



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 AM GMT

PDB ID : 2IUB
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.; Nord-
lund, 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

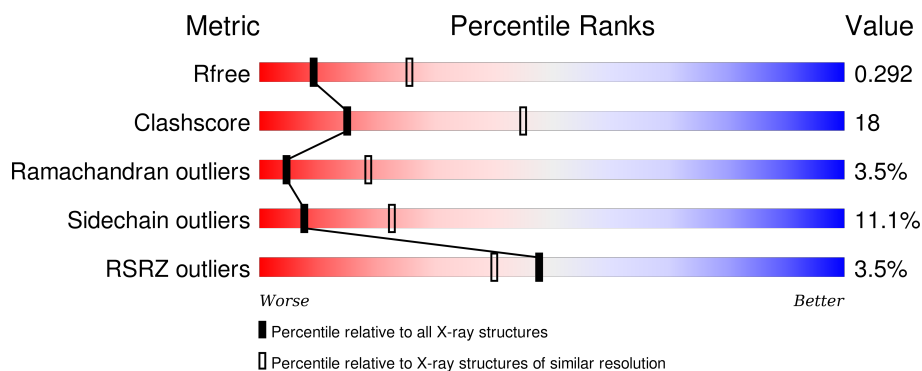
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>55%</div> <div>31%</div> <div>• • 9%</div> </div>
1	B	363	<div> <div>4%</div> <div>54%</div> <div>30%</div> <div>6% • 9%</div> </div>
1	C	363	<div> <div>4%</div> <div>55%</div> <div>31%</div> <div>5% • 9%</div> </div>
1	D	363	<div> <div>3%</div> <div>59%</div> <div>27%</div> <div>• • 9%</div> </div>
1	E	363	<div> <div>2%</div> <div>57%</div> <div>27%</div> <div>5% • 9%</div> </div>

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	1351	-	-	-	X
3	MG	B	1351	-	-	-	X
3	MG	C	1351	-	-	-	X
3	MG	D	1353	-	-	-	X
3	MG	D	1354	-	-	-	X
3	MG	D	1356	-	-	-	X
3	MG	E	1350	-	-	-	X
3	MG	F	1350	-	-	-	X
3	MG	F	1352	-	-	-	X
3	MG	F	1353	-	-	-	X
3	MG	G	1352	-	-	-	X
3	MG	G	1354	-	-	-	X
3	MG	H	1350	-	-	-	X
3	MG	J	1350	-	-	-	X
3	MG	J	1351	-	-	-	X
3	MG	J	1352	-	-	-	X

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 (three-letter code: CL) (formula: Cl).

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

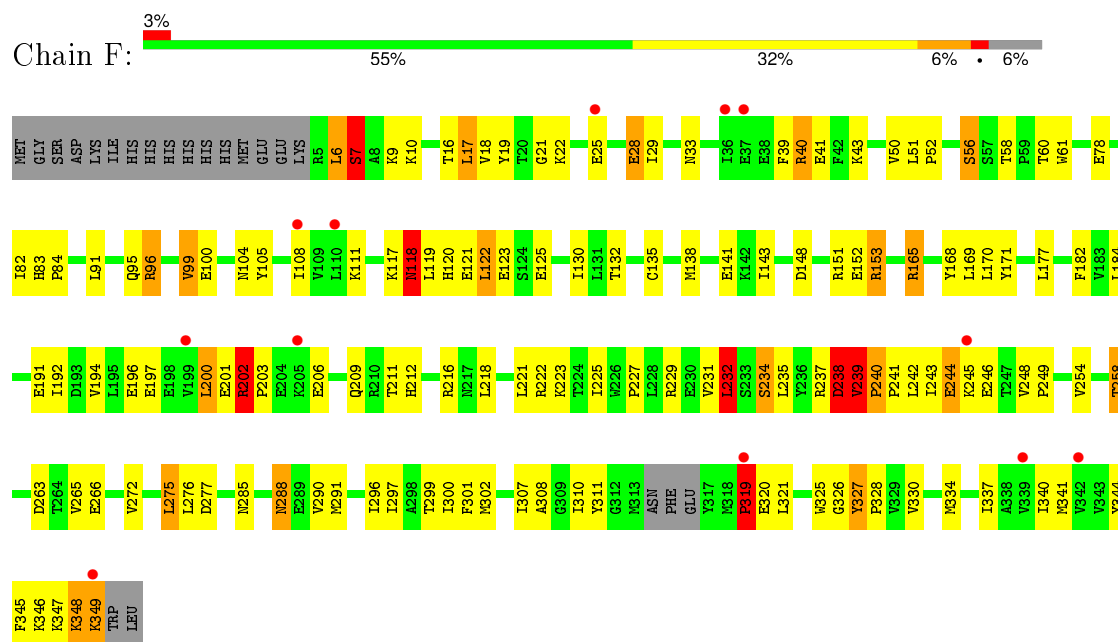
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	3	Total O 3 3	0	0
4	C	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	2	Total O 2 2	0	0

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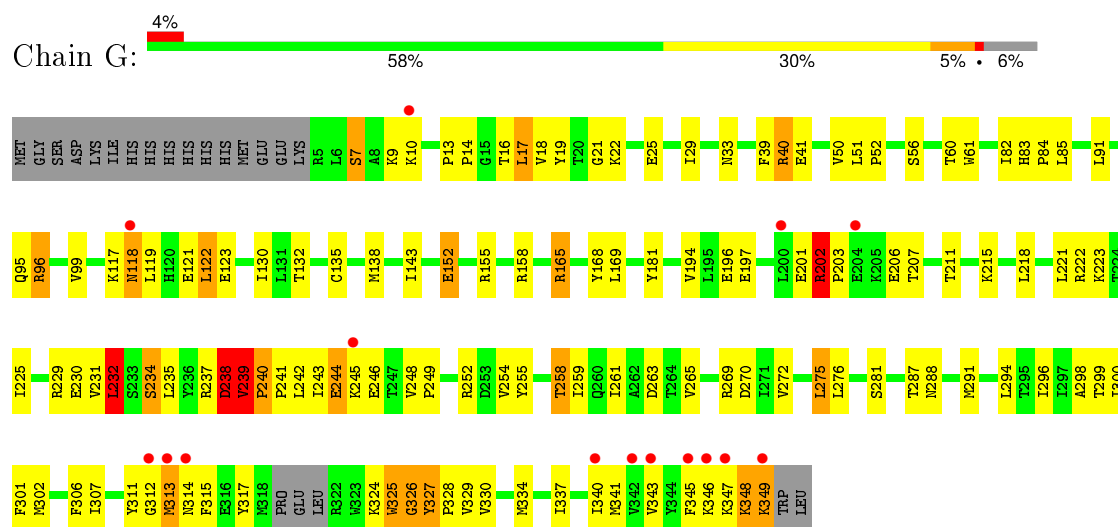
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	2	Total	O	0	0
			2	2		

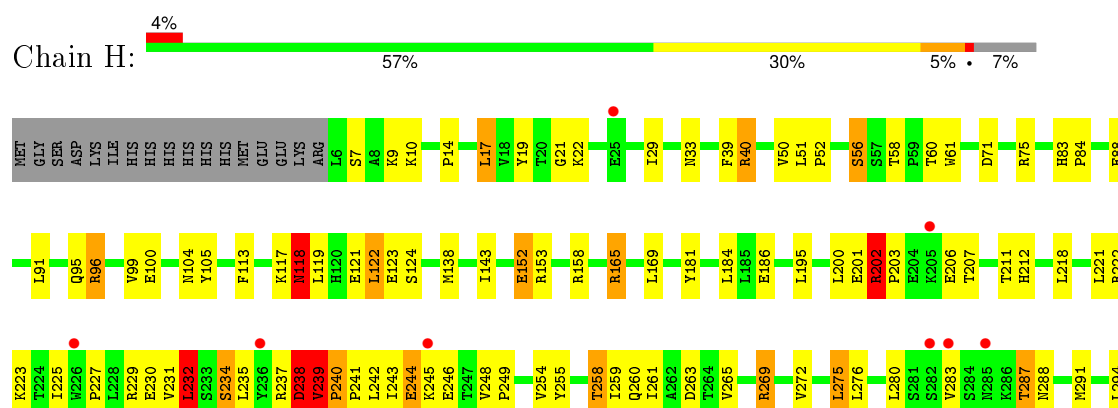
• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

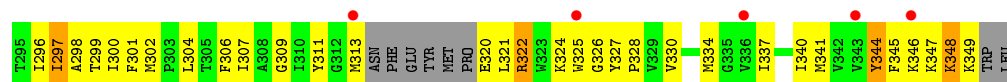


• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

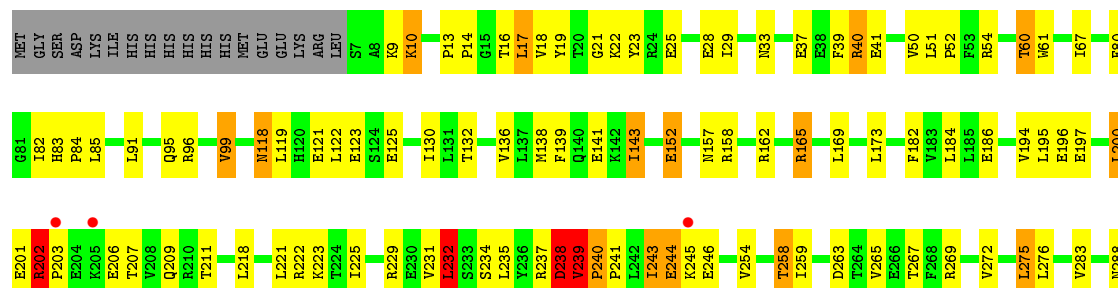


• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

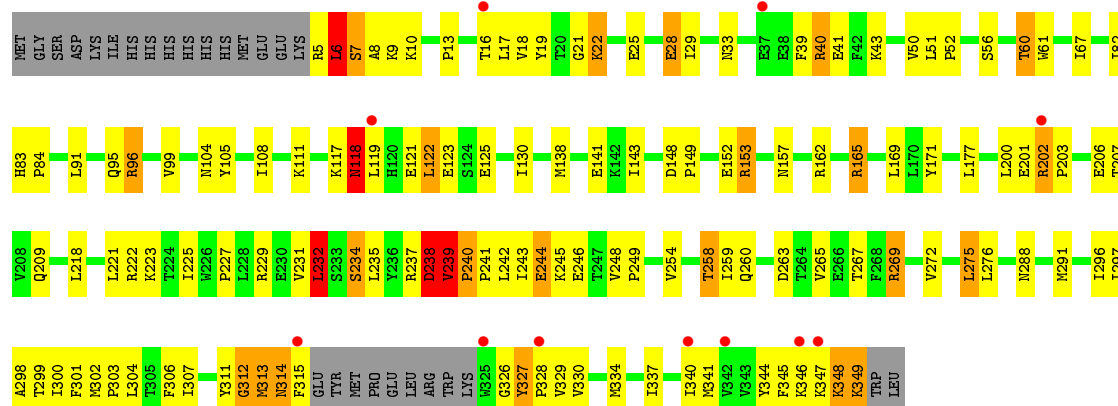




• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN



• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN



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 29.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.90) 90.3 (29.82-2.90)	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 , 0.292	Depositor DCC
R_{free} test set	4921 reflections (5.29%)	DCC
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 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 97917 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.81	1/2792 (0.0%)	0.81	4/3783 (0.1%)
1	B	0.84	0/2784	0.81	4/3773 (0.1%)
1	C	0.85	1/2782 (0.0%)	0.81	5/3770 (0.1%)
1	D	0.84	1/2786 (0.0%)	0.82	4/3776 (0.1%)
1	E	0.84	1/2786 (0.0%)	0.90	6/3776 (0.2%)
1	F	0.84	4/2849 (0.1%)	0.85	5/3861 (0.1%)
1	G	0.85	1/2846 (0.0%)	0.84	6/3858 (0.2%)
1	H	0.88	2/2823 (0.1%)	0.84	4/3826 (0.1%)
1	I	0.84	0/2833	0.83	5/3841 (0.1%)
1	J	0.85	0/2819	0.95	9/3819 (0.2%)
All	All	0.84	11/28100 (0.0%)	0.85	52/38083 (0.1%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	135	CYS	CB-SG	-7.94	1.68	1.82
1	E	100	GLU	CG-CD	6.40	1.61	1.51
1	C	123	GLU	CG-CD	5.63	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	100	GLU	CG-CD	5.57	1.60	1.51
1	H	88	GLU	CG-CD	-5.53	1.43	1.51
1	A	100	GLU	CG-CD	5.51	1.60	1.51
1	F	135	CYS	CB-SG	-5.32	1.73	1.81
1	H	287	THR	N-CA	5.31	1.56	1.46
1	F	326	GLY	CA-C	5.30	1.60	1.51
1	D	135	CYS	CB-SG	-5.22	1.73	1.81
1	F	266	GLU	CG-CD	5.15	1.59	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	J	269	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	J	269	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	E	269	ARG	NE-CZ-NH1	15.27	127.94	120.30
1	J	6	LEU	CA-CB-CG	8.43	134.70	115.30
1	J	269	ARG	CD-NE-CZ	7.88	134.63	123.60
1	E	269	ARG	CD-NE-CZ	7.24	133.74	123.60
1	I	269	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	B	269	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	D	232	LEU	CA-CB-CG	-6.79	99.67	115.30
1	B	232	LEU	CA-CB-CG	-6.78	99.72	115.30
1	F	153	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	F	232	LEU	CA-CB-CG	-6.66	99.98	115.30
1	I	232	LEU	CA-CB-CG	-6.62	100.09	115.30
1	J	122	LEU	CA-CB-CG	6.55	130.36	115.30
1	G	232	LEU	CA-CB-CG	-6.53	100.27	115.30
1	D	122	LEU	CA-CB-CG	6.44	130.12	115.30
1	H	269	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	6	LEU	CA-CB-CG	6.32	129.83	115.30
1	F	319	PRO	N-CA-CB	6.30	110.86	103.30
1	A	269	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	B	269	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	E	232	LEU	CA-CB-CG	-6.21	101.01	115.30
1	D	269	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	B	122	LEU	CA-CB-CG	6.04	129.20	115.30
1	I	312	GLY	N-CA-C	-5.91	98.32	113.10
1	E	122	LEU	CA-CB-CG	5.89	128.84	115.30
1	G	122	LEU	CA-CB-CG	5.87	128.81	115.30
1	J	232	LEU	CA-CB-CG	-5.87	101.80	115.30
1	H	122	LEU	CA-CB-CG	5.67	128.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	F	99	VAL	CB-CA-C	-5.61	100.74	111.40
1	I	99	VAL	CB-CA-C	-5.61	100.75	111.40
1	I	269	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	232	LEU	CA-CB-CG	-5.57	102.48	115.30
1	J	153	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	H	232	LEU	CA-CB-CG	-5.50	102.64	115.30
1	A	232	LEU	CA-CB-CG	-5.49	102.67	115.30
1	C	122	LEU	CA-CB-CG	5.47	127.89	115.30
1	F	122	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	122	LEU	CA-CB-CG	5.39	127.71	115.30
1	G	325	TRP	N-CA-C	-5.33	96.62	111.00
1	C	330	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	H	325	TRP	C-N-CA	5.28	133.39	122.30
1	E	5	ARG	C-N-CA	5.24	134.80	121.70
1	C	269	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	G	269	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	J	312	GLY	N-CA-C	5.16	126.00	113.10
1	C	269	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	G	155	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	J	313	MET	N-CA-C	5.02	124.56	111.00
1	G	324	LYS	N-CA-C	5.02	124.54	111.00

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	108	0
1	B	2728	0	2779	117	0
1	C	2726	0	2778	110	2
1	D	2730	0	2786	93	1
1	E	2730	0	2786	102	2
1	F	2793	0	2826	119	2
1	G	2790	0	2820	106	0
1	H	2767	0	2808	114	2
1	I	2776	0	2808	128	1
1	J	2763	0	2815	116	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	0	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	2	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	980	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 (980) 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:I:320:GLU:CB	1:I:321:LEU:HA	1.72	1.19
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:B:165:ARG:NH1	1:B:243:ILE:HD13	1.70	1.06
1:F:311:TYR:HD2	1:I:313:MET:HE2	1.16	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:G:165:ARG:HH12	1:G:243:ILE:HD13	0.88	1.01
1:A:240:PRO:HB2	1:A:241:PRO:CD	1.89	1.01
1:H:321:LEU:HA	1:H:322:ARG:CB	1.89	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:F:311:TYR:CD2	1:I:313:MET:HE2	1.97	0.98
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: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
1:I:244:GLU:O	1:I:246:GLU:N	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:H:237:ARG:NH2	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:NH2	1:B:237:ARG:HB2	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:HB2	1:F:237:ARG:NH2	1.84	0.91
1:J:237:ARG:HB2	1:J:237:ARG:NH2	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:NH2	1:D:237:ARG:HB2	1.89	0.88
1:I:237:ARG:NH2	1:I:237:ARG:HB2	1.89	0.87
1:A:244:GLU:O	1:A:246:GLU:N	2.07	0.87
1:F:99:VAL:HG22	1:F:231:VAL:HG13	1.57	0.87
1:C:244:GLU:O	1:C:246:GLU:N	2.07	0.87
1:C:237:ARG:HB2	1:C:237:ARG:NH2	1.89	0.86
1:F:308:ALA:HA	1:I:313:MET:HE3	1.57	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:D:99:VAL:HG22	1:D:231:VAL:HG13	1.55	0.86
1:D:240:PRO:HB2	1:D:241:PRO:HD2	1.56	0.86
1:B:244:GLU:O	1:B:246:GLU:N	2.09	0.86
1:G:237:ARG:NH2	1:G:237:ARG:HB2	1.89	0.86
1:D:244:GLU:O	1:D:246:GLU:N	2.09	0.85
1:F:311:TYR:HD2	1:I:313:MET:CE	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:348:LYS:HE2	1:A:349:LYS:H	1.43	0.83
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.61	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:348:LYS:HE2	1:C:349:LYS:H	1.44	0.82
1:C:19:TYR:CZ	1:C:21:GLY:HA3	2.14	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:C:240:PRO:HB2	1:C:241:PRO:HD2	1.61	0.81
1:B:99:VAL:CG2	1:B:231:VAL:HG13	2.11	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:HH21	1:E:237:ARG:HB2	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:240:PRO:HB2	1:H:241:PRO:HD2	1.63	0.80
1:B:99:VAL:HG22	1:B:231:VAL:HG13	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: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:I:337:ILE:HA	1:I:340:ILE:HG12	1.66	0.78
1:H:348:LYS:HE2	1:H:349:LYS:H	1.47	0.78
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:HH21	1:A:237:ARG:HB2	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: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:J:237:ARG:HH21	1:J:237:ARG:HB2	1.49	0.76
1:D:9:LYS:O	1:D:9:LYS:HG3	1.85	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:F:311:TYR:CD2	1:I:313:MET:CE	2.66	0.76
1:H:313:MET:C	1:J:311:TYR:HB3	2.06	0.75
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:237:ARG:HB2	1:H:237:ARG:HH21	1.52	0.75
1:H:99:VAL:CG2	1:H:231:VAL:HG13	2.16	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:F:237:ARG:HH21	1:F:237:ARG:CB	2.00	0.74
1:A:99:VAL:HG22	1:A:231:VAL:HG13	1.68	0.74
1:A:337:ILE:HA	1:A:340:ILE:HG12	1.69	0.74
1:A:253:ASP:OD1	4:A:2002:HOH:O	2.05	0.74
1:A:29:ILE:HG21	1:A:50:VAL:HG11	1.70	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:D:201:GLU:C	1:D:203:PRO:HD3	2.08	0.74
1:F:61:TRP:HB2	1:F:169:LEU:HD21	1.69	0.74
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:H:313:MET:HB3	1:J:311:TYR:CD2	2.24	0.73
1:E:99:VAL:HG22	1:E:231:VAL:HG13	1.70	0.73
1:H:201:GLU:C	1:H:203:PRO:HD3	2.09	0.73
1:F:337:ILE:HA	1:F:340:ILE:HG12	1.70	0.73
1:E:201:GLU:C	1:E:203:PRO:HD3	2.09	0.72
1:H:237:ARG:CB	1:H:237:ARG:HH21	2.02	0.72
1:B:40:ARG:HB2	1:B:40:ARG:HH11	1.53	0.72
1:B:237:ARG:HH21	1:B:237:ARG:HB2	1.51	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:ILE:HG21	1:F:50:VAL:HG11	1.72	0.72
1:G:201:GLU:C	1:G:203:PRO:HD3	2.10	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:J:19:TYR:CZ	1:J:21:GLY:HA3	2.24	0.72
1:A:201:GLU:C	1:A:203:PRO:HD3	2.10	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:F:201:GLU:C	1:F:203:PRO:HD3	2.11	0.71
1:B:201:GLU:C	1:B:203:PRO:HD3	2.11	0.71
1:H:337:ILE:HA	1:H:340:ILE:HG12	1.72	0.71
1:G:9:LYS:HG3	1:G:9:LYS:O	1.89	0.71
1:A:234:SER:O	1:A:238:ASP:HB2	1.89	0.71
1:E:29:ILE:HG21	1:E:50:VAL:HG11	1.71	0.71
1:B:337:ILE:HA	1:B:340:ILE:HG12	1.72	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:B:240:PRO:HB2	1:B:241:PRO:HD3	1.73	0.71
1:A:237:ARG:HH21	1:A:237:ARG:CB	2.04	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:HH21	1:D:237:ARG:HB2	1.56	0.70
1:E:165:ARG:HH12	1:E:243:ILE:CD1	1.93	0.70
1:D:237:ARG:HH21	1:D:237:ARG:CB	2.05	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:B:29:ILE:HG21	1:B:50:VAL:HG11	1.72	0.70
1:G:234:SER:O	1:G:238:ASP:HB2	1.91	0.70
1:H:321:LEU:CA	1:H:322:ARG:CB	2.68	0.70
1:G:263:ASP:HB3	1:H:223:LYS:HD2	1.72	0.70
1:C:29:ILE:HG21	1:C:50:VAL:HG11	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:J:6:LEU:CD2	1:J:8:ALA:H	2.04	0.69
1:H:19:TYR:CZ	1:H:21:GLY:HA3	2.27	0.69
1:I:201:GLU:C	1:I:203:PRO:HD3	2.13	0.69
1:D:234:SER:O	1:D:238:ASP:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:201:GLU:C	1:J:203:PRO:HD3	2.13	0.69
1:F:234:SER:O	1:F:238:ASP:HB2	1.93	0.69
1:F:237:ARG:HH21	1:F:237:ARG:HB2	1.50	0.69
1:H:299:THR:HG21	1:H:345:PHE:CZ	2.27	0.69
1:A:19:TYR:CZ	1:A:21:GLY:HA3	2.28	0.69
1:I:237:ARG:HH21	1:I:237:ARG:CB	2.05	0.69
1:H:240:PRO:HB2	1:H:241:PRO:HD3	1.73	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:A:186:GLU:OE1	1:B:6:LEU:CG	2.35	0.68
1:J:237:ARG:CB	1:J:237:ARG:HH21	2.05	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:E:5:ARG:CB	1:E:6:LEU:HB2	2.24	0.68
1:C:93:VAL:O	1:C:111:LYS:NZ	2.26	0.68
1:H:299:THR:HG21	1:H:345:PHE:CE1	2.28	0.68
1:C:201:GLU:C	1:C:203:PRO:HD3	2.14	0.68
1:B:61:TRP:HB2	1:B:169:LEU:HD21	1.74	0.68
1:H:200:LEU:HD22	1:J:209:GLN:HG3	1.76	0.68
1:F:40:ARG:HH11	1:F:40:ARG:HB2	1.59	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:HB2	1:C:40:ARG:HH11	1.59	0.68
1:I:321:LEU:CB	1:I:322:ARG:CB	2.73	0.67
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:40:ARG:HH11	1:I:40:ARG:HB2	1.59	0.67
1:C:61:TRP:HB2	1:C:169:LEU:HD21	1.75	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:F:308:ALA:HA	1:I:313:MET:CE	2.25	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:304:LEU:HB3	1:J:306:PHE:CE2	2.31	0.66
1:I:237:ARG:HH21	1:I:237:ARG:HB2	1.59	0.66
1:C:237:ARG:HH21	1:C:237:ARG:CB	2.07	0.66
1:B:232:LEU:HD22	1:B:254:VAL:HB	1.77	0.66
1:G:237:ARG:HH21	1:G:237:ARG:HB2	1.61	0.65
1:H:234:SER:O	1:H:238:ASP:HB2	1.96	0.65
1:A:302:MET:HE1	1:B:298:ALA:HA	1.78	0.65
1:A:302:MET:CE	1:B:298:ALA:HA	2.27	0.65
1:J:9:LYS:HG3	1:J:9:LYS:O	1.95	0.65
1:I:320:GLU:CB	1:I:321:LEU:CA	2.62	0.65
1:A:269:ARG:NH1	1:D:270:ASP:OD1	2.30	0.65
1:C:234:SER:O	1:C:238:ASP:HB2	1.97	0.65
1:C:9:LYS:O	1:C:9:LYS:HG3	1.96	0.65
1:J:232:LEU:HD22	1:J:254:VAL:HB	1.77	0.64
1:A:40:ARG:HH11	1:A:40:ARG:HB2	1.61	0.64
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.76	0.64
1:C:240:PRO:HB2	1:C:241:PRO:HD3	1.79	0.64
1:G:237:ARG:HH21	1:G:237:ARG:CB	2.11	0.64
1:F:9:LYS:O	1:F:9:LYS:HG3	1.97	0.64
1:H:9:LYS:HG3	1:H:9:LYS:O	1.96	0.64
1:B:19:TYR:CZ	1:B:21:GLY:HA3	2.32	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: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: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: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:HH11	1:H:40:ARG:HB2	1.63	0.63
1:I:319:PRO:HB3	1:I:320:GLU:HA	1.81	0.63
1:B:299:THR:HG21	1:B:345:PHE:HZ	1.63	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:CB	1:C:237:ARG:NH2	2.62	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:E:286:LYS:O	1:E:287:THR:C	2.38	0.62
1:I:99:VAL:CG2	1:I:231:VAL:HG13	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:TRP:HE1	1:D:138:MET:HE2	1.63	0.61
1:D:40:ARG:HH11	1:D:40:ARG:HB2	1.63	0.61
1:J:6:LEU:HD23	1:J:7:SER:N	2.15	0.61
1:A:311:TYR:HE2	1:A:330:VAL:HG21	1.65	0.61
1:B:9:LYS:O	1:B:9:LYS:HG3	2.00	0.61
1:A:225:ILE:HD13	1:A:265:VAL:HG21	1.82	0.61
1:B:306:PHE:CE2	1:C:304:LEU:HB3	2.36	0.61
1:F:299:THR:HG21	1:F:345:PHE:HZ	1.65	0.61
1:B:118:ASN:HD22	1:B:119:LEU:N	1.99	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:H:347:LYS:O	1:H:348:LYS:HB2	2.02	0.59
1:E:232:LEU:HD22	1:E:254:VAL:HB	1.84	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:J:240:PRO:CB	1:J:241:PRO:HD2	2.29	0.59
1:H:61:TRP:HZ2	1:H:138:MET:HE1	1.67	0.59
1:E:240:PRO:CB	1:E:241:PRO:HD2	2.29	0.59
1:E:61:TRP:HZ2	1:E:138:MET:HE1	1.67	0.59
1:C:299:THR:HG21	1:C:345:PHE:HZ	1.67	0.59
1:C:291:MET:HE1	1:E:291:MET:SD	2.43	0.59
1:I:307:ILE:CD1	1:I:334:MET:HG2	2.24	0.59
1:I:291:MET:SD	1:J:291:MET:HE1	2.43	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:G:299:THR:HG21	1:G:345:PHE:CE1	2.37	0.58
1:H:237:ARG:CZ	1:H:237:ARG:HB2	2.33	0.58
1:D:300:ILE:HG22	1:D:341:MET:HG3	1.84	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:J:326:GLY:C	1:J:328:PRO:HD2	2.24	0.58
1:D:291:MET:SD	1:E:291:MET:HE1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:ILE:HD13	1:H:265:VAL:HG21	1.86	0.58
1:B:237:ARG:CZ	1:B:237:ARG:HB2	2.33	0.57
1:B:229:ARG:HA	1:B:258:THR:HG21	1.86	0.57
1:F:240:PRO:HB2	1:F:241:PRO:HD3	1.81	0.57
1:E:237:ARG:CB	1:E:237:ARG:NH2	2.56	0.57
1:D:237:ARG:NH2	1:D:237:ARG:CB	2.63	0.57
1:H:313:MET:HA	1:J:311:TYR:HB2	1.86	0.57
1:J:313:MET:HG3	1:J:314:ASN:CB	2.34	0.57
1:I:9:LYS:O	1:I:9:LYS:HG3	2.04	0.57
1:G:291:MET:HE1	1:H:291:MET:SD	2.44	0.57
1:B:40:ARG:CB	1:B:40:ARG:HH11	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:H:186:GLU:OE1	1:J:6:LEU:CD2	2.53	0.57
1:H:61:TRP:HB2	1:H:169:LEU:HD21	1.86	0.57
1:A:232:LEU:HD22	1:A:254:VAL:HB	1.86	0.57
1:F:300:ILE:HG22	1:F:341:MET:CG	2.30	0.57
1:A:298:ALA:HA	1:D:302:MET:CE	2.35	0.57
1:G:326:GLY:O	1:G:329:VAL:HB	2.04	0.56
1:A:291:MET:HE1	1:B:291:MET:SD	2.45	0.56
1:I:118:ASN:HD22	1:I:119:LEU:N	2.04	0.56
1:E:17:LEU:HB3	1:E:91:LEU:CD1	2.35	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:E:99:VAL:CG2	1:E:231:VAL:HG13	2.35	0.56
1:G:99:VAL:CG2	1:G:231:VAL:HG13	2.34	0.56
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.86	0.56
1:I:229:ARG:HA	1:I:258:THR:CG2	2.35	0.56
1:E:229:ARG:HA	1:E:258:THR:HG21	1.87	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: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:D:61:TRP:HZ2	1:D:138:MET:HE1	1.71	0.56
1:C:40:ARG:HB2	1:C:40:ARG:NH1	2.21	0.56
1:I:40:ARG:HB2	1:I:40:ARG:NH1	2.20	0.56
1:J:237:ARG:HB2	1:J:237:ARG:CZ	2.36	0.56
1:F:211:THR:HG21	1:F:276:LEU:HD13	1.87	0.56
1:E:40:ARG:HH11	1:E:40:ARG:HB2	1.71	0.56
1:C:347:LYS:O	1:C:348:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:313:MET:CA	1:J:311:TYR:HB3	2.35	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:J:83:HIS:ND1	1:J:84:PRO:CD	2.66	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:E:237:ARG:CZ	1:E:237:ARG:HB2	2.35	0.55
1:I:237:ARG:NH2	1:I:237:ARG:CB	2.62	0.55
1:D:223:LYS:HD2	1:E:263:ASP:HB3	1.88	0.55
1:F:240:PRO:CB	1:F:241:PRO:CD	2.76	0.55
1:D:229:ARG:HA	1:D:258:THR:HG21	1.88	0.55
1:A:229:ARG:HA	1:A:258:THR:HG21	1.87	0.55
1:E:285:ASN:O	1:E:288:ASN:HB2	2.06	0.55
1:A:229:ARG:HA	1:A:258:THR:CG2	2.36	0.55
1:F:308:ALA:CA	1:I:313:MET:HE3	2.34	0.55
1:F:40:ARG:HH11	1:F:40:ARG:CB	2.20	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:I:240:PRO:CB	1:I:241:PRO:CD	2.80	0.55
1:B:347:LYS:O	1:B:348:LYS:HB2	2.07	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:I:229:ARG:HA	1:I:258:THR:HG21	1.88	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:J:347:LYS:O	1:J:348:LYS:HB2	2.07	0.54
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: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
1:J:118:ASN:HD22	1:J:119:LEU:N	2.04	0.54
1:D:347:LYS:O	1:D:348:LYS:HB2	2.07	0.54
1:B:229:ARG:HA	1:B:258:THR:CG2	2.37	0.54
1:A:298:ALA:HA	1:D:302:MET:HE1	1.89	0.54
1:A:51:LEU:N	1:A:52:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:297:ILE:HG12	1:J:299:THR:OG1	2.08	0.54
1:D:82:ILE:HD13	1:D:130:ILE:HD13	1.90	0.54
1:C:152:GLU:HB2	1:C:158:ARG:HH12	1.73	0.54
1:F:40:ARG:HB2	1:F:40:ARG:NH1	2.23	0.54
1:H:313:MET:CA	1:J:311:TYR:CB	2.86	0.54
1:H:232:LEU:HD22	1:H:254:VAL:HB	1.90	0.54
1:A:294:LEU:HD22	1:B:294:LEU:HD11	1.90	0.54
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:D:296:ILE:HA	1:D:299:THR:HG22	1.90	0.53
1:C:299:THR:HA	1:E:297:ILE:HG21	1.88	0.53
1:G:202:ARG:O	1:G:202:ARG:HG3	2.07	0.53
1:F:17:LEU:HD22	1:F:17:LEU:H	1.73	0.53
1:F:290:VAL:HG11	1:I:291:MET:HB3	1.90	0.53
1:I:298:ALA:HA	1:J:302:MET:HE1	1.88	0.53
1:G:240:PRO:CB	1:G:241:PRO:CD	2.79	0.53
1:E:292:LYS:NZ	1:E:348:LYS:HE3	2.22	0.53
1:H:291:MET:HE1	1:J:291:MET:SD	2.49	0.53
1:G:51:LEU:N	1:G:52:PRO:HD2	2.24	0.53
1:H:240:PRO:CB	1:H:241:PRO:HD2	2.34	0.53
1:F:6:LEU:HD12	1:I:186:GLU:HG2	1.89	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:I:240:PRO:CB	1:I:241:PRO:HD2	2.37	0.53
1:H:248:VAL:N	1:H:249:PRO:HD2	2.24	0.53
1:I:300:ILE:HG22	1:I:341:MET:HG3	1.91	0.53
1:G:232:LEU:HD22	1:G:254:VAL:HB	1.91	0.53
1:J:229:ARG:HA	1:J:258:THR:HG21	1.91	0.52
1:I:319:PRO:HA	1:I:320:GLU:O	2.09	0.52
1:D:240:PRO:CB	1:D:241:PRO:CD	2.79	0.52
1:I:300:ILE:HG13	1:I:301:PHE:N	2.24	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:248:VAL:N	1:C:249:PRO:HD2	2.25	0.52
1:E:225:ILE:HD13	1:E:265:VAL:HG21	1.91	0.52
1:D:240:PRO:HB2	1:D:241:PRO:HD3	1.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:TRP:HE1	1:E:138:MET:HE2	1.75	0.52
1:D:14:PRO:HG3	1:E:171:TYR:CZ	2.43	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:I:33:ASN:HB2	1:I:60:THR:HG23	1.91	0.52
1:C:311:TYR:HE2	1:C:330:VAL:HG21	1.75	0.52
1:B:286:LYS:O	1:B:290:VAL:HG23	2.08	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:J:240:PRO:HB2	1:J:241:PRO:HD3	1.85	0.52
1:G:296:ILE:HA	1:G:299:THR:HG22	1.92	0.52
1:A:82:ILE:HD13	1:A:130:ILE:HD13	1.90	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: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:E:6:LEU:O	1:E:7:SER:CB	2.58	0.51
1:G:40:ARG:HB2	1:G:40:ARG:HH11	1.75	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:A:300:ILE:HG13	1:A:301:PHE:N	2.26	0.51
1:H:40:ARG:NH1	1:H:40:ARG:HB2	2.25	0.51
1:G:302:MET:HE1	1:H:298:ALA:HA	1.93	0.51
1:G:248:VAL:N	1:G:249:PRO:HD2	2.25	0.51
1:F:229:ARG:HA	1:F:258:THR:CG2	2.41	0.51
1:A:41:GLU:O	1:A:41:GLU:HG3	2.10	0.51
1:F:16:THR:HG22	1:F:18:VAL:HG23	1.92	0.51
1:C:237:ARG:CZ	1:C:237:ARG:HB2	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:296:ILE:HA	1:C:299:THR:HG22	1.93	0.51
1:A:291:MET:SD	1:D:291:MET:HE1	2.51	0.51
1:G:211:THR:HG21	1:G:276:LEU:HD13	1.93	0.51
1:C:118:ASN:HD22	1:C:119:LEU:N	2.08	0.51
1:D:51:LEU:N	1:D:52:PRO:HD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:GLU:OE1	1:H:212:HIS:NE2	2.41	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:I:298:ALA:HA	1:J:302:MET:CE	2.40	0.50
1:A:33:ASN:HB2	1:A:60:THR:HG23	1.92	0.50
1:I:237:ARG:HB2	1:I:237:ARG:CZ	2.41	0.50
1:C:40:ARG:CB	1:C:40:ARG:HH11	2.23	0.50
1:B:263:ASP:HB3	1:C:223:LYS:HD2	1.92	0.50
1:I:61:TRP:HZ2	1:I:138:MET:HE1	1.77	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:F:229:ARG:HA	1:F:258:THR:HG21	1.94	0.50
1:D:118:ASN:HD22	1:D:119:LEU:N	2.09	0.50
1:B:194:VAL:O	1:B:197:GLU:HB2	2.11	0.50
1:E:347:LYS:O	1:E:348:LYS:HB2	2.11	0.50
1:I:202:ARG:O	1:I:202:ARG:HG3	2.10	0.50
1:D:337:ILE:O	1:D:341:MET:HG2	2.12	0.50
1:J:258:THR:HG22	1:J:259:ILE:N	2.27	0.50
1:C:299:THR:OG1	1:E:297:ILE:HG12	2.11	0.50
1:B:16:THR:HG22	1:B:18:VAL:HG23	1.94	0.50
1:C:61:TRP:HE1	1:C:138:MET:HE2	1.77	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:HG3	1:F:41:GLU:O	2.12	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:F:290:VAL:HG12	1:I:291:MET:HE3	1.93	0.49
1:J:117:LYS:O	1:J:119:LEU:N	2.44	0.49
1:G:294:LEU:HD22	1:H:294:LEU:HD11	1.94	0.49
1:J:104:ASN:O	1:J:105:TYR:HB3	2.11	0.49
1:F:285:ASN:O	1:F:288:ASN:HB2	2.12	0.49
1:F:337:ILE:O	1:F:341:MET:HG2	2.12	0.49
1:E:5:ARG:C	1:E:6:LEU:HD22	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HH11	1:A:40:ARG:CB	2.25	0.49
1:G:255:TYR:O	1:G:258:THR:HG22	2.13	0.49
1:D:132:THR:O	1:D:132:THR:HG23	2.10	0.49
1:G:237:ARG:HB2	1:G:237:ARG:CZ	2.41	0.49
1:G:337:ILE:O	1:G:341:MET:HG2	2.11	0.49
1:E:40:ARG:NH1	1:E:40:ARG:HB2	2.27	0.49
1:E:272:VAL:O	1:E:275:LEU:HB2	2.13	0.49
1:C:270:ASP:OD1	1:E:269:ARG:NH1	2.46	0.49
1:G:313:MET:H	1:G:314:ASN:CB	2.25	0.49
1:J:61:TRP:HE1	1:J:138:MET:HE2	1.77	0.49
1:B:300:ILE:HG13	1:B:301:PHE:N	2.27	0.49
1:A:152:GLU:HB2	1:A:158:ARG:HH12	1.77	0.49
1:C:184:LEU:HD21	1:C:221:LEU:HD11	1.94	0.49
1:G:33:ASN:HB2	1:G:60:THR:HG23	1.94	0.49
1:J:17:LEU:HB3	1:J:91:LEU:CD1	2.43	0.49
1:D:211:THR:HG21	1:D:276:LEU:HD13	1.93	0.49
1:B:153:ARG:CD	1:C:13:PRO:HG3	2.43	0.49
1:I:194:VAL:O	1:I:197:GLU:HB2	2.13	0.49
1:F:327:TYR:N	1:F:328:PRO:HD2	2.28	0.49
1:I:232:LEU:HD22	1:I:254:VAL:HB	1.95	0.49
1:A:186:GLU:CD	1:B:6:LEU:HG	2.30	0.49
1:D:348:LYS:HE2	1:D:349:LYS:N	2.19	0.49
1:G:326:GLY:HA2	1:G:328:PRO:HD2	1.93	0.49
1:D:232:LEU:HD22	1:D:254:VAL:HB	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
1:H:200:LEU:O	1:H:201:GLU:HG3	2.13	0.48
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:B:221:LEU:HG	1:B:225:ILE:CD1	2.43	0.48
1:J:238:ASP:HB3	1:J:239:VAL:H	1.53	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:H:337:ILE:O	1:H:341:MET:HG2	2.13	0.48
1:E:51:LEU:N	1:E:52:PRO:HD2	2.28	0.48
1:A:202:ARG:O	1:A:202:ARG:HG3	2.11	0.48
1:G:300:ILE:HG13	1:G:301:PHE:N	2.28	0.48
1:D:17:LEU:HB3	1:D:91:LEU:CD1	2.43	0.48
1:C:291:MET:HE2	1:E:291:MET:HG2	1.96	0.48
1:H:221:LEU:HG	1:H:225:ILE:CD1	2.43	0.48
1:C:194:VAL:O	1:C:197:GLU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HG3	1:A:9:LYS:O	2.12	0.48
1:A:300:ILE:HG22	1:A:341:MET:HG3	1.96	0.48
1:H:229:ARG:HA	1:H:258:THR:CG2	2.43	0.48
1:D:33:ASN:HB2	1:D:60:THR:HG23	1.95	0.48
1:C:202:ARG:O	1:C:202:ARG:HG3	2.14	0.48
1:C:166:ALA:O	1:C:169:LEU:HB3	2.14	0.48
1:H:181:TYR:HB2	1:H:261:ILE:HD13	1.95	0.48
1:F:300:ILE:HG13	1:F:301:PHE:N	2.29	0.48
1:J:40:ARG:HH11	1:J:40:ARG:CB	2.27	0.48
1:B:82:ILE:HD13	1:B:130:ILE:HD13	1.96	0.48
1:H:272:VAL:O	1:H:275:LEU:HB2	2.14	0.48
1:E:202:ARG:HG3	1:E:202:ARG:O	2.12	0.48
1:F:237:ARG:CZ	1:F:237:ARG:HB2	2.42	0.48
1:C:196:GLU:OE1	1:E:212:HIS:NE2	2.47	0.48
1:C:300:ILE:HG13	1:C:301:PHE:N	2.29	0.47
1:I:311:TYR:CE2	1:I:330:VAL:HG21	2.49	0.47
1:E:120:HIS:HD2	1:E:191:GLU:OE2	1.97	0.47
1:B:195:LEU:HD21	1:B:211:THR:HA	1.96	0.47
1:J:296:ILE:HA	1:J:299:THR:HG22	1.96	0.47
1:B:225:ILE:O	1:B:228:LEU:HB3	2.14	0.47
1:A:103:GLU:HB3	1:A:104:ASN:OD1	2.14	0.47
1:E:242:LEU:O	1:E:243:ILE:C	2.52	0.47
1:E:337:ILE:O	1:E:341:MET:HG2	2.15	0.47
1:G:40:ARG:NH1	1:G:40:ARG:HB2	2.28	0.47
1:H:117:LYS:O	1:H:119:LEU:N	2.46	0.47
1:F:182:PHE:HB3	1:G:7:SER:O	2.15	0.47
1:B:67:ILE:HG21	1:B:139:PHE:HB3	1.97	0.47
1:C:291:MET:CE	1:E:291:MET:HG2	2.45	0.47
1:G:302:MET:CE	1:H:298:ALA:HA	2.43	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:I:327:TYR:CD2	1:J:314:ASN:O	2.68	0.47
1:E:296:ILE:HA	1:E:299:THR:HG22	1.97	0.47
1:J:242:LEU:O	1:J:243:ILE:C	2.53	0.47
1:D:242:LEU:O	1:D:243:ILE:C	2.52	0.47
1:E:244:GLU:C	1:E:246:GLU:N	2.68	0.47
1:A:307:ILE:CD1	1:A:334:MET:HG2	2.35	0.47
1:A:61:TRP:HZ2	1:A:138:MET:HE1	1.78	0.47
1:J:300:ILE:HG13	1:J:301:PHE:N	2.29	0.47
1:H:296:ILE:HA	1:H:299:THR:HG22	1.96	0.47
1:D:40:ARG:HB2	1:D:40:ARG:NH1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:PHE:CE2	1:H:304:LEU:HB3	2.49	0.47
1:B:170:LEU:O	1:B:171:TYR:C	2.53	0.47
1:A:125:GLU:HG3	1:A:141:GLU:HB2	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:A:272:VAL:O	1:A:275:LEU:HB2	2.14	0.47
1:F:302:MET:HE1	1:G:298:ALA:HA	1.96	0.47
1:G:244:GLU:C	1:G:246:GLU:N	2.68	0.47
1:F:244:GLU:C	1:F:246:GLU:N	2.68	0.47
1:J:238:ASP:O	1:J:239:VAL:HG22	2.14	0.47
1:A:221:LEU:HG	1:A:225:ILE:HD12	1.96	0.47
1:D:311:TYR:HE2	1:D:330:VAL:HG21	1.80	0.47
1:A:306:PHE:CE2	1:B:304:LEU:HB3	2.50	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:H:313:MET:HA	1:J:311:TYR:HB3	1.97	0.47
1:E:40:ARG:HH11	1:E:40:ARG:CB	2.27	0.47
1:B:56:SER:HB3	1:B:58:THR:O	2.15	0.47
1:H:230:GLU:HA	1:H:230:GLU:OE1	2.14	0.47
1:A:83:HIS:ND1	1:A:84:PRO:CD	2.70	0.46
1:C:291:MET:HE3	1:E:290:VAL:HG12	1.96	0.46
1:F:225:ILE:HD13	1:F:265:VAL:HG21	1.98	0.46
1:C:61:TRP:HZ2	1:C:138:MET:HE1	1.80	0.46
1:J:125:GLU:HG3	1:J:141:GLU:HB2	1.97	0.46
1:C:286:LYS:O	1:C:287:THR:C	2.53	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:D:237:ARG:HB2	1:D:237:ARG:CZ	2.43	0.46
1:I:301:PHE:CZ	1:J:303:PRO:HB3	2.50	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:A:343:VAL:HG12	1:A:343:VAL:O	2.15	0.46
1:J:61:TRP:HZ2	1:J:138:MET:HE1	1.81	0.46
1:B:33:ASN:HB2	1:B:60:THR:HG23	1.98	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:CZ	1:A:237:ARG:HB2	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:J:99:VAL:HG13	1:J:108:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:118:ASN:HD22	1:A:119:LEU:N	2.14	0.46
1:F:327:TYR:N	1:F:328:PRO:CD	2.79	0.46
1:A:270:ASP:OD1	1:B:269:ARG:NH1	2.49	0.46
1:F:82:ILE:HD13	1:F:130:ILE:HD13	1.97	0.46
1:H:83:HIS:ND1	1:H:84:PRO:CD	2.74	0.46
1:G:221:LEU:HG	1:G:225:ILE:HD12	1.98	0.46
1:G:194:VAL:O	1:G:197:GLU:HB2	2.15	0.46
1:I:211:THR:HG21	1:I:276:LEU:HD13	1.97	0.46
1:H:56:SER:HB3	1:H:58:THR:O	2.16	0.46
1:C:348:LYS:CE	1:C:349:LYS:H	2.22	0.46
1:C:186:GLU:OE1	1:E:7:SER:HB3	2.16	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:G:41:GLU:O	1:G:41:GLU:HG3	2.15	0.45
1:I:337:ILE:O	1:I:341:MET:HG2	2.17	0.45
1:D:14:PRO:HG2	1:E:168:TYR:OH	2.16	0.45
1:H:17:LEU:HD22	1:H:17:LEU:H	1.81	0.45
1:I:276:LEU:HA	1:I:276:LEU:HD12	1.85	0.45
1:F:51:LEU:N	1:F:52:PRO:HD2	2.31	0.45
1:I:13:PRO:HG3	1:J:153:ARG:HD3	1.97	0.45
1:E:41:GLU:O	1:E:41:GLU:HG3	2.15	0.45
1:I:209:GLN:HG3	1:J:200:LEU:HD22	1.99	0.45
1:C:337:ILE:O	1:C:341:MET:HG2	2.16	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: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: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:A:221:LEU:HG	1:A:225:ILE:CD1	2.46	0.45
1:D:96:ARG:CZ	1:E:263:ASP:OD2	2.64	0.45
1:H:302:MET:CE	1:J:298:ALA:HA	2.47	0.45
1:J:96:ARG:HH11	1:J:227:PRO:HG3	1.81	0.45
1:J:300:ILE:HG22	1:J:341:MET:HG3	1.98	0.45
1:B:238:ASP:O	1:B:239:VAL:HG22	2.16	0.45
1:I:225:ILE:CD1	1:I:265:VAL:HG21	2.42	0.45
1:H:153:ARG:HD3	1:J:13:PRO:HG3	1.98	0.45
1:I:244:GLU:C	1:I:246:GLU:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:348:LYS:HE2	1:H:349:LYS:N	2.26	0.45
1:B:118:ASN:ND2	1:B:119:LEU:N	2.65	0.45
2:A:1350:CL:CL	1:B:14:PRO:HD2	2.53	0.45
1:D:17:LEU:H	1:D:17:LEU:HD22	1.82	0.45
1:C:33:ASN:HB2	1:C:60:THR:HG23	1.98	0.45
1:G:242:LEU:O	1:G:243:ILE:C	2.53	0.45
1:A:200:LEU:O	1:A:201:GLU:HG3	2.16	0.45
1:I:296:ILE:HG13	1:I:297:ILE:H	1.81	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:C:330:VAL:O	1:C:334:MET:HG3	2.17	0.45
1:B:330:VAL:O	1:B:334:MET:HG3	2.17	0.45
1:B:61:TRP:HE1	1:B:138:MET:HE2	1.81	0.45
1:I:238:ASP:HB3	1:I:239:VAL:H	1.57	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
1:H:302:MET:HE1	1:J:298:ALA:HA	1.99	0.45
1:D:248:VAL:N	1:D:249:PRO:HD2	2.32	0.45
1:D:348:LYS:CE	1:D:349:LYS:H	2.20	0.44
1:I:195:LEU:HD21	1:I:211:THR:HA	1.99	0.44
1:H:211:THR:HG21	1:H:276:LEU:HD13	1.99	0.44
1:C:294:LEU:HD22	1:E:294:LEU:HD11	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:I:136:VAL:HG11	1:I:173:LEU:HD12	1.98	0.44
1:G:82:ILE:HD13	1:G:130:ILE:HD13	1.98	0.44
1:C:181:TYR:HB2	1:C:261:ILE:HD13	1.99	0.44
1:D:202:ARG:O	1:D:202:ARG:HG3	2.16	0.44
1:G:299:THR:CG2	1:G:345:PHE:CE1	3.00	0.44
1:B:83:HIS:ND1	1:B:84:PRO:CD	2.71	0.44
1:G:270:ASP:OD1	1:H:269:ARG:NH1	2.50	0.44
1:J:33:ASN:HB2	1:J:60:THR:HG23	1.97	0.44
1:E:92:ASN:C	1:E:92:ASN:OD1	2.56	0.44
1:D:225:ILE:HD13	1:D:265:VAL:HG21	1.98	0.44
1:J:337:ILE:O	1:J:341:MET:HG2	2.16	0.44
1:F:209:GLN:HG3	1:I:200:LEU:HD13	1.99	0.44
1:G:61:TRP:HZ2	1:G:138:MET:HE1	1.82	0.44
1:F:194:VAL:O	1:F:197:GLU:HB2	2.18	0.44
1:I:272:VAL:O	1:I:275:LEU:HB2	2.16	0.44
1:J:311:TYR:HE2	1:J:330:VAL:HG21	1.81	0.44
1:C:341:MET:O	1:C:344:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:242:LEU:O	1:H:243:ILE:C	2.55	0.44
1:F:61:TRP:HE1	1:F:138:MET:HE2	1.83	0.44
1:A:302:MET:HE2	1:B:298:ALA:HA	1.99	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:J:16:THR:HG22	1:J:18:VAL:HG23	2.00	0.44
1:I:10:LYS:HD2	1:I:10:LYS:H	1.83	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:A:238:ASP:O	1:A:239:VAL:HG22	2.18	0.44
1:I:311:TYR:HB3	1:J:313:MET:HB2	1.99	0.44
1:A:258:THR:HG22	1:A:259:ILE:N	2.33	0.44
1:F:327:TYR:H	1:F:328:PRO:HD2	1.82	0.44
1:D:297:ILE:HG21	1:E:299:THR:HA	1.99	0.44
1:A:195:LEU:HD21	1:A:211:THR:HA	2.00	0.44
1:E:184:LEU:HD21	1:E:221:LEU:HD11	1.99	0.44
1:I:307:ILE:O	1:I:310:ILE:HG12	2.18	0.43
1:B:312:GLY:O	1:C:311:TYR:HB2	2.18	0.43
1:H:313:MET:O	1:J:311:TYR:HB3	2.18	0.43
1:G:40:ARG:HH11	1:G:40:ARG:CB	2.30	0.43
1:A:248:VAL:N	1:A:249:PRO:HD2	2.33	0.43
1:I:152:GLU:HB2	1:I:158:ARG:HH12	1.83	0.43
1:D:16:THR:HG22	1:D:18:VAL:HG23	2.00	0.43
1:H:202:ARG:HG3	1:H:202:ARG:O	2.17	0.43
1:B:113:PHE:CE1	1:B:124:SER:HB3	2.53	0.43
1:F:348:LYS:CE	1:F:349:LYS:H	2.23	0.43
1:J:299:THR:HG21	1:J:345:PHE:CE1	2.53	0.43
1:J:221:LEU:HG	1:J:225:ILE:CD1	2.48	0.43
1:F:28:GLU:OE1	1:F:43:LYS:HD3	2.18	0.43
1:C:16:THR:HG22	1:C:18:VAL:HG23	1.99	0.43
1:J:272:VAL:O	1:J:275:LEU:HB2	2.18	0.43
1:F:242:LEU:O	1:F:243:ILE:C	2.57	0.43
1:H:330:VAL:O	1:H:334:MET:HG3	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:THR:HG22	1:I:18:VAL:HG23	2.00	0.43
1:G:85:LEU:HA	1:G:85:LEU:HD23	1.86	0.43
1:H:311:TYR:HE2	1:H:330:VAL:HG21	1.84	0.43
1:F:299:THR:HG21	1:F:345:PHE:CZ	2.49	0.43
1:G:252:ARG:NH2	1:H:100:GLU:HG2	2.34	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:I:41:GLU:O	1:I:41:GLU:HG3	2.17	0.43
1:J:202:ARG:O	1:J:202:ARG:HG3	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:B:348:LYS:HE2	1:B:349:LYS:N	2.28	0.43
1:F:272:VAL:O	1:F:275:LEU:HB2	2.19	0.43
1:A:17:LEU:HB3	1:A:91:LEU:CD1	2.48	0.43
1:B:118:ASN:C	1:B:118:ASN:HD22	2.22	0.43
1:F:291:MET:HE1	1:G:291:MET:SD	2.59	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
1:H:237:ARG:HB3	1:H:237:ARG:HH21	1.81	0.43
1:I:237:ARG:HB3	1:I:237:ARG:HH21	1.81	0.43
1:G:19:TYR:CE1	1:G:21:GLY:HA3	2.53	0.43
1:I:61:TRP:CD1	1:I:61:TRP:C	2.92	0.43
1:G:117:LYS:O	1:G:119:LEU:N	2.51	0.43
1:B:230:GLU:HA	1:B:230:GLU:OE1	2.19	0.43
1:I:318:MET:O	1:I:319:PRO:O	2.37	0.43
1:F:311:TYR:CD2	1:I:313:MET:HE1	2.54	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:A:111:LYS:O	1:A:177:LEU:HD21	2.19	0.43
1:A:230:GLU:OE1	1:A:230:GLU:HA	2.19	0.43
1:J:237:ARG:CB	1:J:237:ARG:NH2	2.64	0.42
1:F:348:LYS:HE2	1:F:349:LYS:N	2.23	0.42
1:I:83:HIS:CD2	1:I:85:LEU:HB2	2.54	0.42
1:B:300:ILE:HG22	1:B:341:MET:CG	2.46	0.42
1:H:276:LEU:HD12	1:H:276:LEU:HA	1.81	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:263:ASP:OD2	1:G:96:ARG:NE	2.53	0.42
1:J:51:LEU:N	1:J:52:PRO:HD2	2.34	0.42
1:B:186:GLU:OE1	1:C:6:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:GLU:OE1	1:G:230:GLU:HA	2.18	0.42
1:F:61:TRP:HZ2	1:F:138:MET:HE1	1.83	0.42
1:F:291:MET:SD	1:I:291:MET:HE1	2.59	0.42
1:B:258:THR:HG22	1:B:259:ILE:N	2.34	0.42
1:B:343:VAL:O	1:B:343:VAL:HG12	2.18	0.42
1:J:243:ILE:HG13	1:J:246:GLU:HB2	2.02	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
1:D:117:LYS:O	1:D:119:LEU:N	2.48	0.42
1:H:96:ARG:HH11	1:H:227:PRO:HG3	1.84	0.42
1:E:54:ARG:HG3	1:E:80:PHE:CD1	2.54	0.42
1:C:348:LYS:HE2	1:C:349:LYS:N	2.23	0.42
1:I:341:MET:O	1:I:344:TYR:HB3	2.20	0.42
1:B:202:ARG:HG3	1:B:202:ARG:O	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:H:61:TRP:HE1	1:H:138:MET:HE2	1.85	0.42
1:B:125:GLU:HG3	1:B:141:GLU:HB2	2.01	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:G:307:ILE:CD1	1:G:334:MET:HG2	2.43	0.42
1:D:238:ASP:HB3	1:D:239:VAL:H	1.55	0.42
1:H:298:ALA:O	1:H:302:MET:HG2	2.19	0.42
1:C:255:TYR:O	1:C:258:THR:HG22	2.19	0.42
1:F:212:HIS:NE2	1:I:196:GLU:OE1	2.47	0.42
1:F:311:TYR:HE2	1:F:330:VAL:HG21	1.85	0.42
1:I:348:LYS:CG	1:I:349:LYS:H	2.31	0.42
1:B:348:LYS:CG	1:B:349:LYS:H	2.32	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:A:275:LEU:HA	1:A:275:LEU:HD12	1.90	0.42
1:A:28:GLU:OE1	1:A:43:LYS:HD3	2.20	0.42
1:B:96:ARG:HH11	1:B:227:PRO:HG3	1.84	0.42
1:H:275:LEU:HA	1:H:275:LEU:HD12	1.89	0.42
1:D:111:LYS:O	1:D:177:LEU:HD21	2.19	0.42
1:J:28:GLU:OE1	1:J:43:LYS:HD3	2.20	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:H:309:GLY:C	1:H:311:TYR:H	2.23	0.42
1:B:291:MET:HE3	1:C:290:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:67:ILE:HG21	1:I:139:PHE:HB3	2.02	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:E:61:TRP:CZ2	1:E:138:MET:HE1	2.51	0.42
1:B:238:ASP:HB3	1:B:239:VAL:H	1.51	0.42
1:A:255:TYR:CZ	1:A:259:ILE:HD11	2.55	0.42
1:E:221:LEU:HA	1:E:221:LEU:HD12	1.83	0.42
1:G:272:VAL:O	1:G:275:LEU:HB2	2.20	0.42
1:C:157:ASN:OD1	1:C:162:ARG:HG3	2.20	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:F:200:LEU:O	1:F:201:GLU:HG3	2.19	0.41
1:A:298:ALA:HA	1:D:302:MET:HE2	2.02	0.41
1:J:276:LEU:HA	1:J:276:LEU:HD12	1.83	0.41
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.94	0.41
1:G:313:MET:N	1:G:314:ASN:CB	2.83	0.41
1:A:166:ALA:O	1:A:169:LEU:HB3	2.21	0.41
1:J:118:ASN:HD22	1:J:118:ASN:C	2.23	0.41
1:B:152:GLU:HB2	1:B:158:ARG:HH12	1.85	0.41
1:I:28:GLU:OE2	1:I:143:ILE:HD11	2.20	0.41
1:J:348:LYS:CG	1:J:349:LYS:H	2.32	0.41
1:H:341:MET:O	1:H:344:TYR:HB3	2.20	0.41
1:E:238:ASP:O	1:E:239:VAL:HG22	2.20	0.41
1:G:327:TYR:N	1:G:328:PRO:HD2	2.35	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:152:GLU:HB2	1:D:158:ARG:NH1	2.34	0.41
1:C:152:GLU:HB2	1:C:158:ARG:NH1	2.35	0.41
1:A:148:ASP:O	1:A:152:GLU:HG2	2.20	0.41
1:D:276:LEU:HA	1:D:276:LEU:HD12	1.83	0.41
1:A:194:VAL:O	1:A:197:GLU:HB2	2.19	0.41
1:A:348:LYS:HE2	1:A:349:LYS:N	2.22	0.41
1:E:348:LYS:CE	1:E:349:LYS:H	2.27	0.41
1:G:255:TYR:CZ	1:G:259:ILE:HD11	2.55	0.41
1:B:171:TYR:OH	1:C:14:PRO:HG3	2.20	0.41
1:F:192:ILE:O	1:F:196:GLU:HG2	2.20	0.41
1:D:54:ARG:HG3	1:D:80:PHE:CD1	2.55	0.41
1:B:272:VAL:O	1:B:275:LEU:HB2	2.20	0.41
1:F:132:THR:HG23	1:F:132:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ARG:HA	1:E:68:HIS:CD2	2.54	0.41
1:A:132:THR:HG23	1:A:132:THR:O	2.20	0.41
1:I:132:THR:HG23	1:I:132:THR:O	2.20	0.41
1:B:276:LEU:HD12	1:B:276:LEU:HA	1.83	0.41
1:H:300:ILE:HG13	1:H:301:PHE:N	2.36	0.41
1:B:242:LEU:O	1:B:243:ILE:C	2.59	0.41
1:B:244:GLU:C	1:B:246:GLU:N	2.73	0.41
1:C:83:HIS:ND1	1:C:84:PRO:CD	2.76	0.41
1:F:348:LYS:CG	1:F:349:LYS:H	2.33	0.41
1:E:292:LYS:HZ3	1:E:348:LYS:HE3	1.85	0.41
1:E:229:ARG:CG	1:E:258:THR:HG23	2.51	0.41
1:B:28:GLU:OE1	1:B:43:LYS:HD3	2.20	0.41
1:C:300:ILE:HG22	1:C:341:MET:CG	2.49	0.41
1:C:202:ARG:N	1:C:203:PRO:HD3	2.36	0.41
1:C:291:MET:HB3	1:E:290:VAL:CG1	2.50	0.41
1:F:202:ARG:O	1:F:202:ARG:CG	2.68	0.41
1:C:229:ARG:HA	1:C:258:THR:HG21	2.02	0.41
1:B:104:ASN:O	1:B:105:TYR:HB3	2.21	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:I:348:LYS:HE2	1:I:349:LYS:N	2.25	0.41
1:F:170:LEU:O	1:F:171:TYR:C	2.58	0.41
1:C:116:ASP:OD2	1:C:119:LEU:HB3	2.21	0.41
1:E:202:ARG:O	1:E:202:ARG:CG	2.69	0.41
1:C:73:VAL:HG21	1:C:91:LEU:HD21	2.03	0.41
1:E:117:LYS:O	1:E:119:LEU:N	2.51	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.97	0.41
1:G:343:VAL:HG12	1:G:343:VAL:O	2.20	0.41
1:B:307:ILE:CD1	1:B:334:MET:HG2	2.37	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:I:309:GLY:C	1:I:311:TYR:H	2.23	0.41
1:H:118:ASN:ND2	1:H:119:LEU:N	2.69	0.41
1:G:221:LEU:HD12	1:G:221:LEU:HA	1.80	0.41
1:F:275:LEU:HD12	1:F:275:LEU:HA	1.90	0.41
1:A:6:LEU:HD22	1:A:7:SER:H	1.85	0.41
1:C:10:LYS:HD2	1:C:10:LYS:H	1.86	0.41
1:F:118:ASN:C	1:F:118:ASN:HD22	2.24	0.41
1:E:275:LEU:HA	1:E:275:LEU:HD12	1.93	0.41
1:J:61:TRP:CD1	1:J:61:TRP:C	2.93	0.40
1:I:302:MET:HG2	1:J:302:MET:HE1	2.03	0.40

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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: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:F:319:PRO:C	1:F:321:LEU:O	2.59	0.40
1:E:286:LYS:C	1:E:288:ASN:N	2.75	0.40
1:B:117:LYS:O	1:B:119:LEU:N	2.54	0.40
1:D:118:ASN:ND2	1:D:119:LEU:N	2.70	0.40
1:G:118:ASN:HD22	1:G:119:LEU:N	2.19	0.40
1:C:272:VAL:O	1:C:275:LEU:HB2	2.20	0.40
1:A:242:LEU:O	1:A:243:ILE:C	2.59	0.40
1:C:237:ARG:HH21	1:C:237:ARG:HB3	1.85	0.40
1:G:19:TYR:CZ	1:G:21:GLY:CA	2.97	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: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: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:B:86:VAL:HG13	1:B:107:PHE:CD2	2.57	0.40
1:C:82:ILE:HD13	1:C:130:ILE:HD13	2.03	0.40
1:I:326:GLY:O	1:I:329:VAL:HB	2.20	0.40
1:C:41:GLU:O	1:C:41:GLU:HG3	2.21	0.40
1:C:24:ARG:HA	1:C:68:HIS:CD2	2.56	0.40
1:A:221:LEU:HA	1:A:221:LEU:HD12	1.74	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:A:294:LEU:HD11	1:D:294:LEU:HD22	2.03	0.40
1:H:17:LEU:N	1:H:17:LEU:HD22	2.37	0.40
1:C:276:LEU:HA	1:C:276:LEU:HD12	1.86	0.40
1:G:181:TYR:HB2	1:G:261:ILE:HD13	2.04	0.40
1:E:311:TYR:HE2	1:E:330:VAL:HG21	1.86	0.40
1:C:61:TRP:C	1:C:61:TRP:CD1	2.95	0.40
1:C:238:ASP:C	1:C:239:VAL:HG13	2.41	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%)	5	19
1	B	327/363 (90%)	291 (89%)	28 (9%)	8 (2%)	7	29
1	C	327/363 (90%)	289 (88%)	29 (9%)	9 (3%)	6	24
1	D	327/363 (90%)	289 (88%)	26 (8%)	12 (4%)	4	17
1	E	327/363 (90%)	289 (88%)	25 (8%)	13 (4%)	4	15
1	F	338/363 (93%)	293 (87%)	34 (10%)	11 (3%)	5	20
1	G	338/363 (93%)	292 (86%)	32 (10%)	14 (4%)	3	14
1	H	334/363 (92%)	291 (87%)	32 (10%)	11 (3%)	5	20
1	I	336/363 (93%)	289 (86%)	33 (10%)	14 (4%)	3	13
1	J	332/363 (92%)	291 (88%)	29 (9%)	12 (4%)	4	18
All	All	3313/3630 (91%)	2898 (88%)	300 (9%)	115 (4%)	4	18

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%)	278 (89%)	33 (11%)	8	25
1	B	309/341 (91%)	272 (88%)	37 (12%)	6	18
1	C	309/341 (91%)	275 (89%)	34 (11%)	8	23
1	D	310/341 (91%)	278 (90%)	32 (10%)	9	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	310/341 (91%)	274 (88%)	36 (12%)	7	20
1	F	312/341 (92%)	277 (89%)	35 (11%)	7	22
1	G	311/341 (91%)	278 (89%)	33 (11%)	8	25
1	H	311/341 (91%)	275 (88%)	36 (12%)	7	20
1	I	311/341 (91%)	279 (90%)	32 (10%)	9	26
1	J	312/341 (92%)	274 (88%)	38 (12%)	6	18
All	All	3106/3410 (91%)	2760 (89%)	346 (11%)	8	22

All (346) 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	39	PHE
1	A	40	ARG
1	A	56	SER
1	A	60	THR
1	A	95	GLN
1	A	96	ARG
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	202	ARG
1	A	206	GLU
1	A	218	LEU
1	A	222	ARG
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

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Mol	Chain	Res	Type
1	A	275	LEU
1	A	288	ASN
1	A	327	TYR
1	A	346	LYS
1	B	10	LYS
1	B	17	LEU
1	B	22	LYS
1	B	28	GLU
1	B	39	PHE
1	B	40	ARG
1	B	56	SER
1	B	60	THR
1	B	95	GLN
1	B	96	ARG
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	202	ARG
1	B	206	GLU
1	B	207	THR
1	B	218	LEU
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	258	THR
1	B	260	GLN
1	B	275	LEU
1	B	283	VAL
1	B	288	ASN
1	B	297	ILE
1	B	327	TYR
1	B	346	LYS
1	B	349	LYS
1	C	10	LYS

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Mol	Chain	Res	Type
1	C	17	LEU
1	C	22	LYS
1	C	28	GLU
1	C	39	PHE
1	C	40	ARG
1	C	60	THR
1	C	95	GLN
1	C	96	ARG
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	202	ARG
1	C	206	GLU
1	C	207	THR
1	C	218	LEU
1	C	222	ARG
1	C	232	LEU
1	C	234	SER
1	C	235	LEU
1	C	238	ASP
1	C	239	VAL
1	C	258	THR
1	C	260	GLN
1	C	267	THR
1	C	275	LEU
1	C	288	ASN
1	C	330	VAL
1	C	346	LYS
1	C	349	LYS
1	D	6	LEU
1	D	7	SER
1	D	10	LYS
1	D	17	LEU
1	D	22	LYS
1	D	39	PHE
1	D	40	ARG
1	D	60	THR
1	D	95	GLN

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Mol	Chain	Res	Type
1	D	96	ARG
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	202	ARG
1	D	206	GLU
1	D	207	THR
1	D	218	LEU
1	D	222	ARG
1	D	232	LEU
1	D	234	SER
1	D	235	LEU
1	D	238	ASP
1	D	239	VAL
1	D	249	PRO
1	D	258	THR
1	D	275	LEU
1	D	288	ASN
1	D	346	LYS
1	E	6	LEU
1	E	7	SER
1	E	10	LYS
1	E	17	LEU
1	E	22	LYS
1	E	39	PHE
1	E	40	ARG
1	E	56	SER
1	E	60	THR
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	200	LEU

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Mol	Chain	Res	Type
1	E	202	ARG
1	E	206	GLU
1	E	218	LEU
1	E	222	ARG
1	E	232	LEU
1	E	235	LEU
1	E	238	ASP
1	E	239	VAL
1	E	258	THR
1	E	260	GLN
1	E	275	LEU
1	E	277	ASP
1	E	288	ASN
1	E	297	ILE
1	E	327	TYR
1	E	346	LYS
1	E	349	LYS
1	F	6	LEU
1	F	10	LYS
1	F	17	LEU
1	F	22	LYS
1	F	28	GLU
1	F	39	PHE
1	F	40	ARG
1	F	56	SER
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	218	LEU
1	F	222	ARG
1	F	232	LEU
1	F	234	SER
1	F	235	LEU

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Mol	Chain	Res	Type
1	F	238	ASP
1	F	239	VAL
1	F	258	THR
1	F	275	LEU
1	F	277	ASP
1	F	288	ASN
1	F	297	ILE
1	F	327	TYR
1	F	346	LYS
1	F	349	LYS
1	G	10	LYS
1	G	17	LEU
1	G	22	LYS
1	G	39	PHE
1	G	40	ARG
1	G	56	SER
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	202	ARG
1	G	206	GLU
1	G	207	THR
1	G	215	LYS
1	G	218	LEU
1	G	222	ARG
1	G	232	LEU
1	G	234	SER
1	G	235	LEU
1	G	238	ASP
1	G	239	VAL
1	G	258	THR
1	G	275	LEU
1	G	287	THR
1	G	288	ASN
1	G	327	TYR
1	G	346	LYS

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Mol	Chain	Res	Type
1	G	349	LYS
1	H	7	SER
1	H	10	LYS
1	H	17	LEU
1	H	22	LYS
1	H	39	PHE
1	H	40	ARG
1	H	56	SER
1	H	71	ASP
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	202	ARG
1	H	206	GLU
1	H	207	THR
1	H	218	LEU
1	H	222	ARG
1	H	232	LEU
1	H	234	SER
1	H	235	LEU
1	H	238	ASP
1	H	239	VAL
1	H	258	THR
1	H	260	GLN
1	H	275	LEU
1	H	283	VAL
1	H	287	THR
1	H	288	ASN
1	H	297	ILE
1	H	327	TYR
1	H	346	LYS
1	I	10	LYS
1	I	17	LEU
1	I	22	LYS
1	I	39	PHE
1	I	40	ARG

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Mol	Chain	Res	Type
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	200	LEU
1	I	202	ARG
1	I	206	GLU
1	I	207	THR
1	I	218	LEU
1	I	222	ARG
1	I	232	LEU
1	I	235	LEU
1	I	238	ASP
1	I	239	VAL
1	I	258	THR
1	I	267	THR
1	I	275	LEU
1	I	283	VAL
1	I	288	ASN
1	I	327	TYR
1	I	346	LYS
1	J	6	LEU
1	J	7	SER
1	J	10	LYS
1	J	22	LYS
1	J	28	GLU
1	J	39	PHE
1	J	40	ARG
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

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Mol	Chain	Res	Type
1	J	123	GLU
1	J	143	ILE
1	J	152	GLU
1	J	165	ARG
1	J	202	ARG
1	J	206	GLU
1	J	207	THR
1	J	218	LEU
1	J	222	ARG
1	J	232	LEU
1	J	234	SER
1	J	235	LEU
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	288	ASN
1	J	327	TYR
1	J	346	LYS
1	J	349	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	120	HIS
1	A	217	ASN
1	B	118	ASN
1	B	120	HIS
1	B	217	ASN
1	C	118	ASN
1	C	120	HIS
1	C	217	ASN
1	D	118	ASN
1	D	120	HIS
1	D	217	ASN
1	E	118	ASN
1	E	120	HIS
1	E	217	ASN

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Mol	Chain	Res	Type
1	E	260	GLN
1	F	118	ASN
1	F	120	HIS
1	F	217	ASN
1	G	118	ASN
1	G	120	HIS
1	G	217	ASN
1	H	118	ASN
1	H	120	HIS
1	H	217	ASN
1	I	118	ASN
1	I	120	HIS
1	I	217	ASN
1	J	118	ASN
1	J	120	HIS
1	J	217	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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%)	0.08	14 (4%)	40	33	43, 68, 98, 103	0
1	B	331/363 (91%)	0.18	14 (4%)	40	33	43, 68, 98, 103	0
1	C	331/363 (91%)	0.22	15 (4%)	37	31	43, 68, 98, 103	0
1	D	331/363 (91%)	0.21	12 (3%)	46	38	43, 68, 98, 103	0
1	E	331/363 (91%)	0.14	6 (1%)	71	68	43, 68, 98, 103	0
1	F	342/363 (94%)	0.16	12 (3%)	48	40	43, 69, 98, 103	0
1	G	342/363 (94%)	0.19	15 (4%)	38	32	43, 69, 98, 103	0
1	H	338/363 (93%)	0.20	13 (3%)	44	37	43, 68, 98, 103	0
1	I	340/363 (93%)	0.10	7 (2%)	67	62	43, 69, 98, 103	0
1	J	336/363 (92%)	0.18	11 (3%)	50	42	43, 68, 98, 103	0
All	All	3353/3630 (92%)	0.17	119 (3%)	48	40	43, 68, 98, 103	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	245	LYS	6.6
1	H	282	SER	6.2
1	D	343	VAL	5.0
1	H	343	VAL	4.9
1	B	329	VAL	4.8
1	F	245	LYS	4.7
1	C	343	VAL	4.4
1	F	339	VAL	4.3
1	I	345	PHE	4.2
1	C	332	ALA	4.1
1	C	328	PRO	4.0
1	B	238	ASP	4.0
1	F	205	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	205	LYS	3.7
1	D	245	LYS	3.6
1	G	345	PHE	3.6
1	A	245	LYS	3.5
1	I	342	VAL	3.3
1	A	327	TYR	3.3
1	D	342	VAL	3.3
1	H	336	VAL	3.3
1	C	245	LYS	3.2
1	C	329	VAL	3.2
1	J	328	PRO	3.1
1	E	245	LYS	3.1
1	J	325	TRP	3.1
1	I	344	TYR	3.1
1	B	330	VAL	3.0
1	C	339	VAL	3.0
1	B	245	LYS	2.9
1	G	10	LYS	2.9
1	G	200	LEU	2.9
1	A	347	LYS	2.9
1	J	37	GLU	2.9
1	G	343	VAL	2.9
1	H	285	ASN	2.9
1	A	340	ILE	2.9
1	J	347	LYS	2.8
1	B	328	PRO	2.8
1	G	118	ASN	2.8
1	C	205	LYS	2.8
1	C	345	PHE	2.8
1	B	202	ARG	2.8
1	J	202	ARG	2.8
1	H	283	VAL	2.7
1	J	315	PHE	2.7
1	H	236	TYR	2.7
1	B	340	ILE	2.7
1	D	5	ARG	2.7
1	D	346	LYS	2.7
1	H	245	LYS	2.7
1	G	342	VAL	2.7
1	E	110	LEU	2.7
1	A	343	VAL	2.7
1	G	314	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	128	SER	2.6
1	C	344	TYR	2.6
1	D	36	ILE	2.6
1	B	136	VAL	2.6
1	J	16	THR	2.6
1	J	342	VAL	2.6
1	G	312	GLY	2.6
1	F	342	VAL	2.6
1	I	205	LYS	2.6
1	H	226	TRP	2.6
1	D	330	VAL	2.6
1	E	129	LEU	2.5
1	I	343	VAL	2.5
1	B	346	LYS	2.5
1	F	25	GLU	2.5
1	D	345	PHE	2.5
1	A	26	ASP	2.4
1	B	343	VAL	2.4
1	C	342	VAL	2.4
1	B	37	GLU	2.4
1	H	205	LYS	2.4
1	A	336	VAL	2.4
1	A	333	VAL	2.4
1	E	128	SER	2.4
1	F	108	ILE	2.4
1	G	245	LYS	2.4
1	G	313	MET	2.4
1	A	332	ALA	2.4
1	I	203	PRO	2.4
1	F	199	VAL	2.4
1	F	349	LYS	2.4
1	F	36	ILE	2.3
1	H	346	LYS	2.3
1	C	203	PRO	2.3
1	C	346	LYS	2.3
1	A	138	MET	2.3
1	A	205	LYS	2.3
1	J	119	LEU	2.3
1	H	313	MET	2.3
1	J	340	ILE	2.3
1	E	118	ASN	2.3
1	D	344	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	110	LEU	2.2
1	D	26	ASP	2.2
1	G	349	LYS	2.2
1	C	128	SER	2.2
1	A	246	GLU	2.2
1	H	325	TRP	2.2
1	B	344	TYR	2.2
1	J	346	LYS	2.2
1	C	244	GLU	2.2
1	G	347	LYS	2.1
1	H	25	GLU	2.1
1	F	319	PRO	2.1
1	D	331	LEU	2.1
1	G	204	GLU	2.1
1	B	248	VAL	2.1
1	A	25	GLU	2.1
1	B	21	GLY	2.0
1	F	37	GLU	2.0
1	G	340	ILE	2.0
1	G	346	LYS	2.0
1	C	298	ALA	2.0
1	E	25	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	H	1350	1/1	0.97	0.62	17.32	54,54,54,54	0
3	MG	D	1354	1/1	0.97	0.69	14.58	55,55,55,55	0
3	MG	G	1354	1/1	0.96	0.52	13.33	50,50,50,50	0
3	MG	E	1350	1/1	0.98	0.57	12.75	56,56,56,56	0
3	MG	D	1356	1/1	0.91	0.33	10.81	46,46,46,46	0
3	MG	B	1351	1/1	0.95	0.54	10.64	56,56,56,56	0
3	MG	J	1352	1/1	0.92	0.61	9.67	63,63,63,63	0
3	MG	J	1350	1/1	0.92	0.40	8.58	61,61,61,61	0
3	MG	F	1352	1/1	0.81	0.38	6.98	46,46,46,46	0
3	MG	A	1351	1/1	0.97	0.31	6.15	47,47,47,47	0
3	MG	F	1350	1/1	0.81	0.26	4.69	55,55,55,55	0
3	MG	G	1352	1/1	0.97	0.32	4.65	44,44,44,44	0
3	MG	D	1353	1/1	0.78	0.30	3.37	65,65,65,65	0
3	MG	F	1353	1/1	0.94	0.28	3.26	45,45,45,45	0
3	MG	J	1351	1/1	0.92	0.30	2.97	43,43,43,43	0
3	MG	C	1351	1/1	0.95	0.29	2.24	38,38,38,38	0
3	MG	D	1355	1/1	0.93	0.25	1.60	56,56,56,56	0
3	MG	A	1352	1/1	0.96	0.18	0.03	35,35,35,35	0
2	CL	F	1351	1/1	0.94	0.15	-0.39	61,61,61,61	0
3	MG	G	1353	1/1	0.91	0.18	-0.41	43,43,43,43	0
2	CL	G	1351	1/1	0.96	0.15	-1.24	69,69,69,69	0
2	CL	D	1350	1/1	0.98	0.14	-1.52	42,42,42,42	0
2	CL	B	1350	1/1	0.92	0.10	-1.60	68,68,68,68	0
2	CL	G	1350	1/1	0.97	0.08	-2.93	47,47,47,47	0
2	CL	A	1350	1/1	0.98	0.06	-3.58	50,50,50,50	0
2	CL	D	1351	1/1	0.95	0.08	-5.38	59,59,59,59	0
3	MG	D	1352	1/1	0.86	0.38	-	71,71,71,71	0
3	MG	C	1350	1/1	0.88	0.24	-	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.