2	1:C:349:LYS:H	1.44	0.82
1:I:240:PRO:HB2	1:I:241:PRO:HD2	1.62	0.82
1:C:263:ASP:HB3	1:E:223:LYS:HD2	1.60	0.82
1:H:83:HIS:ND1	1:H:84:PRO:HD2	1.93	0.82
1:G:307:ILE:HD11	1:G:334:MET:HG2	1.61	0.82
1:B:240:PRO:HB2	1:B:241:PRO:HD2	1.62	0.81
1:E:83:HIS:ND1	1:E:84:PRO:HD2	1.95	0.81
1:C:83:HIS:ND1	1:C:84:PRO:HD2	1.94	0.81
1:B:99:VAL:CG2	1:B:231:VAL:HG13	2.11	0.81
1:C:240:PRO:HB2	1:C:241:PRO:HD2	1.61	0.81
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.62	0.81
1:I:19:TYR:CZ	1:I:21:GLY:HA3	2.16	0.80
1:E:237:ARG:HB2	1:E:237:ARG:HH21	1.47	0.80
1:I:99:VAL:HG22	1:I:231:VAL:HG13	1.64	0.80
1:F:348:LYS:HE2	1:F:349:LYS:H	1.45	0.80
1:H:313:MET:C	1:J:311:TYR:HB3	2.06	0.80
1:B:99:VAL:HG22	1:B:231:VAL:HG13	1.63	0.80
1:H:240:PRO:HB2	1:H:241:PRO:HD2	1.63	0.80
1:H:313:MET:HB3	1:J:311:TYR:HD2	1.47	0.80
1:A:223:LYS:HD2	1:D:263:ASP:HB3	1.64	0.80
1:H:320:GLU:O	1:H:322:ARG:CB	2.30	0.80
1:G:348:LYS:HE2	1:G:349:LYS:H	1.46	0.79
1:D:201:GLU:C	1:D:203:PRO:HD3	2.08	0.79
1:H:99:VAL:HG22	1:H:231:VAL:HG13	1.64	0.79
1:B:311:TYR:HE2	1:B:330:VAL:HG21	1.47	0.79
1:I:29:ILE:HG21	1:I:50:VAL:HG11	1.63	0.79
1:F:308:ALA:HA	1:I:313:MET:HE1	1.63	0.78
1:H:348:LYS:HE2	1:H:349:LYS:H	1.47	0.78
1:I:337:ILE:HA	1:I:340:ILE:HG12	1.66	0.78
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:GLU:C	1:H:203:PRO:HD3	2.09	0.78
1:E:237:ARG:HH21	1:E:237:ARG:CB	1.97	0.77
1:I:348:LYS:HE2	1:I:349:LYS:H	1.48	0.77
1:D:299:THR:HG21	1:D:345:PHE:HZ	1.47	0.77
1:E:201:GLU:C	1:E:203:PRO:HD3	2.09	0.77
1:C:99:VAL:HG22	1:C:231:VAL:HG13	1.67	0.77
1:J:29:ILE:HG21	1:J:50:VAL:HG11	1.67	0.77
1:A:237:ARG:HB2	1:A:237:ARG:HH21	1.46	0.77
1:D:83:HIS:ND1	1:D:84:PRO:HD2	1.99	0.77
1:J:99:VAL:HG22	1:J:231:VAL:HG13	1.67	0.77
1:E:348:LYS:HE2	1:E:349:LYS:H	1.49	0.77
1:G:201:GLU:C	1:G:203:PRO:HD3	2.10	0.77
1:A:201:GLU:C	1:A:203:PRO:HD3	2.10	0.76
1:A:299:THR:HG21	1:A:345:PHE:HZ	1.50	0.76
1:E:300:ILE:HG22	1:E:341:MET:HG3	1.66	0.76
1:G:168:TYR:OH	1:H:14:PRO:HG2	1.85	0.76
1:D:9:LYS:HG3	1:D:9:LYS:O	1.85	0.76
1:J:237:ARG:HB2	1:J:237:ARG:HH21	1.49	0.76
1:F:201:GLU:C	1:F:203:PRO:HD3	2.11	0.76
1:B:348:LYS:HE2	1:B:349:LYS:H	1.51	0.76
1:E:307:ILE:HD11	1:E:334:MET:HG2	1.68	0.76
1:J:337:ILE:HA	1:J:340:ILE:HG12	1.67	0.76
1:B:201:GLU:C	1:B:203:PRO:HD3	2.11	0.76
1:C:302:MET:HE2	1:E:298:ALA:HA	1.68	0.76
1:I:83:HIS:ND1	1:I:84:PRO:HD2	2.00	0.75
1:A:263:ASP:HB3	1:B:223:LYS:HD2	1.67	0.75
1:H:99:VAL:CG2	1:H:231:VAL:HG13	2.16	0.75
1:H:237:ARG:HB2	1:H:237:ARG:HH21	1.52	0.75
1:J:61:TRP:HB2	1:J:169:LEU:HD21	1.68	0.75
1:J:5:ARG:HD3	1:J:22:LYS:HB2	1.68	0.75
1:A:99:VAL:HG22	1:A:231:VAL:HG13	1.68	0.74
1:F:237:ARG:CB	1:F:237:ARG:HH21	2.00	0.74
1:A:253:ASP:OD1	4:A:2002:HOH:O	2.05	0.74
1:A:337:ILE:HA	1:A:340:ILE:HG12	1.69	0.74
1:A:29:ILE:HG21	1:A:50:VAL:HG11	1.70	0.74
1:D:298:ALA:HA	1:E:302:MET:HE2	1.69	0.74
1:I:201:GLU:C	1:I:203:PRO:HD3	2.13	0.74
1:E:9:LYS:O	1:E:9:LYS:HG3	1.87	0.74
1:J:348:LYS:HE2	1:J:349:LYS:H	1.53	0.74
1:F:61:TRP:HB2	1:F:169:LEU:HD21	1.69	0.74
1:J:201:GLU:C	1:J:203:PRO:HD3	2.13	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ILE:HA	1:C:340:ILE:HG12	1.70	0.73
1:D:307:ILE:HD11	1:D:334:MET:HG2	1.68	0.73
1:J:234:SER:O	1:J:238:ASP:HB2	1.88	0.73
1:H:263:ASP:HB3	1:J:223:LYS:HD2	1.69	0.73
1:E:99:VAL:HG22	1:E:231:VAL:HG13	1.70	0.73
1:H:313:MET:HB3	1:J:311:TYR:CD2	2.24	0.73
1:F:337:ILE:HA	1:F:340:ILE:HG12	1.70	0.73
1:B:40:ARG:HH11	1:B:40:ARG:HB2	1.53	0.72
1:H:237:ARG:HH21	1:H:237:ARG:CB	2.02	0.72
1:B:237:ARG:HB2	1:B:237:ARG:HH21	1.51	0.72
1:C:201:GLU:C	1:C:203:PRO:HD3	2.14	0.72
1:F:29:ILE:HG21	1:F:50:VAL:HG11	1.72	0.72
1:B:237:ARG:HH21	1:B:237:ARG:CB	2.03	0.72
1:B:299:THR:HG21	1:B:345:PHE:CZ	2.25	0.72
1:B:302:MET:HE2	1:C:298:ALA:HA	1.72	0.72
1:J:19:TYR:CZ	1:J:21:GLY:HA3	2.24	0.72
1:D:14:PRO:HG3	1:E:171:TYR:OH	1.90	0.71
1:E:6:LEU:O	1:E:7:SER:HB3	1.88	0.71
1:J:299:THR:HG21	1:J:345:PHE:CZ	2.24	0.71
4:A:2002:HOH:O	1:B:89:ASP:OD1	2.09	0.71
1:A:234:SER:O	1:A:238:ASP:HB2	1.89	0.71
1:G:9:LYS:O	1:G:9:LYS:HG3	1.89	0.71
1:H:337:ILE:HA	1:H:340:ILE:HG12	1.72	0.71
1:B:337:ILE:HA	1:B:340:ILE:HG12	1.72	0.71
1:E:29:ILE:HG21	1:E:50:VAL:HG11	1.71	0.71
1:G:83:HIS:ND1	1:G:84:PRO:HD2	2.05	0.71
1:G:337:ILE:HA	1:G:340:ILE:HG12	1.73	0.71
1:A:237:ARG:HH21	1:A:237:ARG:CB	2.04	0.71
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.73	0.71
1:F:6:LEU:HB3	1:I:186:GLU:OE1	1.90	0.71
1:F:307:ILE:HD11	1:F:334:MET:HG2	1.73	0.71
1:I:299:THR:HG21	1:I:345:PHE:CZ	2.26	0.70
1:D:237:ARG:HB2	1:D:237:ARG:HH21	1.56	0.70
1:D:237:ARG:HH21	1:D:237:ARG:CB	2.05	0.70
1:E:165:ARG:HH12	1:E:243:ILE:CD1	1.93	0.70
1:B:29:ILE:HG21	1:B:50:VAL:HG11	1.72	0.70
1:D:19:TYR:CZ	1:D:21:GLY:HA3	2.27	0.70
1:D:29:ILE:HG21	1:D:50:VAL:HG11	1.73	0.70
1:F:320:GLU:N	1:F:321:LEU:O	2.25	0.70
1:G:234:SER:O	1:G:238:ASP:HB2	1.91	0.70
1:C:29:ILE:HG21	1:C:50:VAL:HG11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:ASP:HB3	1:H:223:LYS:HD2	1.72	0.70
1:H:29:ILE:HG21	1:H:50:VAL:HG11	1.72	0.70
1:E:337:ILE:HA	1:E:340:ILE:HG12	1.72	0.70
1:H:310:ILE:HG22	1:J:334:MET:HE1	1.73	0.70
1:H:19:TYR:CZ	1:H:21:GLY:HA3	2.27	0.69
1:J:6:LEU:CD2	1:J:8:ALA:H	2.04	0.69
1:D:234:SER:O	1:D:238:ASP:HB2	1.92	0.69
1:D:337:ILE:HA	1:D:340:ILE:HG12	1.73	0.69
1:B:300:ILE:HG22	1:B:341:MET:HG3	1.75	0.69
1:F:234:SER:O	1:F:238:ASP:HB2	1.93	0.69
1:A:19:TYR:CZ	1:A:21:GLY:HA3	2.28	0.69
1:F:237:ARG:HB2	1:F:237:ARG:HH21	1.50	0.69
1:H:299:THR:HG21	1:H:345:PHE:CZ	2.27	0.69
1:I:237:ARG:CB	1:I:237:ARG:HH21	2.05	0.69
1:C:300:ILE:HG22	1:C:341:MET:HG3	1.75	0.69
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.74	0.69
1:H:240:PRO:HB2	1:H:241:PRO:HD3	1.73	0.69
1:A:186:GLU:OE1	1:B:6:LEU:CG	2.35	0.68
1:D:99:VAL:CG2	1:D:231:VAL:HG13	2.23	0.68
1:G:61:TRP:HB2	1:G:169:LEU:HD21	1.75	0.68
1:J:237:ARG:HH21	1:J:237:ARG:CB	2.05	0.68
1:C:93:VAL:O	1:C:111:LYS:NZ	2.26	0.68
1:E:5:ARG:CB	1:E:6:LEU:HB2	2.24	0.68
1:B:61:TRP:HB2	1:B:169:LEU:HD21	1.74	0.68
1:H:299:THR:HG21	1:H:345:PHE:CE1	2.28	0.68
1:F:40:ARG:HH11	1:F:40:ARG:HB2	1.59	0.68
1:H:200:LEU:HD22	1:J:209:GLN:HG3	1.76	0.68
1:I:61:TRP:HB2	1:I:169:LEU:HD21	1.76	0.68
1:B:200:LEU:HD22	1:C:209:GLN:HG3	1.76	0.68
1:C:40:ARG:HH11	1:C:40:ARG:HB2	1.59	0.68
1:F:302:MET:HE2	1:G:298:ALA:HA	1.76	0.68
1:B:234:SER:O	1:B:238:ASP:HB2	1.94	0.67
1:G:99:VAL:HG22	1:G:231:VAL:HG13	1.76	0.67
1:I:321:LEU:CB	1:I:322:ARG:CB	2.73	0.67
1:C:61:TRP:HB2	1:C:169:LEU:HD21	1.75	0.67
1:I:40:ARG:HH11	1:I:40:ARG:HB2	1.59	0.67
1:I:225:ILE:HD13	1:I:265:VAL:HG21	1.74	0.67
1:J:307:ILE:HD11	1:J:334:MET:HG2	1.75	0.67
1:F:6:LEU:HD13	1:F:7:SER:H	1.58	0.67
1:G:29:ILE:HG21	1:G:50:VAL:HG11	1.77	0.67
1:E:286:LYS:O	1:E:287:THR:C	2.38	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:PRO:CB	1:B:241:PRO:CD	2.73	0.66
1:F:83:HIS:ND1	1:F:84:PRO:HD2	2.10	0.66
1:F:308:ALA:HA	1:I:313:MET:CE	2.25	0.66
1:H:321:LEU:CA	1:H:322:ARG:CB	2.68	0.66
1:A:304:LEU:HB3	1:D:306:PHE:CE2	2.31	0.66
1:E:234:SER:O	1:E:238:ASP:HB2	1.95	0.66
1:F:99:VAL:CG2	1:F:231:VAL:HG13	2.24	0.66
1:A:165:ARG:HH12	1:A:243:ILE:CD1	1.92	0.66
1:I:304:LEU:HB3	1:J:306:PHE:CE2	2.31	0.66
1:C:237:ARG:CB	1:C:237:ARG:HH21	2.07	0.66
1:I:237:ARG:HB2	1:I:237:ARG:HH21	1.59	0.66
1:C:291:MET:HE2	1:E:291:MET:HG2	1.76	0.66
1:B:232:LEU:HD22	1:B:254:VAL:HB	1.77	0.66
1:F:311:TYR:CD2	1:I:313:MET:CE	2.66	0.65
1:G:237:ARG:HB2	1:G:237:ARG:HH21	1.61	0.65
1:H:234:SER:O	1:H:238:ASP:HB2	1.96	0.65
1:J:9:LYS:O	1:J:9:LYS:HG3	1.95	0.65
1:A:269:ARG:NH1	1:D:270:ASP:OD1	2.30	0.65
1:F:298:ALA:HA	1:I:302:MET:HE2	1.79	0.65
1:I:320:GLU:CB	1:I:321:LEU:CA	2.62	0.65
1:C:9:LYS:O	1:C:9:LYS:HG3	1.96	0.65
1:C:234:SER:O	1:C:238:ASP:HB2	1.97	0.65
1:A:40:ARG:HH11	1:A:40:ARG:HB2	1.61	0.64
1:J:232:LEU:HD22	1:J:254:VAL:HB	1.77	0.64
1:C:240:PRO:HB2	1:C:241:PRO:HD3	1.79	0.64
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.76	0.64
1:G:237:ARG:HH21	1:G:237:ARG:CB	2.11	0.64
1:F:9:LYS:HG3	1:F:9:LYS:O	1.97	0.64
1:H:9:LYS:O	1:H:9:LYS:HG3	1.96	0.64
1:B:19:TYR:CZ	1:B:21:GLY:HA3	2.32	0.64
1:D:61:TRP:HE1	1:D:138:MET:HE2	1.61	0.64
1:I:14:PRO:HG3	1:J:171:TYR:OH	1.98	0.64
1:H:165:ARG:HH12	1:H:243:ILE:CD1	1.93	0.64
1:J:99:VAL:CG2	1:J:231:VAL:HG13	2.27	0.64
1:C:299:THR:HG21	1:C:345:PHE:CZ	2.33	0.64
1:G:326:GLY:CA	1:G:328:PRO:HD2	2.28	0.64
1:I:299:THR:HG21	1:I:345:PHE:HZ	1.60	0.64
1:J:40:ARG:HH11	1:J:40:ARG:HB2	1.61	0.64
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.76	0.63
1:G:300:ILE:HG22	1:G:341:MET:HG3	1.80	0.63
1:H:40:ARG:HB2	1:H:40:ARG:HH11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:THR:HG21	1:B:345:PHE:HZ	1.63	0.63
1:I:319:PRO:HB3	1:I:320:GLU:HA	1.81	0.63
1:J:326:GLY:C	1:J:328:PRO:HD2	2.24	0.63
1:F:223:LYS:HD2	1:I:263:ASP:HB3	1.81	0.62
1:I:234:SER:O	1:I:238:ASP:HB2	1.99	0.62
1:F:263:ASP:HB3	1:G:223:LYS:HD2	1.81	0.62
1:C:237:ARG:NH2	1:C:237:ARG:CB	2.62	0.62
1:E:61:TRP:HE1	1:E:138:MET:HE2	1.64	0.62
1:C:99:VAL:CG2	1:C:231:VAL:HG13	2.29	0.62
1:I:297:ILE:HG21	1:J:299:THR:HA	1.82	0.62
1:I:99:VAL:CG2	1:I:231:VAL:HG13	2.29	0.62
1:D:40:ARG:HH11	1:D:40:ARG:HB2	1.63	0.61
1:A:311:TYR:HE2	1:A:330:VAL:HG21	1.65	0.61
1:F:290:VAL:HG12	1:I:291:MET:HE3	1.82	0.61
1:J:6:LEU:HD23	1:J:7:SER:N	2.15	0.61
1:A:225:ILE:HD13	1:A:265:VAL:HG21	1.82	0.61
1:B:9:LYS:O	1:B:9:LYS:HG3	2.00	0.61
1:B:306:PHE:CE2	1:C:304:LEU:HB3	2.36	0.61
1:B:118:ASN:HD22	1:B:119:LEU:N	1.99	0.61
1:F:299:THR:HG21	1:F:345:PHE:HZ	1.65	0.61
1:H:240:PRO:CB	1:H:241:PRO:CD	2.74	0.60
1:H:313:MET:HA	1:J:311:TYR:CB	2.31	0.60
1:I:311:TYR:HE2	1:I:330:VAL:HG21	1.66	0.60
1:G:240:PRO:CB	1:G:241:PRO:HD2	2.32	0.60
1:H:237:ARG:NH2	1:H:237:ARG:CB	2.61	0.60
1:E:232:LEU:HD22	1:E:254:VAL:HB	1.84	0.59
1:H:347:LYS:O	1:H:348:LYS:HB2	2.02	0.59
1:C:225:ILE:HD13	1:C:265:VAL:HG21	1.84	0.59
1:C:232:LEU:HD22	1:C:254:VAL:HB	1.83	0.59
1:A:302:MET:CE	1:B:298:ALA:HA	2.27	0.59
1:J:240:PRO:CB	1:J:241:PRO:HD2	2.29	0.59
1:E:240:PRO:CB	1:E:241:PRO:HD2	2.29	0.59
1:C:299:THR:HG21	1:C:345:PHE:HZ	1.67	0.59
1:I:307:ILE:CD1	1:I:334:MET:HG2	2.24	0.59
1:B:40:ARG:HB2	1:B:40:ARG:NH1	2.17	0.59
1:A:347:LYS:O	1:A:348:LYS:HB2	2.03	0.58
1:A:240:PRO:CB	1:A:241:PRO:CD	2.73	0.58
1:C:240:PRO:CB	1:C:241:PRO:CD	2.77	0.58
1:F:240:PRO:CB	1:F:241:PRO:HD2	2.33	0.58
1:D:300:ILE:HG22	1:D:341:MET:HG3	1.84	0.58
1:G:299:THR:HG21	1:G:345:PHE:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:237:ARG:HB2	1:H:237:ARG:CZ	2.33	0.58
1:B:240:PRO:CB	1:B:241:PRO:HD2	2.31	0.58
1:I:240:PRO:HB2	1:I:241:PRO:HD3	1.85	0.58
1:A:99:VAL:CG2	1:A:231:VAL:HG13	2.34	0.58
1:J:326:GLY:O	1:J:329:VAL:HB	2.04	0.58
1:F:319:PRO:O	1:F:321:LEU:O	2.22	0.58
1:H:225:ILE:HD13	1:H:265:VAL:HG21	1.86	0.58
1:B:229:ARG:HA	1:B:258:THR:HG21	1.86	0.57
1:B:237:ARG:HB2	1:B:237:ARG:CZ	2.33	0.57
1:D:237:ARG:NH2	1:D:237:ARG:CB	2.63	0.57
1:E:237:ARG:NH2	1:E:237:ARG:CB	2.56	0.57
1:F:240:PRO:HB2	1:F:241:PRO:HD3	1.81	0.57
1:H:313:MET:HA	1:J:311:TYR:HB2	1.86	0.57
1:I:9:LYS:HG3	1:I:9:LYS:O	2.04	0.57
1:J:313:MET:HG3	1:J:314:ASN:CB	2.34	0.57
1:B:40:ARG:HH11	1:B:40:ARG:CB	2.18	0.57
1:D:14:PRO:HG3	1:E:171:TYR:CE2	2.39	0.57
1:D:229:ARG:HA	1:D:258:THR:CG2	2.34	0.57
1:G:299:THR:HA	1:H:297:ILE:HG21	1.85	0.57
1:A:232:LEU:HD22	1:A:254:VAL:HB	1.86	0.57
1:H:61:TRP:HB2	1:H:169:LEU:HD21	1.86	0.57
1:H:186:GLU:OE1	1:J:6:LEU:CD2	2.53	0.57
1:C:302:MET:HE3	1:E:301:PHE:HB2	1.87	0.57
1:F:300:ILE:HG22	1:F:341:MET:CG	2.30	0.57
1:I:302:MET:HG2	1:J:302:MET:HE1	1.87	0.57
1:G:326:GLY:O	1:G:329:VAL:HB	2.04	0.56
1:E:17:LEU:HB3	1:E:91:LEU:CD1	2.35	0.56
1:I:118:ASN:HD22	1:I:119:LEU:N	2.04	0.56
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.86	0.56
1:E:99:VAL:CG2	1:E:231:VAL:HG13	2.35	0.56
1:E:229:ARG:HA	1:E:258:THR:HG21	1.87	0.56
1:E:240:PRO:CB	1:E:241:PRO:CD	2.72	0.56
1:F:237:ARG:NH2	1:F:237:ARG:CB	2.60	0.56
1:G:99:VAL:CG2	1:G:231:VAL:HG13	2.34	0.56
1:I:229:ARG:HA	1:I:258:THR:CG2	2.35	0.56
1:D:300:ILE:HG13	1:D:301:PHE:N	2.20	0.56
1:F:118:ASN:HD22	1:F:119:LEU:N	2.04	0.56
1:C:40:ARG:HB2	1:C:40:ARG:NH1	2.21	0.56
1:G:237:ARG:NH2	1:G:237:ARG:CB	2.65	0.56
1:H:186:GLU:OE1	1:J:6:LEU:HD23	2.06	0.56
1:I:40:ARG:HB2	1:I:40:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ARG:HH11	1:E:40:ARG:HB2	1.71	0.56
1:F:211:THR:HG21	1:F:276:LEU:HD13	1.87	0.56
1:J:237:ARG:HB2	1:J:237:ARG:CZ	2.36	0.56
1:C:347:LYS:O	1:C:348:LYS:HB2	2.05	0.56
1:E:229:ARG:HA	1:E:258:THR:CG2	2.34	0.56
1:J:225:ILE:HD13	1:J:265:VAL:HG21	1.87	0.56
1:A:168:TYR:OH	1:B:14:PRO:HG2	2.06	0.56
1:E:16:THR:HG22	1:E:18:VAL:HG23	1.87	0.56
1:H:313:MET:CA	1:J:311:TYR:HB3	2.35	0.56
1:J:83:HIS:ND1	1:J:84:PRO:CD	2.66	0.56
1:D:223:LYS:HD2	1:E:263:ASP:HB3	1.88	0.55
1:E:237:ARG:HB2	1:E:237:ARG:CZ	2.35	0.55
1:I:237:ARG:NH2	1:I:237:ARG:CB	2.62	0.55
1:A:229:ARG:HA	1:A:258:THR:HG21	1.87	0.55
1:D:229:ARG:HA	1:D:258:THR:HG21	1.88	0.55
1:F:240:PRO:CB	1:F:241:PRO:CD	2.76	0.55
1:A:229:ARG:HA	1:A:258:THR:CG2	2.36	0.55
1:E:285:ASN:O	1:E:288:ASN:HB2	2.06	0.55
1:F:40:ARG:HH11	1:F:40:ARG:CB	2.20	0.55
1:H:310:ILE:CG2	1:J:334:MET:HE1	2.36	0.55
1:B:221:LEU:HG	1:B:225:ILE:HD12	1.89	0.55
1:I:82:ILE:HD13	1:I:130:ILE:HD13	1.88	0.55
1:J:229:ARG:HA	1:J:258:THR:CG2	2.36	0.55
1:I:296:ILE:HA	1:I:299:THR:HG22	1.88	0.55
1:B:347:LYS:O	1:B:348:LYS:HB2	2.07	0.55
1:I:240:PRO:CB	1:I:241:PRO:CD	2.80	0.55
1:I:229:ARG:HA	1:I:258:THR:HG21	1.88	0.55
1:J:240:PRO:CB	1:J:241:PRO:CD	2.75	0.55
1:J:299:THR:HG21	1:J:345:PHE:HZ	1.67	0.55
1:A:240:PRO:CB	1:A:241:PRO:HD2	2.31	0.55
1:D:152:GLU:HB2	1:D:158:ARG:HH12	1.72	0.55
1:G:17:LEU:HB3	1:G:91:LEU:CD1	2.37	0.55
1:C:200:LEU:HD22	1:E:209:GLN:HG3	1.88	0.54
1:I:40:ARG:HH11	1:I:40:ARG:CB	2.20	0.54
1:J:347:LYS:O	1:J:348:LYS:HB2	2.07	0.54
1:C:291:MET:HE3	1:E:290:VAL:HG12	1.88	0.54
1:H:221:LEU:HG	1:H:225:ILE:HD12	1.89	0.54
1:J:41:GLU:HG3	1:J:41:GLU:O	2.08	0.54
1:C:240:PRO:CB	1:C:241:PRO:HD2	2.36	0.54
1:G:347:LYS:O	1:G:348:LYS:HB2	2.07	0.54
1:I:347:LYS:O	1:I:348:LYS:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:ASN:HD22	1:J:119:LEU:N	2.04	0.54
1:A:51:LEU:N	1:A:52:PRO:HD2	2.23	0.54
1:B:229:ARG:HA	1:B:258:THR:CG2	2.37	0.54
1:D:347:LYS:O	1:D:348:LYS:HB2	2.07	0.54
1:E:5:ARG:C	1:E:6:LEU:HD12	2.31	0.54
1:D:240:PRO:CB	1:D:241:PRO:HD2	2.34	0.54
1:H:238:ASP:O	1:H:239:VAL:HG22	2.07	0.54
1:C:152:GLU:HB2	1:C:158:ARG:HH12	1.73	0.54
1:D:82:ILE:HD13	1:D:130:ILE:HD13	1.90	0.54
1:I:297:ILE:HG12	1:J:299:THR:OG1	2.08	0.54
1:F:40:ARG:HB2	1:F:40:ARG:NH1	2.23	0.54
1:A:294:LEU:HD22	1:B:294:LEU:HD11	1.90	0.54
1:H:232:LEU:HD22	1:H:254:VAL:HB	1.90	0.54
1:H:313:MET:CA	1:J:311:TYR:CB	2.86	0.54
1:A:186:GLU:CD	1:B:6:LEU:HG	2.30	0.53
1:C:291:MET:HB3	1:E:290:VAL:HG11	1.91	0.53
1:F:117:LYS:O	1:F:119:LEU:N	2.41	0.53
1:B:311:TYR:CE2	1:B:330:VAL:HG21	2.35	0.53
1:C:299:THR:HA	1:E:297:ILE:HG21	1.88	0.53
1:D:296:ILE:HA	1:D:299:THR:HG22	1.90	0.53
1:F:17:LEU:H	1:F:17:LEU:HD22	1.73	0.53
1:F:290:VAL:HG11	1:I:291:MET:HB3	1.90	0.53
1:E:292:LYS:NZ	1:E:348:LYS:HE3	2.22	0.53
1:G:51:LEU:N	1:G:52:PRO:HD2	2.24	0.53
1:G:240:PRO:CB	1:G:241:PRO:CD	2.79	0.53
1:D:61:TRP:HZ2	1:D:138:MET:HE1	1.74	0.53
1:F:6:LEU:HD12	1:I:186:GLU:HG2	1.89	0.53
1:H:240:PRO:CB	1:H:241:PRO:HD2	2.34	0.53
1:C:237:ARG:HB2	1:C:237:ARG:HH21	1.61	0.53
1:G:311:TYR:HE2	1:G:330:VAL:HG21	1.74	0.53
1:B:17:LEU:HB3	1:B:91:LEU:CD1	2.39	0.53
1:C:125:GLU:HG3	1:C:141:GLU:HB2	1.91	0.53
1:H:248:VAL:N	1:H:249:PRO:HD2	2.24	0.53
1:I:240:PRO:CB	1:I:241:PRO:HD2	2.37	0.53
1:G:232:LEU:HD22	1:G:254:VAL:HB	1.91	0.53
1:I:300:ILE:HG22	1:I:341:MET:HG3	1.91	0.53
1:A:291:MET:HE2	1:B:291:MET:HG2	1.90	0.53
1:J:229:ARG:HA	1:J:258:THR:HG21	1.91	0.52
1:A:99:VAL:HG13	1:A:108:ILE:HG12	1.90	0.52
1:B:157:ASN:OD1	1:B:162:ARG:HG3	2.10	0.52
1:C:61:TRP:HZ2	1:C:138:MET:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:N	1:C:249:PRO:HD2	2.25	0.52
1:D:240:PRO:CB	1:D:241:PRO:CD	2.79	0.52
1:E:225:ILE:HD13	1:E:265:VAL:HG21	1.91	0.52
1:F:291:MET:HE3	1:G:290:VAL:HG12	1.91	0.52
1:I:300:ILE:HG13	1:I:301:PHE:N	2.24	0.52
1:I:319:PRO:HA	1:I:320:GLU:O	2.09	0.52
1:B:291:MET:HE3	1:C:290:VAL:HG12	1.90	0.52
1:D:14:PRO:HG3	1:E:171:TYR:CZ	2.43	0.52
1:D:240:PRO:HB2	1:D:241:PRO:HD3	1.85	0.52
1:E:286:LYS:O	1:E:289:GLU:N	2.41	0.52
1:F:125:GLU:HG3	1:F:141:GLU:HB2	1.91	0.52
1:G:202:ARG:O	1:G:202:ARG:HG3	2.07	0.52
1:I:33:ASN:HB2	1:I:60:THR:HG23	1.91	0.52
1:B:286:LYS:O	1:B:290:VAL:HG23	2.08	0.52
1:C:311:TYR:HE2	1:C:330:VAL:HG11	1.75	0.52
1:D:25:GLU:OE2	1:I:23:TYR:HD1	1.93	0.52
1:A:299:THR:HG21	1:A:345:PHE:CE1	2.43	0.52
1:C:238:ASP:O	1:C:239:VAL:HG22	2.09	0.52
1:F:17:LEU:HB3	1:F:91:LEU:CD1	2.39	0.52
1:I:125:GLU:HG3	1:I:141:GLU:HB2	1.92	0.52
1:F:347:LYS:O	1:F:348:LYS:HB2	2.10	0.52
1:H:17:LEU:HB3	1:H:91:LEU:CD1	2.40	0.52
1:D:242:LEU:O	1:D:243:ILE:C	2.52	0.52
1:G:296:ILE:HA	1:G:299:THR:HG22	1.92	0.52
1:J:240:PRO:HB2	1:J:241:PRO:HD3	1.85	0.52
1:A:82:ILE:HD13	1:A:130:ILE:HD13	1.90	0.52
1:E:244:GLU:C	1:E:246:GLU:N	2.68	0.52
1:A:337:ILE:O	1:A:341:MET:HG2	2.10	0.52
1:J:40:ARG:HB2	1:J:40:ARG:NH1	2.24	0.52
1:J:242:LEU:O	1:J:243:ILE:C	2.53	0.52
1:A:311:TYR:CE2	1:A:330:VAL:HG21	2.45	0.51
1:F:202:ARG:O	1:F:202:ARG:HG3	2.10	0.51
1:F:244:GLU:C	1:F:246:GLU:N	2.68	0.51
1:G:244:GLU:C	1:G:246:GLU:N	2.68	0.51
1:E:6:LEU:O	1:E:7:SER:CB	2.58	0.51
1:F:153:ARG:CD	1:G:13:PRO:HG3	2.40	0.51
1:F:232:LEU:HD22	1:F:254:VAL:HB	1.92	0.51
1:G:40:ARG:HB2	1:G:40:ARG:HH11	1.75	0.51
1:A:300:ILE:HG13	1:A:301:PHE:N	2.26	0.51
1:H:40:ARG:HB2	1:H:40:ARG:NH1	2.25	0.51
1:A:41:GLU:O	1:A:41:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LYS:O	1:C:287:THR:C	2.53	0.51
1:F:16:THR:HG22	1:F:18:VAL:HG23	1.92	0.51
1:F:229:ARG:HA	1:F:258:THR:CG2	2.41	0.51
1:G:248:VAL:N	1:G:249:PRO:HD2	2.25	0.51
1:H:61:TRP:HZ2	1:H:138:MET:HE1	1.75	0.51
1:B:170:LEU:O	1:B:171:TYR:C	2.53	0.51
1:C:237:ARG:HB2	1:C:237:ARG:CZ	2.41	0.51
1:F:171:TYR:OH	1:G:14:PRO:HG3	2.09	0.51
1:E:300:ILE:HG13	1:E:301:PHE:N	2.25	0.51
1:G:132:THR:HG23	1:G:132:THR:O	2.11	0.51
1:C:118:ASN:HD22	1:C:119:LEU:N	2.08	0.51
1:C:296:ILE:HA	1:C:299:THR:HG22	1.93	0.51
1:D:51:LEU:N	1:D:52:PRO:HD2	2.26	0.51
1:G:196:GLU:OE1	1:H:212:HIS:NE2	2.41	0.51
1:G:211:THR:HG21	1:G:276:LEU:HD13	1.93	0.51
1:I:51:LEU:N	1:I:52:PRO:HD2	2.26	0.51
1:F:7:SER:O	1:I:182:PHE:HB3	2.11	0.51
1:I:184:LEU:HD21	1:I:221:LEU:HD11	1.93	0.51
1:A:33:ASN:HB2	1:A:60:THR:HG23	1.92	0.50
1:E:242:LEU:O	1:E:243:ILE:C	2.52	0.50
1:B:263:ASP:HB3	1:C:223:LYS:HD2	1.92	0.50
1:C:40:ARG:HH11	1:C:40:ARG:CB	2.23	0.50
1:I:237:ARG:HB2	1:I:237:ARG:CZ	2.41	0.50
1:H:33:ASN:HB2	1:H:60:THR:HG23	1.94	0.50
1:A:297:ILE:HG21	1:D:299:THR:HA	1.92	0.50
1:H:51:LEU:N	1:H:52:PRO:HD2	2.25	0.50
1:H:118:ASN:HD22	1:H:119:LEU:N	2.09	0.50
1:B:99:VAL:HG13	1:B:108:ILE:HG12	1.93	0.50
1:D:125:GLU:HG3	1:D:141:GLU:HB2	1.92	0.50
1:H:306:PHE:CE2	1:J:304:LEU:HB3	2.46	0.50
1:B:194:VAL:O	1:B:197:GLU:HB2	2.11	0.50
1:D:118:ASN:HD22	1:D:119:LEU:N	2.09	0.50
1:E:292:LYS:HZ3	1:E:348:LYS:HE3	1.77	0.50
1:F:229:ARG:HA	1:F:258:THR:HG21	1.94	0.50
1:D:337:ILE:O	1:D:341:MET:HG2	2.12	0.50
1:E:347:LYS:O	1:E:348:LYS:HB2	2.11	0.50
1:F:302:MET:HE1	1:G:302:MET:HG2	1.92	0.50
1:I:202:ARG:O	1:I:202:ARG:HG3	2.10	0.50
1:J:61:TRP:HE1	1:J:138:MET:HE2	1.75	0.50
1:J:258:THR:HG22	1:J:259:ILE:N	2.27	0.50
1:B:16:THR:HG22	1:B:18:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:OG1	1:E:297:ILE:HG12	2.11	0.50
1:A:40:ARG:HB2	1:A:40:ARG:NH1	2.24	0.50
1:B:153:ARG:HD3	1:C:13:PRO:HG3	1.94	0.50
1:F:41:GLU:O	1:F:41:GLU:HG3	2.12	0.50
1:I:244:GLU:C	1:I:246:GLU:N	2.68	0.50
1:A:299:THR:HA	1:B:297:ILE:HG21	1.94	0.49
1:F:153:ARG:HD3	1:G:13:PRO:HG3	1.94	0.49
1:A:310:ILE:O	1:A:312:GLY:HA2	2.12	0.49
1:D:238:ASP:O	1:D:239:VAL:HG22	2.12	0.49
1:G:242:LEU:O	1:G:243:ILE:C	2.53	0.49
1:G:294:LEU:HD22	1:H:294:LEU:HD11	1.94	0.49
1:J:117:LYS:O	1:J:119:LEU:N	2.44	0.49
1:F:285:ASN:O	1:F:288:ASN:HB2	2.12	0.49
1:A:40:ARG:HH11	1:A:40:ARG:CB	2.25	0.49
1:D:132:THR:O	1:D:132:THR:HG23	2.10	0.49
1:F:337:ILE:O	1:F:341:MET:HG2	2.12	0.49
1:G:255:TYR:O	1:G:258:THR:HG22	2.13	0.49
1:G:237:ARG:HB2	1:G:237:ARG:CZ	2.41	0.49
1:G:291:MET:HE1	1:H:291:MET:SD	2.53	0.49
1:G:337:ILE:O	1:G:341:MET:HG2	2.11	0.49
1:C:270:ASP:OD1	1:E:269:ARG:NH1	2.46	0.49
1:E:40:ARG:HB2	1:E:40:ARG:NH1	2.27	0.49
1:E:272:VAL:O	1:E:275:LEU:HB2	2.13	0.49
1:A:152:GLU:HB2	1:A:158:ARG:HH12	1.77	0.49
1:B:300:ILE:HG13	1:B:301:PHE:N	2.27	0.49
1:C:184:LEU:HD21	1:C:221:LEU:HD11	1.94	0.49
1:D:211:THR:HG21	1:D:276:LEU:HD13	1.93	0.49
1:E:92:ASN:OD1	1:E:92:ASN:C	2.56	0.49
1:G:33:ASN:HB2	1:G:60:THR:HG23	1.94	0.49
1:G:313:MET:H	1:G:314:ASN:CB	2.25	0.49
1:J:17:LEU:HB3	1:J:91:LEU:CD1	2.43	0.49
1:B:153:ARG:CD	1:C:13:PRO:HG3	2.43	0.49
1:F:327:TYR:N	1:F:328:PRO:HD2	2.28	0.49
1:I:194:VAL:O	1:I:197:GLU:HB2	2.13	0.49
1:I:232:LEU:HD22	1:I:254:VAL:HB	1.95	0.49
1:D:232:LEU:HD22	1:D:254:VAL:HB	1.93	0.49
1:D:348:LYS:HE2	1:D:349:LYS:N	2.19	0.49
1:F:302:MET:HE3	1:G:301:PHE:HB2	1.94	0.49
1:G:326:GLY:HA2	1:G:328:PRO:HD2	1.93	0.49
1:B:337:ILE:O	1:B:341:MET:HG2	2.12	0.49
1:C:99:VAL:HG13	1:C:108:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:THR:HG21	1:C:276:LEU:HD13	1.94	0.48
1:E:298:ALA:O	1:E:302:MET:HG2	2.13	0.48
1:H:200:LEU:O	1:H:201:GLU:HG3	2.13	0.48
1:B:221:LEU:HG	1:B:225:ILE:CD1	2.43	0.48
1:H:242:LEU:O	1:H:243:ILE:C	2.55	0.48
1:G:229:ARG:HA	1:G:258:THR:CG2	2.44	0.48
1:I:223:LYS:HD2	1:J:263:ASP:HB3	1.94	0.48
1:J:238:ASP:HB3	1:J:239:VAL:H	1.53	0.48
1:A:202:ARG:O	1:A:202:ARG:HG3	2.11	0.48
1:E:51:LEU:N	1:E:52:PRO:HD2	2.28	0.48
1:H:337:ILE:O	1:H:341:MET:HG2	2.13	0.48
1:D:17:LEU:HB3	1:D:91:LEU:CD1	2.43	0.48
1:G:300:ILE:HG13	1:G:301:PHE:N	2.28	0.48
1:A:9:LYS:HG3	1:A:9:LYS:O	2.12	0.48
1:C:194:VAL:O	1:C:197:GLU:HB2	2.14	0.48
1:C:244:GLU:C	1:C:246:GLU:N	2.71	0.48
1:F:242:LEU:O	1:F:243:ILE:C	2.57	0.48
1:H:221:LEU:HG	1:H:225:ILE:CD1	2.43	0.48
1:A:300:ILE:HG22	1:A:341:MET:HG3	1.96	0.48
1:D:33:ASN:HB2	1:D:60:THR:HG23	1.95	0.48
1:H:229:ARG:HA	1:H:258:THR:CG2	2.43	0.48
1:J:104:ASN:O	1:J:105:TYR:HB3	2.11	0.48
1:A:244:GLU:C	1:A:246:GLU:N	2.72	0.48
1:C:166:ALA:O	1:C:169:LEU:HB3	2.14	0.48
1:H:61:TRP:HE1	1:H:138:MET:HE2	1.79	0.48
1:H:181:TYR:HB2	1:H:261:ILE:HD13	1.95	0.48
1:B:82:ILE:HD13	1:B:130:ILE:HD13	1.96	0.48
1:E:202:ARG:O	1:E:202:ARG:HG3	2.12	0.48
1:F:300:ILE:HG13	1:F:301:PHE:N	2.29	0.48
1:H:272:VAL:O	1:H:275:LEU:HB2	2.14	0.48
1:J:40:ARG:HH11	1:J:40:ARG:CB	2.27	0.48
1:B:118:ASN:HD22	1:B:118:ASN:C	2.22	0.48
1:C:196:GLU:OE1	1:E:212:HIS:NE2	2.47	0.48
1:F:237:ARG:HB2	1:F:237:ARG:CZ	2.42	0.48
1:B:195:LEU:HD21	1:B:211:THR:HA	1.96	0.47
1:C:202:ARG:HG3	1:C:202:ARG:O	2.14	0.47
1:C:300:ILE:HG13	1:C:301:PHE:N	2.29	0.47
1:E:120:HIS:HD2	1:E:191:GLU:OE2	1.97	0.47
1:I:311:TYR:CE2	1:I:330:VAL:HG21	2.49	0.47
1:A:302:MET:HE1	1:B:302:MET:HG2	1.95	0.47
1:B:225:ILE:O	1:B:228:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:TRP:CD1	1:I:61:TRP:C	2.92	0.47
1:J:296:ILE:HA	1:J:299:THR:HG22	1.96	0.47
1:A:103:GLU:HB3	1:A:104:ASN:OD1	2.14	0.47
1:B:67:ILE:HG21	1:B:139:PHE:HB3	1.97	0.47
1:E:337:ILE:O	1:E:341:MET:HG2	2.15	0.47
1:F:182:PHE:HB3	1:G:7:SER:O	2.15	0.47
1:G:40:ARG:HB2	1:G:40:ARG:NH1	2.28	0.47
1:H:117:LYS:O	1:H:119:LEU:N	2.46	0.47
1:B:296:ILE:HA	1:B:299:THR:HG22	1.96	0.47
1:C:238:ASP:HB3	1:C:239:VAL:H	1.55	0.47
1:E:296:ILE:HA	1:E:299:THR:HG22	1.97	0.47
1:I:327:TYR:CD2	1:J:314:ASN:O	2.68	0.47
1:A:125:GLU:HG3	1:A:141:GLU:HB2	1.96	0.47
1:A:272:VAL:O	1:A:275:LEU:HB2	2.14	0.47
1:A:307:ILE:CD1	1:A:334:MET:HG2	2.35	0.47
1:D:40:ARG:HB2	1:D:40:ARG:NH1	2.27	0.47
1:G:306:PHE:CE2	1:H:304:LEU:HB3	2.49	0.47
1:H:233:SER:HG	1:H:237:ARG:HH12	1.61	0.47
1:H:296:ILE:HA	1:H:299:THR:HG22	1.96	0.47
1:J:148:ASP:N	1:J:149:PRO:HD2	2.29	0.47
1:J:157:ASN:OD1	1:J:162:ARG:HG3	2.14	0.47
1:J:300:ILE:HG13	1:J:301:PHE:N	2.29	0.47
1:A:221:LEU:HG	1:A:225:ILE:HD12	1.96	0.47
1:A:306:PHE:CE2	1:B:304:LEU:HB3	2.50	0.47
1:D:311:TYR:HE2	1:D:330:VAL:HG21	1.80	0.47
1:J:238:ASP:O	1:J:239:VAL:HG22	2.14	0.47
1:B:299:THR:HG21	1:B:345:PHE:CE1	2.49	0.47
1:G:225:ILE:HD13	1:G:265:VAL:HG21	1.96	0.47
1:B:56:SER:HB3	1:B:58:THR:O	2.15	0.47
1:E:40:ARG:HH11	1:E:40:ARG:CB	2.27	0.47
1:H:230:GLU:OE1	1:H:230:GLU:HA	2.14	0.47
1:H:313:MET:HA	1:J:311:TYR:HB3	1.97	0.47
1:A:83:HIS:ND1	1:A:84:PRO:CD	2.70	0.46
1:F:225:ILE:HD13	1:F:265:VAL:HG21	1.98	0.46
1:H:309:GLY:C	1:H:311:TYR:H	2.23	0.46
1:A:28:GLU:OE2	1:A:143:ILE:HD11	2.15	0.46
1:B:51:LEU:N	1:B:52:PRO:HD2	2.30	0.46
1:F:301:PHE:HB2	1:I:302:MET:HE3	1.96	0.46
1:G:291:MET:HE3	1:G:291:MET:HB3	1.85	0.46
1:J:125:GLU:HG3	1:J:141:GLU:HB2	1.97	0.46
1:A:343:VAL:HG12	1:A:343:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ARG:HB2	1:D:237:ARG:CZ	2.43	0.46
1:E:33:ASN:HB2	1:E:60:THR:HG23	1.97	0.46
1:E:211:THR:HG21	1:E:276:LEU:HD13	1.96	0.46
1:I:17:LEU:HB3	1:I:91:LEU:CD1	2.46	0.46
1:I:301:PHE:CZ	1:J:303:PRO:HB3	2.50	0.46
1:B:33:ASN:HB2	1:B:60:THR:HG23	1.98	0.46
1:I:291:MET:SD	1:J:291:MET:HE1	2.55	0.46
1:J:118:ASN:HD22	1:J:118:ASN:C	2.23	0.46
1:E:238:ASP:HB3	1:E:239:VAL:H	1.53	0.46
1:I:157:ASN:OD1	1:I:162:ARG:HG3	2.15	0.46
1:A:237:ARG:HB2	1:A:237:ARG:CZ	2.43	0.46
1:A:296:ILE:HA	1:A:299:THR:HG22	1.97	0.46
1:B:299:THR:HA	1:C:297:ILE:HG21	1.98	0.46
1:A:118:ASN:HD22	1:A:119:LEU:N	2.14	0.46
1:F:263:ASP:OD2	1:G:96:ARG:CZ	2.64	0.46
1:F:296:ILE:HA	1:F:299:THR:HG22	1.97	0.46
1:G:152:GLU:HB2	1:G:158:ARG:HH12	1.81	0.46
1:J:99:VAL:HG13	1:J:108:ILE:HG12	1.98	0.46
1:A:270:ASP:OD1	1:B:269:ARG:NH1	2.49	0.46
1:B:242:LEU:O	1:B:243:ILE:C	2.59	0.46
1:B:244:GLU:C	1:B:246:GLU:N	2.73	0.46
1:D:291:MET:HE3	1:D:291:MET:HB3	1.82	0.46
1:F:82:ILE:HD13	1:F:130:ILE:HD13	1.97	0.46
1:F:327:TYR:N	1:F:328:PRO:CD	2.79	0.46
1:G:194:VAL:O	1:G:197:GLU:HB2	2.15	0.46
1:G:221:LEU:HG	1:G:225:ILE:HD12	1.98	0.46
1:H:56:SER:HB3	1:H:58:THR:O	2.16	0.46
1:H:83:HIS:ND1	1:H:84:PRO:CD	2.74	0.46
1:I:211:THR:HG21	1:I:276:LEU:HD13	1.97	0.46
1:C:186:GLU:OE1	1:E:7:SER:HB3	2.16	0.46
1:C:348:LYS:CE	1:C:349:LYS:H	2.22	0.46
1:F:170:LEU:O	1:F:171:TYR:C	2.58	0.46
1:H:255:TYR:CZ	1:H:259:ILE:HD11	2.51	0.46
1:C:229:ARG:HA	1:C:258:THR:CG2	2.47	0.45
1:D:291:MET:SD	1:E:291:MET:HE1	2.56	0.45
1:G:41:GLU:O	1:G:41:GLU:HG3	2.15	0.45
1:D:14:PRO:HG2	1:E:168:TYR:OH	2.16	0.45
1:E:41:GLU:O	1:E:41:GLU:HG3	2.15	0.45
1:F:51:LEU:N	1:F:52:PRO:HD2	2.31	0.45
1:H:17:LEU:HD22	1:H:17:LEU:H	1.81	0.45
1:I:13:PRO:HG3	1:J:153:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:GLN:HG3	1:J:200:LEU:HD22	1.99	0.45
1:I:276:LEU:HD12	1:I:276:LEU:HA	1.85	0.45
1:I:337:ILE:O	1:I:341:MET:HG2	2.17	0.45
1:A:117:LYS:O	1:A:119:LEU:N	2.49	0.45
1:C:51:LEU:N	1:C:52:PRO:HD2	2.31	0.45
1:C:337:ILE:O	1:C:341:MET:HG2	2.16	0.45
1:F:118:ASN:HD22	1:F:118:ASN:C	2.24	0.45
1:F:307:ILE:O	1:F:310:ILE:HG12	2.16	0.45
1:H:40:ARG:HH11	1:H:40:ARG:CB	2.27	0.45
1:A:221:LEU:HG	1:A:225:ILE:CD1	2.46	0.45
1:C:61:TRP:HE1	1:C:138:MET:HE2	1.80	0.45
1:D:96:ARG:CZ	1:E:263:ASP:OD2	2.64	0.45
1:F:61:TRP:HE1	1:F:138:MET:HE2	1.81	0.45
1:G:348:LYS:HE2	1:G:349:LYS:N	2.24	0.45
1:H:299:THR:HA	1:J:297:ILE:HG21	1.99	0.45
1:I:309:GLY:C	1:I:311:TYR:H	2.23	0.45
1:J:61:TRP:CD1	1:J:61:TRP:C	2.93	0.45
1:J:96:ARG:HH11	1:J:227:PRO:HG3	1.81	0.45
1:B:238:ASP:O	1:B:239:VAL:HG22	2.16	0.45
1:E:286:LYS:C	1:E:288:ASN:N	2.75	0.45
1:F:319:PRO:C	1:F:321:LEU:O	2.59	0.45
1:J:300:ILE:HG22	1:J:341:MET:HG3	1.98	0.45
1:A:242:LEU:O	1:A:243:ILE:C	2.59	0.45
1:H:153:ARG:HD3	1:J:13:PRO:HG3	1.98	0.45
1:I:225:ILE:CD1	1:I:265:VAL:HG21	2.42	0.45
2:A:1350:CL:CL	1:B:14:PRO:HD2	2.53	0.45
1:B:118:ASN:ND2	1:B:119:LEU:N	2.65	0.45
1:C:33:ASN:HB2	1:C:60:THR:HG23	1.98	0.45
1:D:17:LEU:H	1:D:17:LEU:HD22	1.82	0.45
1:E:61:TRP:HZ2	1:E:138:MET:HE1	1.81	0.45
1:H:348:LYS:HE2	1:H:349:LYS:N	2.26	0.45
1:A:200:LEU:O	1:A:201:GLU:HG3	2.16	0.45
1:C:61:TRP:CD1	1:C:61:TRP:C	2.95	0.45
1:C:238:ASP:C	1:C:239:VAL:HG13	2.41	0.45
1:F:238:ASP:O	1:F:239:VAL:HG22	2.16	0.45
1:H:152:GLU:HB2	1:H:158:ARG:HH12	1.80	0.45
1:I:296:ILE:HG13	1:I:297:ILE:H	1.81	0.45
1:B:330:VAL:O	1:B:334:MET:HG3	2.17	0.45
1:C:330:VAL:O	1:C:334:MET:HG3	2.17	0.45
1:D:40:ARG:HH11	1:D:40:ARG:CB	2.28	0.45
1:F:248:VAL:N	1:F:249:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:ASP:HB3	1:I:239:VAL:H	1.57	0.45
1:D:248:VAL:N	1:D:249:PRO:HD2	2.32	0.45
1:C:294:LEU:HD22	1:E:294:LEU:HD11	1.98	0.44
1:D:348:LYS:CE	1:D:349:LYS:H	2.20	0.44
1:F:310:ILE:HG22	1:G:334:MET:HE1	1.99	0.44
1:H:211:THR:HG21	1:H:276:LEU:HD13	1.99	0.44
1:H:244:GLU:C	1:H:246:GLU:N	2.71	0.44
1:I:195:LEU:HD21	1:I:211:THR:HA	1.99	0.44
1:C:181:TYR:HB2	1:C:261:ILE:HD13	1.99	0.44
1:C:291:MET:CE	1:E:291:MET:HG2	2.45	0.44
1:D:202:ARG:O	1:D:202:ARG:HG3	2.16	0.44
1:G:82:ILE:HD13	1:G:130:ILE:HD13	1.98	0.44
1:I:61:TRP:HE1	1:I:138:MET:HE2	1.81	0.44
1:I:136:VAL:HG11	1:I:173:LEU:HD12	1.98	0.44
1:J:221:LEU:HG	1:J:225:ILE:HD12	1.99	0.44
1:J:248:VAL:N	1:J:249:PRO:HD2	2.32	0.44
1:B:83:HIS:ND1	1:B:84:PRO:CD	2.71	0.44
1:D:225:ILE:HD13	1:D:265:VAL:HG21	1.98	0.44
1:G:270:ASP:OD1	1:H:269:ARG:NH1	2.50	0.44
1:G:299:THR:CG2	1:G:345:PHE:CE1	3.00	0.44
1:J:33:ASN:HB2	1:J:60:THR:HG23	1.97	0.44
1:F:194:VAL:O	1:F:197:GLU:HB2	2.18	0.44
1:F:209:GLN:HG3	1:I:200:LEU:HD13	1.99	0.44
1:I:272:VAL:O	1:I:275:LEU:HB2	2.16	0.44
1:J:337:ILE:O	1:J:341:MET:HG2	2.16	0.44
1:A:61:TRP:HZ2	1:A:138:MET:HE1	1.82	0.44
1:C:341:MET:O	1:C:344:TYR:HB3	2.18	0.44
1:D:309:GLY:C	1:D:311:TYR:H	2.25	0.44
1:J:311:TYR:HE2	1:J:330:VAL:HG21	1.81	0.44
1:B:61:TRP:HE1	1:B:138:MET:HE2	1.82	0.44
1:B:237:ARG:NH2	1:B:237:ARG:CB	2.61	0.44
1:C:298:ALA:O	1:C:302:MET:HG2	2.17	0.44
1:J:61:TRP:HZ2	1:J:138:MET:HE1	1.83	0.44
1:G:348:LYS:CE	1:G:349:LYS:H	2.24	0.44
1:I:54:ARG:HG3	1:I:80:PHE:CD1	2.53	0.44
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.72	0.44
1:H:326:GLY:H	1:H:328:PRO:HD2	1.82	0.44
1:I:10:LYS:H	1:I:10:LYS:HD2	1.83	0.44
1:J:16:THR:HG22	1:J:18:VAL:HG23	2.00	0.44
1:A:195:LEU:HD21	1:A:211:THR:HA	2.00	0.44
1:A:238:ASP:O	1:A:239:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:THR:HG22	1:A:259:ILE:N	2.33	0.44
1:A:312:GLY:O	1:B:311:TYR:HB2	2.18	0.44
1:D:99:VAL:HG13	1:D:108:ILE:HG12	1.99	0.44
1:D:297:ILE:HG21	1:E:299:THR:HA	1.99	0.44
1:E:184:LEU:HD21	1:E:221:LEU:HD11	1.99	0.44
1:F:327:TYR:H	1:F:328:PRO:HD2	1.82	0.44
1:I:242:LEU:O	1:I:243:ILE:C	2.61	0.44
1:I:311:TYR:HB3	1:J:313:MET:HB2	1.99	0.44
1:A:248:VAL:N	1:A:249:PRO:HD2	2.33	0.43
1:B:113:PHE:CE1	1:B:124:SER:HB3	2.53	0.43
1:B:312:GLY:O	1:C:311:TYR:HB2	2.18	0.43
1:D:16:THR:HG22	1:D:18:VAL:HG23	2.00	0.43
1:G:40:ARG:HH11	1:G:40:ARG:CB	2.30	0.43
1:H:202:ARG:HG3	1:H:202:ARG:O	2.17	0.43
1:H:313:MET:O	1:J:311:TYR:HB3	2.18	0.43
1:I:152:GLU:HB2	1:I:158:ARG:HH12	1.83	0.43
1:I:307:ILE:O	1:I:310:ILE:HG12	2.18	0.43
1:F:348:LYS:CE	1:F:349:LYS:H	2.23	0.43
1:J:221:LEU:HG	1:J:225:ILE:CD1	2.48	0.43
1:J:299:THR:HG21	1:J:345:PHE:CE1	2.53	0.43
1:C:16:THR:HG22	1:C:18:VAL:HG23	1.99	0.43
1:D:244:GLU:C	1:D:246:GLU:N	2.74	0.43
1:E:291:MET:HE3	1:E:291:MET:HB3	1.87	0.43
1:F:28:GLU:OE1	1:F:43:LYS:HD3	2.18	0.43
1:J:272:VAL:O	1:J:275:LEU:HB2	2.18	0.43
1:E:157:ASN:OD1	1:E:162:ARG:HG3	2.18	0.43
1:G:16:THR:HG22	1:G:18:VAL:HG23	1.99	0.43
1:G:85:LEU:HD23	1:G:85:LEU:HA	1.86	0.43
1:G:300:ILE:HG22	1:G:341:MET:CG	2.47	0.43
1:H:195:LEU:HD21	1:H:211:THR:HA	2.00	0.43
1:H:330:VAL:O	1:H:334:MET:HG3	2.18	0.43
1:I:16:THR:HG22	1:I:18:VAL:HG23	2.00	0.43
1:C:242:LEU:O	1:C:243:ILE:C	2.61	0.43
1:F:56:SER:HB3	1:F:58:THR:O	2.18	0.43
1:F:148:ASP:OD1	1:F:151:ARG:NH1	2.52	0.43
1:F:299:THR:HG21	1:F:345:PHE:CZ	2.49	0.43
1:F:309:GLY:C	1:F:311:TYR:H	2.25	0.43
1:G:252:ARG:NH2	1:H:100:GLU:HG2	2.34	0.43
1:H:311:TYR:HE2	1:H:330:VAL:HG21	1.84	0.43
1:I:41:GLU:O	1:I:41:GLU:HG3	2.17	0.43
1:J:202:ARG:HG3	1:J:202:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:244:GLU:C	1:J:246:GLU:N	2.68	0.43
1:A:17:LEU:HB3	1:A:91:LEU:CD1	2.48	0.43
1:B:348:LYS:HE2	1:B:349:LYS:N	2.28	0.43
1:D:94:HIS:C	1:E:260:GLN:HE22	2.27	0.43
1:F:272:VAL:O	1:F:275:LEU:HB2	2.19	0.43
1:G:240:PRO:HB2	1:G:241:PRO:HD3	1.90	0.43
1:I:348:LYS:CE	1:I:349:LYS:H	2.26	0.43
1:J:82:ILE:HD13	1:J:130:ILE:HD13	2.01	0.43
1:G:238:ASP:O	1:G:239:VAL:HG22	2.18	0.43
4:A:2002:HOH:O	1:B:89:ASP:CG	2.60	0.43
1:B:230:GLU:OE1	1:B:230:GLU:HA	2.19	0.43
1:G:19:TYR:CE1	1:G:21:GLY:HA3	2.53	0.43
1:G:117:LYS:O	1:G:119:LEU:N	2.51	0.43
1:H:237:ARG:HH21	1:H:237:ARG:HB3	1.81	0.43
1:I:237:ARG:HH21	1:I:237:ARG:HB3	1.81	0.43
1:A:111:LYS:O	1:A:177:LEU:HD21	2.19	0.43
1:B:61:TRP:CD1	1:B:61:TRP:C	2.97	0.43
1:B:348:LYS:CE	1:B:349:LYS:H	2.27	0.43
1:F:238:ASP:HB3	1:F:239:VAL:H	1.55	0.43
1:G:170:LEU:O	1:G:171:TYR:C	2.61	0.43
1:I:318:MET:O	1:I:319:PRO:O	2.37	0.43
1:B:300:ILE:HG22	1:B:341:MET:CG	2.46	0.42
1:C:17:LEU:HB3	1:C:91:LEU:CD1	2.49	0.42
1:D:184:LEU:HD21	1:D:221:LEU:HD11	2.01	0.42
1:E:125:GLU:HG3	1:E:141:GLU:HB2	2.00	0.42
1:F:348:LYS:HE2	1:F:349:LYS:N	2.23	0.42
1:H:276:LEU:HD12	1:H:276:LEU:HA	1.81	0.42
1:I:83:HIS:CD2	1:I:85:LEU:HB2	2.54	0.42
1:J:237:ARG:NH2	1:J:237:ARG:CB	2.64	0.42
1:J:309:GLY:C	1:J:311:TYR:H	2.27	0.42
1:B:186:GLU:OE1	1:C:6:LEU:N	2.52	0.42
1:F:263:ASP:OD2	1:G:96:ARG:NE	2.53	0.42
1:G:230:GLU:OE1	1:G:230:GLU:HA	2.18	0.42
1:G:309:GLY:C	1:G:311:TYR:H	2.26	0.42
1:J:51:LEU:N	1:J:52:PRO:HD2	2.34	0.42
1:B:258:THR:HG22	1:B:259:ILE:N	2.34	0.42
1:B:343:VAL:HG12	1:B:343:VAL:O	2.18	0.42
1:D:117:LYS:O	1:D:119:LEU:N	2.48	0.42
1:E:54:ARG:HG3	1:E:80:PHE:CD1	2.54	0.42
1:F:99:VAL:HG13	1:F:108:ILE:HG12	2.01	0.42
1:G:202:ARG:O	1:G:202:ARG:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:ARG:HH11	1:H:227:PRO:HG3	1.84	0.42
1:J:243:ILE:HG13	1:J:246:GLU:HB2	2.02	0.42
1:B:125:GLU:HG3	1:B:141:GLU:HB2	2.01	0.42
1:B:202:ARG:O	1:B:202:ARG:HG3	2.20	0.42
1:B:202:ARG:N	1:B:203:PRO:HD3	2.34	0.42
1:C:200:LEU:O	1:C:201:GLU:HG3	2.19	0.42
1:C:348:LYS:HE2	1:C:349:LYS:N	2.23	0.42
1:D:28:GLU:OE1	1:D:43:LYS:HD3	2.19	0.42
1:D:157:ASN:OD1	1:D:162:ARG:HG3	2.18	0.42
1:F:96:ARG:HH11	1:F:227:PRO:HG3	1.83	0.42
1:I:341:MET:O	1:I:344:TYR:HB3	2.20	0.42
1:A:291:MET:HE3	1:A:291:MET:HB3	1.87	0.42
1:C:255:TYR:O	1:C:258:THR:HG22	2.19	0.42
1:C:291:MET:HE1	1:E:291:MET:SD	2.59	0.42
1:D:238:ASP:HB3	1:D:239:VAL:H	1.55	0.42
1:F:212:HIS:NE2	1:I:196:GLU:OE1	2.47	0.42
1:G:307:ILE:CD1	1:G:334:MET:HG2	2.43	0.42
1:H:298:ALA:O	1:H:302:MET:HG2	2.19	0.42
1:A:28:GLU:OE1	1:A:43:LYS:HD3	2.20	0.42
1:A:230:GLU:OE1	1:A:230:GLU:HA	2.19	0.42
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.90	0.42
1:A:298:ALA:HA	1:D:302:MET:CE	2.35	0.42
1:B:96:ARG:HH11	1:B:227:PRO:HG3	1.84	0.42
1:B:348:LYS:CG	1:B:349:LYS:H	2.32	0.42
1:E:309:GLY:C	1:E:311:TYR:H	2.27	0.42
1:E:327:TYR:CD1	1:E:327:TYR:C	2.97	0.42
1:F:311:TYR:HE2	1:F:330:VAL:HG21	1.85	0.42
1:G:300:ILE:HG22	1:G:341:MET:CB	2.50	0.42
1:H:184:LEU:HD21	1:H:221:LEU:HD11	2.02	0.42
1:I:291:MET:HG2	1:J:291:MET:HE2	2.02	0.42
1:I:348:LYS:CG	1:I:349:LYS:H	2.31	0.42
1:A:136:VAL:HG11	1:A:173:LEU:HD12	2.01	0.42
1:A:212:HIS:NE2	1:D:196:GLU:OE1	2.47	0.42
1:B:95:GLN:O	1:B:96:ARG:C	2.63	0.42
1:D:111:LYS:O	1:D:177:LEU:HD21	2.19	0.42
1:D:118:ASN:HD22	1:D:118:ASN:C	2.28	0.42
1:H:275:LEU:HD12	1:H:275:LEU:HA	1.89	0.42
1:J:28:GLU:OE1	1:J:43:LYS:HD3	2.20	0.42
1:E:148:ASP:O	1:E:152:GLU:HG2	2.19	0.42
1:H:104:ASN:O	1:H:105:TYR:HB3	2.19	0.42
1:I:67:ILE:HG21	1:I:139:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:VAL:O	1:I:111:LYS:NZ	2.47	0.42
1:I:94:HIS:C	1:J:260:GLN:HE22	2.28	0.42
1:I:298:ALA:O	1:I:302:MET:HG2	2.20	0.42
1:J:111:LYS:O	1:J:177:LEU:HD21	2.20	0.42
1:A:255:TYR:CZ	1:A:259:ILE:HD11	2.55	0.42
1:B:238:ASP:HB3	1:B:239:VAL:H	1.51	0.42
1:C:157:ASN:OD1	1:C:162:ARG:HG3	2.20	0.42
1:E:221:LEU:HA	1:E:221:LEU:HD12	1.83	0.42
1:F:104:ASN:O	1:F:105:TYR:HB3	2.20	0.42
1:F:184:LEU:HD21	1:F:221:LEU:HD11	2.01	0.42
1:G:272:VAL:O	1:G:275:LEU:HB2	2.20	0.42
1:I:61:TRP:HZ2	1:I:138:MET:HE1	1.85	0.42
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.94	0.41
1:F:200:LEU:O	1:F:201:GLU:HG3	2.19	0.41
1:J:276:LEU:HD12	1:J:276:LEU:HA	1.83	0.41
1:A:166:ALA:O	1:A:169:LEU:HB3	2.21	0.41
1:B:152:GLU:HB2	1:B:158:ARG:HH12	1.85	0.41
1:G:313:MET:N	1:G:314:ASN:CB	2.83	0.41
1:I:28:GLU:OE2	1:I:143:ILE:HD11	2.20	0.41
1:A:148:ASP:O	1:A:152:GLU:HG2	2.20	0.41
1:A:194:VAL:O	1:A:197:GLU:HB2	2.19	0.41
1:C:152:GLU:HB2	1:C:158:ARG:NH1	2.35	0.41
1:D:152:GLU:HB2	1:D:158:ARG:NH1	2.34	0.41
1:D:229:ARG:HA	1:D:258:THR:HG23	2.03	0.41
1:D:229:ARG:CG	1:D:258:THR:HG23	2.50	0.41
1:D:276:LEU:HD12	1:D:276:LEU:HA	1.83	0.41
1:E:238:ASP:O	1:E:239:VAL:HG22	2.20	0.41
1:G:61:TRP:CD1	1:G:61:TRP:C	2.97	0.41
1:G:327:TYR:N	1:G:328:PRO:HD2	2.35	0.41
1:H:341:MET:O	1:H:344:TYR:HB3	2.20	0.41
1:J:348:LYS:CG	1:J:349:LYS:H	2.32	0.41
1:A:348:LYS:HE2	1:A:349:LYS:N	2.22	0.41
1:B:171:TYR:OH	1:C:14:PRO:HG3	2.20	0.41
1:B:272:VAL:O	1:B:275:LEU:HB2	2.20	0.41
1:D:54:ARG:HG3	1:D:80:PHE:CD1	2.55	0.41
1:E:348:LYS:CE	1:E:349:LYS:H	2.27	0.41
1:F:132:THR:HG23	1:F:132:THR:O	2.20	0.41
1:F:192:ILE:O	1:F:196:GLU:HG2	2.20	0.41
1:G:255:TYR:CZ	1:G:259:ILE:HD11	2.55	0.41
1:A:132:THR:O	1:A:132:THR:HG23	2.20	0.41
1:B:276:LEU:HD12	1:B:276:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:O	1:D:171:TYR:C	2.62	0.41
1:E:24:ARG:HA	1:E:68:HIS:CD2	2.54	0.41
1:H:300:ILE:HG13	1:H:301:PHE:N	2.36	0.41
1:I:132:THR:O	1:I:132:THR:HG23	2.20	0.41
1:B:28:GLU:OE1	1:B:43:LYS:HD3	2.20	0.41
1:C:83:HIS:ND1	1:C:84:PRO:CD	2.76	0.41
1:E:229:ARG:CG	1:E:258:THR:HG23	2.51	0.41
1:F:348:LYS:CG	1:F:349:LYS:H	2.33	0.41
2:F:1351:CL:CL	1:J:168:TYR:OH	2.73	0.41
1:I:309:GLY:C	1:I:311:TYR:N	2.77	0.41
1:B:104:ASN:O	1:B:105:TYR:HB3	2.21	0.41
1:C:202:ARG:N	1:C:203:PRO:HD3	2.36	0.41
1:C:229:ARG:HA	1:C:258:THR:HG21	2.02	0.41
1:C:291:MET:HB3	1:E:290:VAL:CG1	2.50	0.41
1:C:300:ILE:HG22	1:C:341:MET:CG	2.49	0.41
1:D:238:ASP:C	1:D:239:VAL:HG13	2.45	0.41
1:E:170:LEU:O	1:E:171:TYR:C	2.63	0.41
1:F:33:ASN:HB2	1:F:60:THR:HG23	2.02	0.41
1:F:120:HIS:HD2	1:F:191:GLU:OE2	2.03	0.41
1:F:202:ARG:O	1:F:202:ARG:CG	2.68	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.97	0.41
1:C:73:VAL:HG21	1:C:91:LEU:HD21	2.03	0.41
1:C:116:ASP:OD2	1:C:119:LEU:HB3	2.21	0.41
1:E:117:LYS:O	1:E:119:LEU:N	2.51	0.41
1:E:202:ARG:O	1:E:202:ARG:CG	2.69	0.41
1:G:343:VAL:HG12	1:G:343:VAL:O	2.20	0.41
1:H:291:MET:HE1	1:J:291:MET:SD	2.61	0.41
1:I:118:ASN:HD22	1:I:118:ASN:C	2.28	0.41
1:I:348:LYS:HE2	1:I:349:LYS:N	2.25	0.41
1:J:170:LEU:O	1:J:171:TYR:C	2.63	0.41
1:A:6:LEU:HD22	1:A:7:SER:H	1.85	0.41
1:B:307:ILE:CD1	1:B:334:MET:HG2	2.37	0.41
1:C:10:LYS:H	1:C:10:LYS:HD2	1.86	0.41
1:F:275:LEU:HD12	1:F:275:LEU:HA	1.90	0.41
1:G:221:LEU:HD12	1:G:221:LEU:HA	1.80	0.41
1:H:118:ASN:ND2	1:H:119:LEU:N	2.69	0.41
1:I:202:ARG:N	1:I:203:PRO:HD3	2.35	0.41
1:I:327:TYR:CE2	1:J:315:PHE:O	2.74	0.41
1:E:61:TRP:NE1	1:E:138:MET:HE2	2.34	0.41
1:E:275:LEU:HD12	1:E:275:LEU:HA	1.93	0.41
1:G:291:MET:HE2	1:H:291:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:ARG:HD2	1:I:196:GLU:OE1	2.21	0.40
1:G:281:SER:OG	1:H:280:LEU:HD13	2.21	0.40
1:H:113:PHE:CD1	1:H:124:SER:HB3	2.56	0.40
1:A:334:MET:HE1	1:D:310:ILE:HG22	2.03	0.40
1:B:117:LYS:O	1:B:119:LEU:N	2.54	0.40
1:C:118:ASN:HD22	1:C:118:ASN:C	2.29	0.40
1:C:272:VAL:O	1:C:275:LEU:HB2	2.20	0.40
1:D:118:ASN:ND2	1:D:119:LEU:N	2.70	0.40
1:F:61:TRP:HZ2	1:F:138:MET:HE1	1.85	0.40
1:G:61:TRP:HZ2	1:G:138:MET:HE1	1.86	0.40
1:G:118:ASN:HD22	1:G:119:LEU:N	2.19	0.40
1:I:318:MET:HA	1:I:319:PRO:HD2	1.82	0.40
1:I:319:PRO:CB	1:I:320:GLU:HA	2.48	0.40
1:J:331:LEU:HD23	1:J:334:MET:HE2	2.03	0.40
1:A:291:MET:HE3	1:B:290:VAL:HG12	2.03	0.40
1:B:86:VAL:HG13	1:B:107:PHE:CD2	2.57	0.40
1:C:24:ARG:HA	1:C:68:HIS:CD2	2.56	0.40
1:C:82:ILE:HD13	1:C:130:ILE:HD13	2.03	0.40
1:C:237:ARG:HH21	1:C:237:ARG:HB3	1.85	0.40
1:C:255:TYR:CZ	1:C:259:ILE:HD11	2.56	0.40
1:D:221:LEU:HA	1:D:221:LEU:HD12	1.78	0.40
1:E:17:LEU:H	1:E:17:LEU:HD22	1.86	0.40
1:F:168:TYR:OH	1:G:14:PRO:HG2	2.21	0.40
1:G:19:TYR:CZ	1:G:21:GLY:CA	2.97	0.40
1:G:61:TRP:HE1	1:G:138:MET:HE2	1.86	0.40
1:H:313:MET:CA	1:J:311:TYR:HB2	2.49	0.40
1:I:200:LEU:O	1:I:201:GLU:HG3	2.21	0.40
1:I:326:GLY:O	1:I:329:VAL:HB	2.20	0.40
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.74	0.40
1:A:294:LEU:HD11	1:D:294:LEU:HD22	2.03	0.40
1:A:327:TYR:CD1	1:A:327:TYR:C	2.99	0.40
1:C:276:LEU:HD12	1:C:276:LEU:HA	1.86	0.40
1:D:291:MET:HG2	1:E:291:MET:HE2	2.04	0.40
1:E:311:TYR:HE2	1:E:330:VAL:HG21	1.86	0.40
1:G:181:TYR:HB2	1:G:261:ILE:HD13	2.04	0.40
1:H:17:LEU:HD22	1:H:17:LEU:N	2.37	0.40
1:I:118:ASN:ND2	1:I:119:LEU:N	2.68	0.40
1:I:258:THR:HG22	1:I:259:ILE:N	2.37	0.40
1:F:111:LYS:O	1:F:177:LEU:HD21	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLU:OE2	1:E:348:LYS:CA[2_555]	1.99	0.21
1:F:78:GLU:OE1	1:H:202:ARG:NH1[2_546]	2.00	0.20
1:D:38:GLU:OE1	1:H:75:ARG:CD[2_546]	2.05	0.15
1:C:37:GLU:OE2	1:E:348:LYS:N[2_555]	2.11	0.09
1:F:348:LYS:CA	1:I:37:GLU:OE2[2_556]	2.14	0.06

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	327/363 (90%)	284 (87%)	32 (10%)	11 (3%)	3	12
1	B	327/363 (90%)	291 (89%)	28 (9%)	8 (2%)	4	18
1	C	327/363 (90%)	289 (88%)	29 (9%)	9 (3%)	4	15
1	D	327/363 (90%)	289 (88%)	26 (8%)	12 (4%)	2	11
1	E	327/363 (90%)	289 (88%)	25 (8%)	13 (4%)	2	9
1	F	338/363 (93%)	293 (87%)	34 (10%)	11 (3%)	3	13
1	G	338/363 (93%)	292 (86%)	32 (10%)	14 (4%)	2	9
1	H	334/363 (92%)	291 (87%)	32 (10%)	11 (3%)	3	13
1	I	336/363 (93%)	289 (86%)	33 (10%)	14 (4%)	2	9
1	J	332/363 (92%)	291 (88%)	29 (9%)	12 (4%)	2	11
All	All	3313/3630 (91%)	2898 (88%)	300 (9%)	115 (4%)	3	12

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	PRO
1	A	244	GLU
1	A	245	LYS
1	A	348	LYS
1	B	7	SER

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Mol	Chain	Res	Type
1	B	240	PRO
1	B	244	GLU
1	B	245	LYS
1	B	348	LYS
1	C	240	PRO
1	C	244	GLU
1	C	245	LYS
1	C	348	LYS
1	D	240	PRO
1	D	244	GLU
1	D	245	LYS
1	D	348	LYS
1	E	6	LEU
1	E	240	PRO
1	E	244	GLU
1	E	245	LYS
1	E	348	LYS
1	F	7	SER
1	F	240	PRO
1	F	244	GLU
1	F	245	LYS
1	F	348	LYS
1	G	240	PRO
1	G	244	GLU
1	G	245	LYS
1	G	325	TRP
1	G	348	LYS
1	H	240	PRO
1	H	244	GLU
1	H	245	LYS
1	H	322	ARG
1	H	324	LYS
1	H	348	LYS
1	I	240	PRO
1	I	244	GLU
1	I	245	LYS
1	I	319	PRO
1	I	324	LYS
1	I	348	LYS
1	J	240	PRO
1	J	244	GLU
1	J	245	LYS

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Mol	Chain	Res	Type
1	J	348	LYS
1	A	7	SER
1	A	238	ASP
1	D	238	ASP
1	E	7	SER
1	E	25	GLU
1	E	238	ASP
1	E	287	THR
1	G	7	SER
1	G	238	ASP
1	G	313	MET
1	G	317	TYR
1	H	238	ASP
1	I	238	ASP
1	I	323	TRP
1	B	238	ASP
1	C	25	GLU
1	C	238	ASP
1	D	25	GLU
1	D	287	THR
1	F	25	GLU
1	F	118	ASN
1	F	238	ASP
1	I	320	GLU
1	J	238	ASP
1	J	314	ASN
1	J	327	TYR
1	A	25	GLU
1	A	239	VAL
1	B	25	GLU
1	B	239	VAL
1	C	239	VAL
1	D	239	VAL
1	E	95	GLN
1	E	239	VAL
1	F	239	VAL
1	F	344	TYR
1	G	239	VAL
1	G	315	PHE
1	H	118	ASN
1	H	239	VAL
1	I	25	GLU

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Mol	Chain	Res	Type
1	I	239	VAL
1	J	25	GLU
1	J	118	ASN
1	J	239	VAL
1	J	312	GLY
1	A	202	ARG
1	A	344	TYR
1	C	327	TYR
1	D	202	ARG
1	D	344	TYR
1	E	202	ARG
1	E	344	TYR
1	G	25	GLU
1	G	202	ARG
1	H	202	ARG
1	H	344	TYR
1	J	344	TYR
1	A	118	ASN
1	C	344	TYR
1	D	118	ASN
1	F	202	ARG
1	G	312	GLY
1	I	344	TYR
1	I	243	ILE
1	D	243	ILE
1	I	202	ARG

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	311/341 (91%)	269 (86%)	42 (14%)	4	12
1	B	309/341 (91%)	262 (85%)	47 (15%)	3	9
1	C	309/341 (91%)	265 (86%)	44 (14%)	3	11
1	D	310/341 (91%)	267 (86%)	43 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	310/341 (91%)	268 (86%)	42 (14%)	4	12
1	F	312/341 (92%)	273 (88%)	39 (12%)	4	15
1	G	311/341 (91%)	268 (86%)	43 (14%)	3	12
1	H	311/341 (91%)	266 (86%)	45 (14%)	3	10
1	I	311/341 (91%)	270 (87%)	41 (13%)	4	13
1	J	312/341 (92%)	268 (86%)	44 (14%)	3	11
All	All	3106/3410 (91%)	2676 (86%)	430 (14%)	3	12

All (430) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	SER
1	A	10	LYS
1	A	17	LEU
1	A	22	LYS
1	A	36	ILE
1	A	40	ARG
1	A	47	VAL
1	A	56	SER
1	A	60	THR
1	A	95	GLN
1	A	96	ARG
1	A	99	VAL
1	A	118	ASN
1	A	121	GLU
1	A	122	LEU
1	A	123	GLU
1	A	143	ILE
1	A	152	GLU
1	A	165	ARG
1	A	199	VAL
1	A	200	LEU
1	A	202	ARG
1	A	206	GLU
1	A	207	THR
1	A	209	GLN
1	A	213	GLN
1	A	218	LEU
1	A	222	ARG

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Mol	Chain	Res	Type
1	A	228	LEU
1	A	232	LEU
1	A	235	LEU
1	A	237	ARG
1	A	238	ASP
1	A	239	VAL
1	A	258	THR
1	A	267	THR
1	A	275	LEU
1	A	283	VAL
1	A	287	THR
1	A	288	ASN
1	A	297	ILE
1	B	10	LYS
1	B	17	LEU
1	B	22	LYS
1	B	28	GLU
1	B	36	ILE
1	B	40	ARG
1	B	47	VAL
1	B	50	VAL
1	B	56	SER
1	B	60	THR
1	B	67	ILE
1	B	95	GLN
1	B	96	ARG
1	B	99	VAL
1	B	118	ASN
1	B	121	GLU
1	B	122	LEU
1	B	123	GLU
1	B	143	ILE
1	B	152	GLU
1	B	165	ARG
1	B	198	GLU
1	B	200	LEU
1	B	202	ARG
1	B	206	GLU
1	B	207	THR
1	B	209	GLN
1	B	213	GLN
1	B	218	LEU

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Mol	Chain	Res	Type
1	B	222	ARG
1	B	232	LEU
1	B	234	SER
1	B	235	LEU
1	B	237	ARG
1	B	238	ASP
1	B	239	VAL
1	B	254	VAL
1	B	258	THR
1	B	260	GLN
1	B	266	GLU
1	B	267	THR
1	B	275	LEU
1	B	283	VAL
1	B	287	THR
1	B	288	ASN
1	B	297	ILE
1	B	327	TYR
1	C	10	LYS
1	C	17	LEU
1	C	22	LYS
1	C	36	ILE
1	C	40	ARG
1	C	47	VAL
1	C	60	THR
1	C	95	GLN
1	C	96	ARG
1	C	99	VAL
1	C	118	ASN
1	C	121	GLU
1	C	122	LEU
1	C	123	GLU
1	C	143	ILE
1	C	152	GLU
1	C	165	ARG
1	C	198	GLU
1	C	200	LEU
1	C	202	ARG
1	C	206	GLU
1	C	207	THR
1	C	209	GLN
1	C	213	GLN

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Mol	Chain	Res	Type
1	C	215	LYS
1	C	218	LEU
1	C	222	ARG
1	C	228	LEU
1	C	232	LEU
1	C	234	SER
1	C	235	LEU
1	C	237	ARG
1	C	238	ASP
1	C	239	VAL
1	C	254	VAL
1	C	258	THR
1	C	260	GLN
1	C	267	THR
1	C	275	LEU
1	C	283	VAL
1	C	287	THR
1	C	288	ASN
1	C	297	ILE
1	C	330	VAL
1	D	6	LEU
1	D	7	SER
1	D	10	LYS
1	D	17	LEU
1	D	22	LYS
1	D	36	ILE
1	D	40	ARG
1	D	47	VAL
1	D	50	VAL
1	D	60	THR
1	D	67	ILE
1	D	95	GLN
1	D	96	ARG
1	D	99	VAL
1	D	118	ASN
1	D	121	GLU
1	D	122	LEU
1	D	123	GLU
1	D	143	ILE
1	D	152	GLU
1	D	165	ARG
1	D	198	GLU

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Mol	Chain	Res	Type
1	D	200	LEU
1	D	202	ARG
1	D	206	GLU
1	D	207	THR
1	D	209	GLN
1	D	215	LYS
1	D	218	LEU
1	D	222	ARG
1	D	232	LEU
1	D	234	SER
1	D	235	LEU
1	D	237	ARG
1	D	238	ASP
1	D	239	VAL
1	D	258	THR
1	D	267	THR
1	D	275	LEU
1	D	283	VAL
1	D	287	THR
1	D	288	ASN
1	D	297	ILE
1	E	7	SER
1	E	10	LYS
1	E	17	LEU
1	E	22	LYS
1	E	36	ILE
1	E	40	ARG
1	E	47	VAL
1	E	50	VAL
1	E	60	THR
1	E	67	ILE
1	E	95	GLN
1	E	96	ARG
1	E	118	ASN
1	E	121	GLU
1	E	122	LEU
1	E	123	GLU
1	E	143	ILE
1	E	152	GLU
1	E	165	ARG
1	E	198	GLU
1	E	200	LEU

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Mol	Chain	Res	Type
1	E	202	ARG
1	E	206	GLU
1	E	207	THR
1	E	209	GLN
1	E	213	GLN
1	E	218	LEU
1	E	222	ARG
1	E	232	LEU
1	E	235	LEU
1	E	237	ARG
1	E	238	ASP
1	E	239	VAL
1	E	258	THR
1	E	260	GLN
1	E	267	THR
1	E	275	LEU
1	E	283	VAL
1	E	287	THR
1	E	288	ASN
1	E	297	ILE
1	E	327	TYR
1	F	6	LEU
1	F	10	LYS
1	F	17	LEU
1	F	22	LYS
1	F	36	ILE
1	F	40	ARG
1	F	47	VAL
1	F	67	ILE
1	F	95	GLN
1	F	96	ARG
1	F	118	ASN
1	F	121	GLU
1	F	122	LEU
1	F	123	GLU
1	F	143	ILE
1	F	152	GLU
1	F	165	ARG
1	F	200	LEU
1	F	202	ARG
1	F	206	GLU
1	F	207	THR

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Mol	Chain	Res	Type
1	F	209	GLN
1	F	218	LEU
1	F	222	ARG
1	F	232	LEU
1	F	235	LEU
1	F	237	ARG
1	F	238	ASP
1	F	239	VAL
1	F	258	THR
1	F	260	GLN
1	F	266	GLU
1	F	267	THR
1	F	275	LEU
1	F	283	VAL
1	F	287	THR
1	F	288	ASN
1	F	297	ILE
1	F	327	TYR
1	G	10	LYS
1	G	17	LEU
1	G	22	LYS
1	G	36	ILE
1	G	40	ARG
1	G	47	VAL
1	G	50	VAL
1	G	56	SER
1	G	60	THR
1	G	95	GLN
1	G	96	ARG
1	G	118	ASN
1	G	121	GLU
1	G	122	LEU
1	G	123	GLU
1	G	143	ILE
1	G	152	GLU
1	G	165	ARG
1	G	200	LEU
1	G	202	ARG
1	G	206	GLU
1	G	207	THR
1	G	209	GLN
1	G	213	GLN

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Mol	Chain	Res	Type
1	G	215	LYS
1	G	218	LEU
1	G	222	ARG
1	G	228	LEU
1	G	232	LEU
1	G	234	SER
1	G	235	LEU
1	G	237	ARG
1	G	238	ASP
1	G	239	VAL
1	G	258	THR
1	G	267	THR
1	G	275	LEU
1	G	283	VAL
1	G	287	THR
1	G	288	ASN
1	G	296	ILE
1	G	297	ILE
1	G	327	TYR
1	H	7	SER
1	H	10	LYS
1	H	17	LEU
1	H	22	LYS
1	H	40	ARG
1	H	47	VAL
1	H	50	VAL
1	H	56	SER
1	H	60	THR
1	H	95	GLN
1	H	96	ARG
1	H	118	ASN
1	H	121	GLU
1	H	122	LEU
1	H	123	GLU
1	H	143	ILE
1	H	152	GLU
1	H	165	ARG
1	H	198	GLU
1	H	200	LEU
1	H	202	ARG
1	H	206	GLU
1	H	207	THR

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Mol	Chain	Res	Type
1	H	209	GLN
1	H	213	GLN
1	H	218	LEU
1	H	222	ARG
1	H	228	LEU
1	H	232	LEU
1	H	234	SER
1	H	235	LEU
1	H	237	ARG
1	H	238	ASP
1	H	239	VAL
1	H	254	VAL
1	H	258	THR
1	H	260	GLN
1	H	267	THR
1	H	275	LEU
1	H	283	VAL
1	H	287	THR
1	H	288	ASN
1	H	296	ILE
1	H	297	ILE
1	H	327	TYR
1	I	10	LYS
1	I	17	LEU
1	I	22	LYS
1	I	36	ILE
1	I	39	PHE
1	I	40	ARG
1	I	47	VAL
1	I	50	VAL
1	I	60	THR
1	I	95	GLN
1	I	96	ARG
1	I	118	ASN
1	I	121	GLU
1	I	122	LEU
1	I	123	GLU
1	I	143	ILE
1	I	152	GLU
1	I	165	ARG
1	I	198	GLU
1	I	200	LEU

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Mol	Chain	Res	Type
1	I	202	ARG
1	I	206	GLU
1	I	207	THR
1	I	209	GLN
1	I	218	LEU
1	I	222	ARG
1	I	228	LEU
1	I	232	LEU
1	I	235	LEU
1	I	237	ARG
1	I	238	ASP
1	I	239	VAL
1	I	258	THR
1	I	260	GLN
1	I	267	THR
1	I	275	LEU
1	I	283	VAL
1	I	288	ASN
1	I	296	ILE
1	I	297	ILE
1	I	327	TYR
1	J	6	LEU
1	J	7	SER
1	J	10	LYS
1	J	22	LYS
1	J	28	GLU
1	J	36	ILE
1	J	40	ARG
1	J	47	VAL
1	J	56	SER
1	J	60	THR
1	J	67	ILE
1	J	95	GLN
1	J	96	ARG
1	J	118	ASN
1	J	121	GLU
1	J	122	LEU
1	J	123	GLU
1	J	143	ILE
1	J	152	GLU
1	J	165	ARG
1	J	200	LEU

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Mol	Chain	Res	Type
1	J	202	ARG
1	J	206	GLU
1	J	207	THR
1	J	209	GLN
1	J	213	GLN
1	J	218	LEU
1	J	222	ARG
1	J	232	LEU
1	J	235	LEU
1	J	237	ARG
1	J	238	ASP
1	J	239	VAL
1	J	258	THR
1	J	260	GLN
1	J	267	THR
1	J	269	ARG
1	J	275	LEU
1	J	283	VAL
1	J	287	THR
1	J	288	ASN
1	J	296	ILE
1	J	297	ILE
1	J	327	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	118	ASN
1	A	120	HIS
1	A	213	GLN
1	A	217	ASN
1	B	74	GLN
1	B	94	HIS
1	B	95	GLN
1	B	118	ASN
1	B	120	HIS
1	B	213	GLN
1	B	217	ASN
1	B	260	GLN
1	C	118	ASN
1	C	120	HIS

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Mol	Chain	Res	Type
1	C	212	HIS
1	C	213	GLN
1	C	217	ASN
1	C	260	GLN
1	D	74	GLN
1	D	94	HIS
1	D	118	ASN
1	D	120	HIS
1	D	213	GLN
1	D	217	ASN
1	D	260	GLN
1	E	94	HIS
1	E	118	ASN
1	E	120	HIS
1	E	213	GLN
1	E	217	ASN
1	E	260	GLN
1	F	74	GLN
1	F	94	HIS
1	F	118	ASN
1	F	120	HIS
1	F	213	GLN
1	F	217	ASN
1	F	260	GLN
1	G	94	HIS
1	G	118	ASN
1	G	120	HIS
1	G	213	GLN
1	G	217	ASN
1	G	260	GLN
1	H	94	HIS
1	H	118	ASN
1	H	120	HIS
1	H	213	GLN
1	H	217	ASN
1	H	260	GLN
1	I	74	GLN
1	I	94	HIS
1	I	118	ASN
1	I	120	HIS
1	I	217	ASN
1	I	260	GLN

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Mol	Chain	Res	Type
1	J	74	GLN
1	J	94	HIS
1	J	118	ASN
1	J	120	HIS
1	J	212	HIS
1	J	213	GLN
1	J	217	ASN
1	J	260	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 28 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 ⓘ

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	331/363 (91%)	0.36	10 (3%)	52	43	43, 68, 98, 103	0
1	B	331/363 (91%)	0.47	18 (5%)	31	24	43, 68, 98, 103	0
1	C	331/363 (91%)	0.38	6 (1%)	67	59	43, 68, 98, 103	0
1	D	331/363 (91%)	0.55	15 (4%)	38	30	43, 68, 98, 103	0
1	E	331/363 (91%)	0.44	9 (2%)	56	47	43, 68, 98, 103	0
1	F	342/363 (94%)	0.42	9 (2%)	57	48	43, 69, 98, 103	0
1	G	342/363 (94%)	0.49	18 (5%)	32	25	43, 69, 98, 103	0
1	H	338/363 (93%)	0.59	18 (5%)	32	25	43, 68, 98, 103	0
1	I	340/363 (93%)	0.36	6 (1%)	67	59	43, 69, 98, 103	0
1	J	336/363 (92%)	0.35	7 (2%)	63	54	43, 68, 98, 103	0
All	All	3353/3630 (92%)	0.44	116 (3%)	47	38	43, 68, 98, 103	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	282	SER	5.3
1	H	231	VAL	5.3
1	E	284	SER	4.7
1	D	312	GLY	4.2
1	H	285	ASN	4.1
1	H	284	SER	3.9
1	C	326	GLY	3.9
1	D	205	LYS	3.7
1	D	343	VAL	3.5
1	H	286	LYS	3.5
1	H	283	VAL	3.5
1	A	96	ARG	3.3
1	F	199	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	238	ASP	3.2
1	I	245	LYS	3.1
1	B	248	VAL	3.1
1	E	305	THR	3.1
1	H	279	TYR	3.0
1	B	282	SER	3.0
1	C	207	THR	3.0
1	E	308	ALA	3.0
1	G	118	ASN	2.9
1	H	225	ILE	2.9
1	H	36	ILE	2.9
1	D	26	ASP	2.9
1	G	348	LYS	2.9
1	G	26	ASP	2.9
1	G	201	GLU	2.8
1	B	5	ARG	2.8
1	F	205	LYS	2.8
1	C	241	PRO	2.8
1	D	308	ALA	2.7
1	J	308	ALA	2.7
1	E	285	ASN	2.7
1	H	278	VAL	2.7
1	H	96	ARG	2.7
1	B	144	GLY	2.7
1	A	327	TYR	2.6
1	C	343	VAL	2.6
1	A	312	GLY	2.6
1	B	204	GLU	2.6
1	D	284	SER	2.6
1	B	236	TYR	2.6
1	G	208	VAL	2.6
1	G	318	MET	2.6
1	G	284	SER	2.5
1	J	314	ASN	2.5
1	J	282	SER	2.5
1	D	348	LYS	2.5
1	H	280	LEU	2.4
1	H	35	SER	2.4
1	F	223	LYS	2.4
1	G	182	PHE	2.4
1	B	277	ASP	2.4
1	C	312	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	312	GLY	2.4
1	A	246	GLU	2.4
1	B	21	GLY	2.4
1	G	193	ASP	2.4
1	C	284	SER	2.4
1	H	313	MET	2.4
1	D	304	LEU	2.4
1	G	243	ILE	2.3
1	I	26	ASP	2.3
1	F	337	ILE	2.3
1	E	309	GLY	2.3
1	F	245	LYS	2.3
1	H	281	SER	2.3
1	G	241	PRO	2.3
1	H	237	ARG	2.3
1	B	208	VAL	2.3
1	D	38	GLU	2.2
1	A	284	SER	2.2
1	J	309	GLY	2.2
1	D	25	GLU	2.2
1	E	266	GLU	2.2
1	G	197	GLU	2.2
1	A	237	ARG	2.2
1	D	330	VAL	2.2
1	G	281	SER	2.2
1	G	200	LEU	2.2
1	I	243	ILE	2.2
1	B	241	PRO	2.2
1	H	203	PRO	2.2
1	I	145	ASP	2.2
1	A	256	ASP	2.1
1	B	26	ASP	2.1
1	F	326	GLY	2.1
1	I	345	PHE	2.1
1	F	339	VAL	2.1
1	I	146	VAL	2.1
1	B	224	THR	2.1
1	G	312	GLY	2.1
1	J	315	PHE	2.1
1	J	8	ALA	2.1
1	B	243	ILE	2.1
1	D	243	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	152	GLU	2.1
1	A	119	LEU	2.1
1	G	345	PHE	2.1
1	H	8	ALA	2.1
1	J	220	GLU	2.1
1	D	291	MET	2.1
1	A	270	ASP	2.1
1	B	96	ARG	2.1
1	D	71	ASP	2.1
1	F	317	TYR	2.1
1	A	302	MET	2.0
1	B	239	VAL	2.0
1	D	196	GLU	2.0
1	E	349	LYS	2.0
1	G	245	LYS	2.0
1	B	93	VAL	2.0
1	E	199	VAL	2.0
1	B	8	ALA	2.0
1	G	278	VAL	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
3	MG	J	1350	1/1	0.76	0.23	61,61,61,61	0
3	MG	D	1353	1/1	0.81	0.21	65,65,65,65	0
3	MG	J	1352	1/1	0.84	0.45	63,63,63,63	0
3	MG	D	1352	1/1	0.85	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	J	1351	1/1	0.86	0.18	43,43,43,43	0
3	MG	F	1350	1/1	0.86	0.15	55,55,55,55	0
3	MG	C	1350	1/1	0.88	0.16	43,43,43,43	0
3	MG	D	1355	1/1	0.89	0.21	56,56,56,56	0
3	MG	F	1352	1/1	0.89	0.30	46,46,46,46	0
3	MG	F	1353	1/1	0.89	0.17	45,45,45,45	0
3	MG	G	1353	1/1	0.91	0.10	43,43,43,43	0
3	MG	G	1354	1/1	0.91	0.26	50,50,50,50	0
3	MG	H	1350	1/1	0.91	0.37	54,54,54,54	0
3	MG	D	1356	1/1	0.92	0.20	46,46,46,46	0
3	MG	C	1351	1/1	0.92	0.17	38,38,38,38	0
3	MG	G	1352	1/1	0.93	0.18	44,44,44,44	0
3	MG	B	1351	1/1	0.94	0.32	56,56,56,56	0
3	MG	D	1354	1/1	0.94	0.30	55,55,55,55	0
2	CL	F	1351	1/1	0.95	0.06	61,61,61,61	0
3	MG	A	1351	1/1	0.95	0.13	47,47,47,47	0
2	CL	B	1350	1/1	0.95	0.05	68,68,68,68	0
2	CL	D	1351	1/1	0.95	0.07	59,59,59,59	0
3	MG	A	1352	1/1	0.96	0.14	35,35,35,35	0
3	MG	E	1350	1/1	0.96	0.35	56,56,56,56	0
2	CL	G	1351	1/1	0.97	0.04	69,69,69,69	0
2	CL	A	1350	1/1	0.97	0.04	50,50,50,50	0
2	CL	G	1350	1/1	0.98	0.03	47,47,47,47	0
2	CL	D	1350	1/1	0.99	0.04	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.