



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:54 PM UTC

PDB ID : 4HVZ / pdb_00004hvx
Title : Crystal structure of brucella abortus immunogenic BP26 protein
Authors : Kim, D.; Park, J.; Oh, B.; Song, J.
Deposited on : 2012-11-07
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

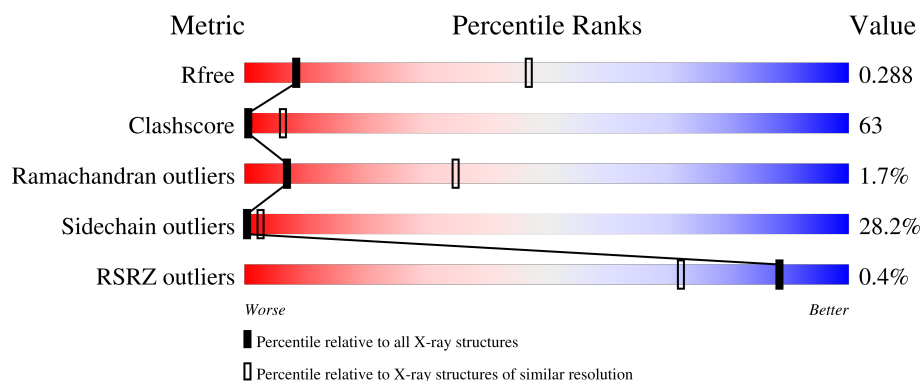
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	224	28%46%19% . .
1	B	224	% 24%50%19% . .
1	C	224	23%45%25% . .
1	D	224	22%46%24% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6340 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 26 kDa periplasmic immunogenic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			
1	B	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			
1	C	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			
1	D	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			

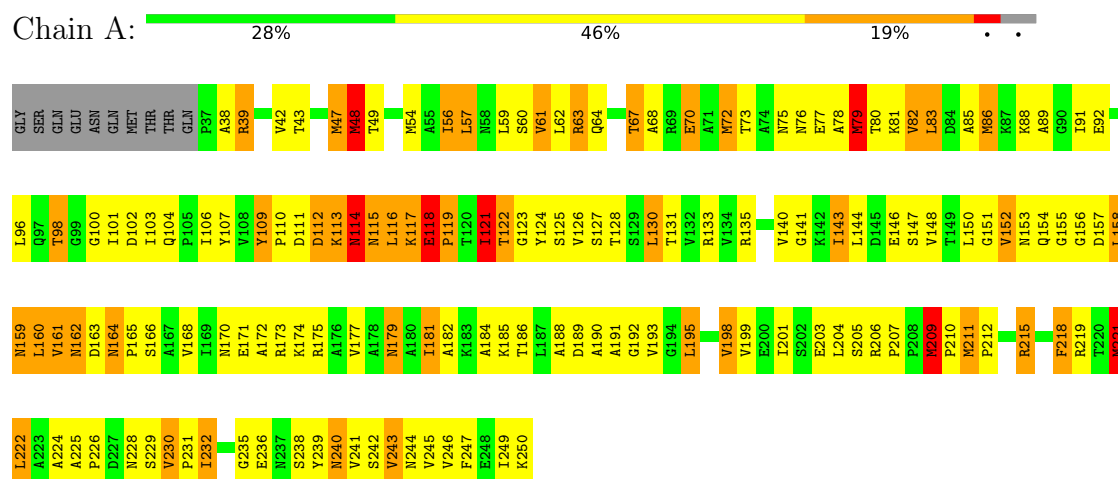
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q44642
A	28	SER	-	expression tag	UNP Q44642
B	27	GLY	-	expression tag	UNP Q44642
B	28	SER	-	expression tag	UNP Q44642
C	27	GLY	-	expression tag	UNP Q44642
C	28	SER	-	expression tag	UNP Q44642
D	27	GLY	-	expression tag	UNP Q44642
D	28	SER	-	expression tag	UNP Q44642

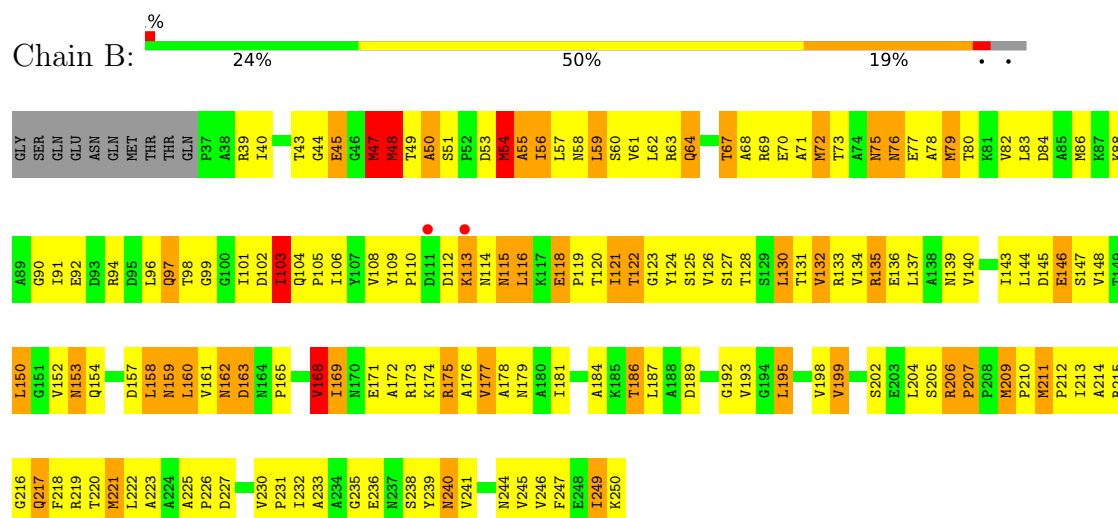
3 Residue-property plots [i](#)

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

- Molecule 1: 26 kDa periplasmic immunogenic protein

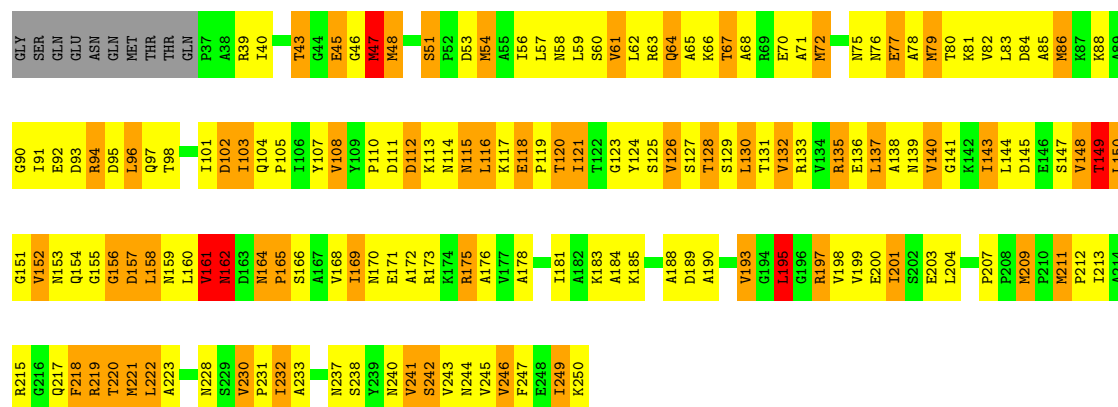


- Molecule 1: 26 kDa periplasmic immunogenic protein

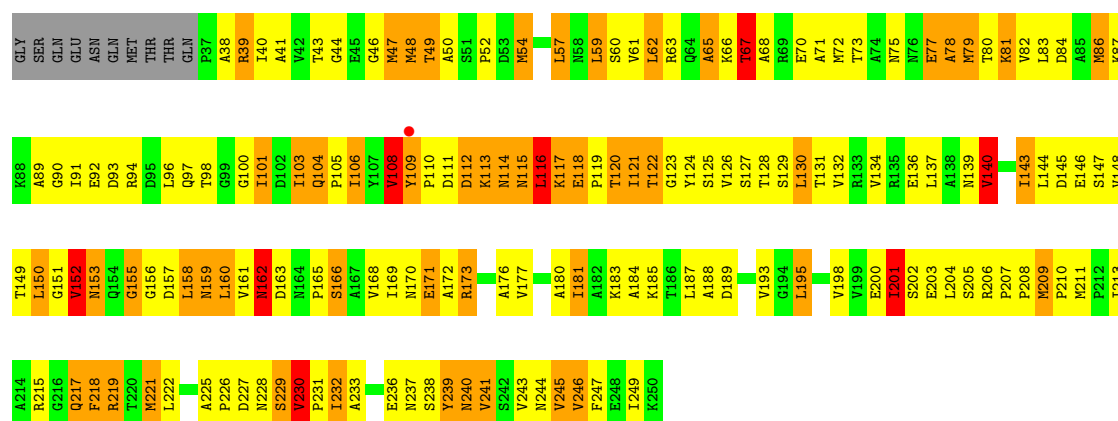
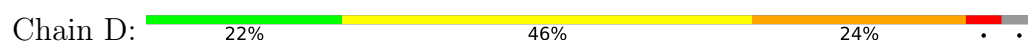


- Molecule 1: 26 kDa periplasmic immunogenic protein





- Molecule 1: 26 kDa periplasmic immunogenic protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	203.09Å 203.09Å 207.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.50 29.96 – 3.50	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.96-3.50) 88.6 (29.96-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.45 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.283 0.242 , 0.288	Depositor DCC
R_{free} test set	2682 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	117.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h 0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6340	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.16	16/1602 (1.0%)	1.36	17/2172 (0.8%)
1	B	1.17	17/1602 (1.1%)	1.34	19/2172 (0.9%)
1	C	1.24	19/1602 (1.2%)	1.46	22/2172 (1.0%)
1	D	1.21	19/1602 (1.2%)	1.44	34/2172 (1.6%)
All	All	1.20	71/6408 (1.1%)	1.40	92/8688 (1.1%)

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	A	0	3
1	D	0	3
All	All	0	6

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	MET	CG-SD	8.83	2.02	1.80
1	C	47	MET	SD-CE	8.41	2.00	1.79
1	B	209	MET	CG-SD	8.39	2.01	1.80
1	A	221	MET	SD-CE	8.33	2.00	1.79
1	A	86	MET	CG-SD	8.30	2.01	1.80
1	B	48	MET	SD-CE	8.15	2.00	1.79
1	D	79	MET	CG-SD	8.12	2.01	1.80
1	A	221	MET	CG-SD	8.05	2.00	1.80
1	D	72	MET	SD-CE	8.03	1.99	1.79
1	A	48	MET	SD-CE	7.91	1.99	1.79
1	C	211	MET	SD-CE	7.87	1.99	1.79
1	A	72	MET	CG-SD	7.86	2.00	1.80
1	B	72	MET	SD-CE	7.78	1.99	1.79
1	B	79	MET	CG-SD	7.77	2.00	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	MET	SD-CE	7.64	1.98	1.79
1	A	79	MET	CG-SD	7.62	1.99	1.80
1	C	72	MET	CG-SD	7.56	1.99	1.80
1	C	221	MET	SD-CE	7.55	1.98	1.79
1	A	72	MET	SD-CE	7.54	1.98	1.79
1	A	54	MET	SD-CE	7.47	1.98	1.79
1	D	86	MET	SD-CE	7.47	1.98	1.79
1	D	86	MET	CG-SD	7.46	1.99	1.80
1	C	86	MET	CG-SD	7.45	1.99	1.80
1	C	72	MET	SD-CE	7.44	1.98	1.79
1	B	54	MET	SD-CE	7.36	1.98	1.79
1	D	211	MET	SD-CE	7.35	1.98	1.79
1	C	209	MET	SD-CE	7.32	1.97	1.79
1	B	209	MET	SD-CE	7.30	1.97	1.79
1	C	54	MET	SD-CE	7.30	1.97	1.79
1	D	47	MET	SD-CE	7.27	1.97	1.79
1	B	86	MET	SD-CE	7.26	1.97	1.79
1	A	79	MET	SD-CE	7.24	1.97	1.79
1	A	211	MET	SD-CE	7.15	1.97	1.79
1	D	209	MET	SD-CE	7.12	1.97	1.79
1	D	221	MET	SD-CE	7.11	1.97	1.79
1	A	48	MET	CG-SD	7.10	1.98	1.80
1	A	209	MET	SD-CE	7.09	1.97	1.79
1	C	209	MET	CG-SD	7.07	1.98	1.80
1	D	54	MET	SD-CE	7.06	1.97	1.79
1	B	221	MET	SD-CE	7.04	1.97	1.79
1	C	86	MET	SD-CE	7.02	1.97	1.79
1	C	79	MET	CG-SD	7.00	1.98	1.80
1	C	54	MET	CG-SD	6.91	1.98	1.80
1	B	47	MET	SD-CE	6.85	1.96	1.79
1	B	221	MET	CG-SD	6.81	1.97	1.80
1	B	47	MET	CG-SD	6.79	1.97	1.80
1	D	79	MET	SD-CE	6.76	1.96	1.79
1	B	86	MET	CG-SD	6.73	1.97	1.80
1	C	79	MET	SD-CE	6.69	1.96	1.79
1	B	48	MET	CG-SD	6.67	1.97	1.80
1	A	54	MET	CG-SD	6.62	1.97	1.80
1	D	209	MET	CG-SD	6.62	1.97	1.80
1	B	211	MET	SD-CE	6.46	1.95	1.79
1	D	48	MET	SD-CE	6.37	1.95	1.79
1	C	221	MET	CG-SD	6.36	1.96	1.80
1	A	86	MET	SD-CE	6.33	1.95	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	MET	SD-CE	6.33	1.95	1.79
1	D	221	MET	CG-SD	6.33	1.96	1.80
1	C	48	MET	SD-CE	6.32	1.95	1.79
1	C	48	MET	CG-SD	6.28	1.96	1.80
1	C	211	MET	CG-SD	6.23	1.96	1.80
1	D	211	MET	CG-SD	6.22	1.96	1.80
1	C	47	MET	CG-SD	6.18	1.96	1.80
1	B	54	MET	CG-SD	6.16	1.96	1.80
1	A	211	MET	CG-SD	5.98	1.95	1.80
1	D	72	MET	CG-SD	5.67	1.95	1.80
1	D	47	MET	CG-SD	5.61	1.94	1.80
1	D	48	MET	CG-SD	5.46	1.94	1.80
1	D	108	VAL	CA-CB	-5.42	1.47	1.54
1	C	126	VAL	CA-CB	-5.34	1.48	1.54
1	B	72	MET	CG-SD	5.17	1.93	1.80

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	GLU	CA-C-N	13.30	133.47	119.90
1	C	118	GLU	C-N-CA	13.30	133.47	119.90
1	A	206	ARG	CA-C-N	11.59	132.32	120.38
1	A	206	ARG	C-N-CA	11.59	132.32	120.38
1	B	115	ASN	N-CA-C	9.96	121.39	108.24
1	C	46	GLY	N-CA-C	-9.23	97.20	110.96
1	B	211	MET	CA-C-N	-9.21	110.50	119.90
1	B	211	MET	C-N-CA	-9.21	110.50	119.90
1	D	206	ARG	CA-C-N	9.06	129.71	120.38
1	D	206	ARG	C-N-CA	9.06	129.71	120.38
1	A	225	ALA	CA-C-N	8.48	129.00	119.93
1	A	225	ALA	C-N-CA	8.48	129.00	119.93
1	B	153	ASN	N-CA-C	8.03	121.08	108.79
1	C	156	GLY	N-CA-C	-7.99	103.41	114.67
1	B	217	GLN	N-CA-C	-7.96	103.68	113.15
1	D	109	TYR	CA-C-N	7.88	128.36	119.93
1	D	109	TYR	C-N-CA	7.88	128.36	119.93
1	D	177	VAL	CB-CA-C	-7.65	102.09	111.88
1	D	50	ALA	N-CA-C	7.61	119.59	108.86
1	B	207	PRO	CA-C-N	7.32	128.99	119.84
1	B	207	PRO	C-N-CA	7.32	128.99	119.84
1	A	164	ASN	CA-C-N	7.26	128.91	119.84
1	A	164	ASN	C-N-CA	7.26	128.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	SER	N-CA-C	-7.08	101.41	110.19
1	C	165	PRO	N-CA-C	-7.08	104.30	113.57
1	B	122	THR	N-CA-C	6.90	122.55	113.30
1	D	181	ILE	N-CA-C	-6.87	103.62	110.62
1	D	201	ILE	CB-CA-C	-6.84	100.28	110.82
1	D	121	ILE	CB-CA-C	-6.81	102.21	111.33
1	A	229	SER	N-CA-C	-6.71	99.45	109.86
1	A	119	PRO	N-CA-C	6.65	121.03	111.13
1	C	107	TYR	N-CA-C	6.59	119.89	109.81
1	D	111	ASP	CA-C-N	-6.39	112.57	122.16
1	D	111	ASP	C-N-CA	-6.39	112.57	122.16
1	A	235	GLY	N-CA-C	-6.35	107.13	114.69
1	C	195	LEU	N-CA-C	6.34	119.80	109.59
1	A	104	GLN	N-CA-C	6.33	115.59	108.25
1	C	90	GLY	N-CA-C	6.30	123.83	114.95
1	D	207	PRO	CA-C-N	6.29	126.81	120.14
1	D	207	PRO	C-N-CA	6.29	126.81	120.14
1	D	157	ASP	N-CA-C	-6.21	105.53	113.23
1	C	135	ARG	N-CA-C	-6.16	102.23	110.55
1	C	164	ASN	CB-CA-C	6.13	116.24	110.17
1	C	61	VAL	N-CA-C	6.12	116.43	107.37
1	A	118	GLU	CA-C-N	-6.11	114.48	120.52
1	A	118	GLU	C-N-CA	-6.11	114.48	120.52
1	D	158	LEU	CA-CB-CG	-6.09	95.00	116.30
1	D	209	MET	CA-C-N	-6.08	113.70	119.90
1	D	209	MET	C-N-CA	-6.08	113.70	119.90
1	A	109	TYR	CA-C-N	6.03	126.34	119.83
1	A	109	TYR	C-N-CA	6.03	126.34	119.83
1	B	206	ARG	CA-C-N	5.99	126.55	120.38
1	B	206	ARG	C-N-CA	5.99	126.55	120.38
1	D	118	GLU	N-CA-C	-5.89	100.39	109.41
1	D	162	ASN	N-CA-C	5.86	117.12	108.86
1	D	230	VAL	CA-C-N	-5.71	113.88	119.76
1	D	230	VAL	C-N-CA	-5.71	113.88	119.76
1	D	172	ALA	N-CA-C	-5.69	105.17	111.71
1	D	89	ALA	N-CA-C	-5.68	106.02	113.17
1	C	164	ASN	CA-C-N	5.64	125.17	119.19
1	C	164	ASN	C-N-CA	5.64	125.17	119.19
1	D	94	ARG	N-CA-C	-5.64	104.53	111.75
1	D	104	GLN	CA-C-N	5.64	125.65	119.90
1	D	104	GLN	C-N-CA	5.64	125.65	119.90
1	B	169	ILE	N-CA-C	-5.61	104.40	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	VAL	CB-CA-C	-5.58	104.73	112.04
1	D	67	THR	N-CA-C	5.50	117.21	108.79
1	D	113	LYS	CA-C-N	5.47	131.99	121.54
1	D	113	LYS	C-N-CA	5.47	131.99	121.54
1	A	107	TYR	N-CA-C	5.46	118.16	110.14
1	D	81	LYS	N-CA-C	-5.43	105.05	110.97
1	C	197	ARG	N-CA-C	-5.41	103.48	110.19
1	B	121	ILE	N-CA-C	5.36	115.91	108.84
1	C	51	SER	CA-C-N	5.32	125.22	119.85
1	C	51	SER	C-N-CA	5.32	125.22	119.85
1	B	118	GLU	CA-C-N	5.31	125.77	120.14
1	B	118	GLU	C-N-CA	5.31	125.77	120.14
1	B	55	ALA	N-CA-C	-5.29	100.68	108.99
1	C	246	VAL	N-CA-C	5.29	115.60	107.77
1	C	115	ASN	N-CA-C	-5.27	106.62	113.16
1	C	207	PRO	CA-C-N	5.26	125.17	119.85
1	C	207	PRO	C-N-CA	5.26	125.17	119.85
1	C	94	ARG	N-CA-C	-5.26	105.66	111.71
1	D	78	ALA	N-CA-C	-5.26	105.96	112.38
1	B	50	ALA	N-CA-C	5.25	116.50	108.42
1	B	103	ILE	N-CA-C	5.21	115.09	107.37
1	D	140	VAL	N-CA-C	5.20	118.40	111.44
1	C	162	ASN	N-CA-C	-5.16	101.47	109.72
1	A	121	ILE	N-CA-C	5.12	115.71	107.73
1	A	63	ARG	N-CA-C	-5.11	101.93	109.18
1	D	155	GLY	N-CA-C	5.02	121.75	114.67
1	B	64	GLN	N-CA-C	5.01	117.42	109.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASP	Peptide
1	A	114	ASN	Peptide
1	A	228	ASN	Peptide
1	D	112	ASP	Peptide
1	D	217	GLN	Peptide
1	D	65	ALA	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	1585	0	1629	217	0
1	B	1585	0	1629	208	1
1	C	1585	0	1629	235	3
1	D	1585	0	1629	226	3
All	All	6340	0	6516	812	4

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 63.

All (812) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:MET:CG	1:A:86:MET:SD	2.01	1.47
1:B:209:MET:CG	1:B:209:MET:SD	2.01	1.47
1:D:54:MET:CG	1:D:54:MET:SD	2.02	1.44
1:B:118:GLU:HG3	1:B:119:PRO:HD2	1.27	1.14
1:A:62:LEU:HB3	1:A:127:SER:HB2	1.28	1.14
1:B:47:MET:HE2	1:B:47:MET:HA	1.27	1.13
1:C:103:ILE:H	1:C:103:ILE:CD1	1.62	1.10
1:C:175:ARG:HH11	1:C:175:ARG:HB2	1.13	1.06
1:D:65:ALA:HB2	1:D:71:ALA:CB	1.85	1.05
1:C:103:ILE:HD12	1:C:103:ILE:N	1.64	1.05
1:C:103:ILE:HG23	1:C:126:VAL:CG2	1.87	1.05
1:D:65:ALA:CB	1:D:71:ALA:HB2	1.87	1.04
1:D:98:THR:HG22	1:D:130:LEU:HA	1.38	1.04
1:A:83:LEU:HD12	1:A:83:LEU:H	1.20	1.04
1:D:48:MET:HE1	1:D:171:GLU:HG2	1.39	1.04
1:C:175:ARG:HB2	1:C:175:ARG:NH1	1.73	1.02
1:D:91:ILE:HD11	1:D:143:ILE:HG21	1.41	1.02
1:A:182:ALA:HA	1:A:185:LYS:HE2	1.39	1.01
1:A:59:LEU:HB3	1:A:152:VAL:HG11	1.40	1.00
1:C:67:THR:HG22	1:C:70:GLU:OE1	1.60	0.99
1:B:103:ILE:H	1:C:158:LEU:HD21	1.23	0.99
1:A:61:VAL:HG23	1:A:152:VAL:HG22	1.42	0.99
1:A:121:ILE:HD12	1:A:121:ILE:H	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:HH11	1:C:175:ARG:CB	1.76	0.98
1:D:151:GLY:O	1:D:152:VAL:HG22	1.63	0.98
1:D:63:ARG:HH12	1:D:81:LYS:NZ	1.61	0.98
1:D:63:ARG:HH12	1:D:81:LYS:HZ1	1.00	0.97
1:C:114:ASN:HB3	1:C:116:LEU:CD1	1.96	0.95
1:C:103:ILE:H	1:C:103:ILE:HD12	0.81	0.95
1:A:230:VAL:HG12	1:A:231:PRO:HD2	1.46	0.95
1:A:193:VAL:HG11	1:A:249:ILE:HG23	1.46	0.95
1:C:79:MET:O	1:C:82:VAL:HG12	1.65	0.94
1:A:161:VAL:HG23	1:A:162:ASN:N	1.82	0.94
1:C:101:ILE:HD13	1:C:128:THR:HB	1.46	0.94
1:B:91:ILE:HD11	1:B:143:ILE:HD12	1.48	0.94
1:C:152:VAL:HG12	1:C:153:ASN:N	1.82	0.94
1:D:65:ALA:HB2	1:D:71:ALA:HB2	0.95	0.94
1:D:200:GLU:HB3	1:D:246:VAL:HG23	1.47	0.93
1:A:91:ILE:HG13	1:A:96:LEU:HD11	1.51	0.93
1:C:114:ASN:HB3	1:C:116:LEU:HD11	1.51	0.92
1:D:115:ASN:C	1:D:117:LYS:H	1.78	0.92
1:B:218:PHE:HD1	1:B:219:ARG:H	1.00	0.92
1:B:54:MET:HE2	1:B:135:ARG:HA	1.53	0.90
1:D:134:VAL:HG11	1:D:140:VAL:HG23	1.53	0.90
1:B:210:PRO:HB3	1:B:239:TYR:CE2	2.08	0.89
1:C:108:VAL:HG23	1:C:120:THR:HG23	1.54	0.89
1:C:91:ILE:HG23	1:C:96:LEU:HD23	1.52	0.89
1:D:140:VAL:HA	1:D:143:ILE:CD1	2.04	0.88
1:B:218:PHE:HD1	1:B:219:ARG:N	1.71	0.87
1:B:108:VAL:O	1:B:119:PRO:HA	1.75	0.86
1:B:47:MET:HA	1:B:47:MET:CE	2.04	0.86
1:C:61:VAL:HG22	1:C:128:THR:O	1.74	0.85
1:C:64:GLN:HB3	1:C:125:SER:HA	1.59	0.84
1:D:77:GLU:OE1	1:D:78:ALA:N	2.11	0.84
1:A:189:ASP:O	1:A:192:GLY:N	2.12	0.83
1:A:131:THR:HG23	1:B:233:ALA:HB2	1.60	0.83
1:D:200:GLU:HB3	1:D:246:VAL:CG2	2.09	0.83
1:C:157:ASP:HB3	1:D:218:PHE:CZ	2.13	0.83
1:B:110:PRO:HA	1:B:114:ASN:ND2	1.94	0.82
1:C:152:VAL:HG12	1:C:153:ASN:H	1.43	0.82
1:D:65:ALA:HB1	1:D:67:THR:H	1.44	0.82
1:D:67:THR:HG23	1:D:70:GLU:HB3	1.60	0.82
1:A:67:THR:HG22	1:A:70:GLU:OE1	1.79	0.82
1:C:218:PHE:CE2	1:C:219:ARG:HG2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HD11	1:B:154:GLN:NE2	1.94	0.82
1:D:57:LEU:HD21	1:D:132:VAL:HB	1.60	0.82
1:C:75:ASN:HD21	1:C:128:THR:HG22	1.43	0.81
1:D:198:VAL:HG22	1:D:247:PHE:CE2	2.15	0.81
1:B:53:ASP:O	1:B:54:MET:HE3	1.81	0.81
1:D:63:ARG:NH2	1:D:81:LYS:HZ2	1.78	0.81
1:D:147:SER:O	1:D:150:LEU:N	2.14	0.81
1:A:181:ILE:HG22	1:A:182:ALA:N	1.96	0.80
1:D:59:LEU:HD13	1:D:130:LEU:HD23	1.64	0.80
1:C:103:ILE:HG23	1:C:126:VAL:HG23	1.63	0.80
1:C:63:ARG:HH12	1:C:81:LYS:HZ1	1.26	0.80
1:B:133:ARG:HH21	1:C:231:PRO:HD3	1.44	0.80
1:B:169:ILE:HD11	1:B:239:TYR:CD2	2.15	0.80
1:C:103:ILE:HG23	1:C:126:VAL:HG22	1.63	0.80
1:D:48:MET:HG2	1:D:168:VAL:HG23	1.64	0.80
1:C:147:SER:HB3	1:C:152:VAL:HG11	1.62	0.80
1:B:233:ALA:O	1:B:236:GLU:HB2	1.81	0.80
1:A:60:SER:O	1:A:152:VAL:HG13	1.81	0.79
1:D:237:ASN:HB3	1:D:239:TYR:HE1	1.48	0.79
1:B:48:MET:CE	1:B:48:MET:HA	2.13	0.79
1:D:63:ARG:HH22	1:D:81:LYS:HZ2	1.28	0.79
1:B:131:THR:CG2	1:C:233:ALA:HA	2.14	0.78
1:C:63:ARG:HH12	1:C:81:LYS:NZ	1.81	0.78
1:A:114:ASN:O	1:A:115:ASN:HB2	1.83	0.78
1:A:67:THR:HG22	1:A:70:GLU:CG	2.13	0.78
1:B:45:GLU:OE1	1:B:45:GLU:N	2.16	0.78
1:B:60:SER:H	1:B:153:ASN:ND2	1.81	0.78
1:B:105:PRO:HG3	1:C:154:GLN:NE2	1.98	0.78
1:B:57:LEU:HB3	1:B:59:LEU:HD21	1.65	0.77
1:B:102:ASP:OD2	1:C:158:LEU:HD11	1.84	0.77
1:B:159:ASN:OD1	1:B:159:ASN:N	2.11	0.77
1:D:198:VAL:HG22	1:D:247:PHE:CD2	2.19	0.77
1:A:83:LEU:HD12	1:A:83:LEU:N	1.99	0.77
1:C:215:ARG:O	1:C:218:PHE:CD2	2.37	0.77
1:D:63:ARG:NH1	1:D:81:LYS:NZ	2.32	0.77
1:A:101:ILE:CG2	1:B:160:LEU:HD21	2.15	0.77
1:A:102:ASP:OD1	1:A:102:ASP:O	2.03	0.77
1:B:233:ALA:N	1:B:236:GLU:OE2	2.17	0.77
1:D:92:GLU:HG3	1:D:93:ASP:H	1.50	0.77
1:C:45:GLU:HB2	1:C:241:VAL:O	1.83	0.77
1:D:59:LEU:HD12	1:D:130:LEU:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:TYR:CE2	1:D:119:PRO:HG2	2.20	0.77
1:B:103:ILE:N	1:C:158:LEU:HD21	2.00	0.76
1:D:96:LEU:HD21	1:D:132:VAL:HG22	1.67	0.76
1:C:123:GLY:O	1:C:124:TYR:CD1	2.37	0.76
1:C:105:PRO:HG3	1:D:155:GLY:HA3	1.68	0.76
1:C:116:LEU:HD12	1:C:116:LEU:O	1.86	0.76
1:C:157:ASP:HB3	1:D:218:PHE:HZ	1.50	0.76
1:A:210:PRO:O	1:A:212:PRO:HD3	1.86	0.75
1:B:189:ASP:O	1:B:192:GLY:N	2.18	0.75
1:A:82:VAL:HG22	1:A:150:LEU:HD13	1.68	0.75
1:C:130:LEU:HD21	1:C:132:VAL:HG23	1.69	0.75
1:A:165:PRO:O	1:A:168:VAL:N	2.19	0.75
1:B:152:VAL:HG12	1:B:153:ASN:ND2	2.02	0.75
1:A:43:THR:HG22	1:A:244:ASN:OD1	1.87	0.74
1:D:63:ARG:HH22	1:D:81:LYS:NZ	1.85	0.74
1:B:116:LEU:O	1:B:116:LEU:HD22	1.87	0.74
1:A:166:SER:O	1:A:170:ASN:HB2	1.87	0.74
1:A:57:LEU:HD23	1:A:57:LEU:N	2.02	0.73
1:B:109:TYR:CD2	1:B:119:PRO:HB3	2.22	0.73
1:A:102:ASP:HB2	1:B:158:LEU:HD21	1.69	0.73
1:A:230:VAL:HG12	1:A:231:PRO:CD	2.18	0.73
1:C:60:SER:H	1:C:153:ASN:ND2	1.87	0.73
1:D:92:GLU:HG3	1:D:93:ASP:N	2.03	0.73
1:A:67:THR:HG22	1:A:70:GLU:HG2	1.70	0.72
1:A:193:VAL:HG11	1:A:249:ILE:CG2	2.17	0.72
1:A:103:ILE:HG22	1:A:126:VAL:HG22	1.71	0.71
1:B:72:MET:O	1:B:76:ASN:N	2.22	0.71
1:C:123:GLY:C	1:C:124:TYR:CD1	2.68	0.71
1:D:109:TYR:HE2	1:D:119:PRO:HG2	1.55	0.71
1:B:161:VAL:HG22	1:B:162:ASN:H	1.56	0.71
1:D:48:MET:CE	1:D:171:GLU:HB3	2.21	0.71
1:D:80:THR:HA	1:D:83:LEU:HB2	1.73	0.70
1:B:240:ASN:OD1	1:B:240:ASN:N	2.24	0.70
1:D:77:GLU:CD	1:D:78:ALA:N	2.50	0.70
1:B:56:ILE:O	1:B:159:ASN:ND2	2.25	0.70
1:C:143:ILE:O	1:C:143:ILE:HD12	1.92	0.70
1:A:79:MET:HE3	1:A:79:MET:HA	1.74	0.69
1:D:140:VAL:HA	1:D:143:ILE:HD11	1.74	0.69
1:D:57:LEU:CD2	1:D:132:VAL:HB	2.22	0.69
1:B:48:MET:HA	1:B:48:MET:HE2	1.76	0.68
1:B:91:ILE:CG2	1:B:96:LEU:HD11	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLY:C	1:D:124:TYR:HD1	2.02	0.68
1:A:110:PRO:N	1:A:116:LEU:HD11	2.08	0.68
1:B:79:MET:HE3	1:B:98:THR:HG21	1.76	0.67
1:C:54:MET:HE1	1:C:133:ARG:HG2	1.76	0.67
1:A:193:VAL:CG1	1:A:249:ILE:HG23	2.21	0.67
1:D:48:MET:HE1	1:D:171:GLU:CG	2.20	0.67
1:D:109:TYR:CD2	1:D:119:PRO:CG	2.77	0.67
1:D:233:ALA:O	1:D:236:GLU:HG3	1.95	0.67
1:A:63:ARG:NH2	1:A:81:LYS:HZ2	1.91	0.67
1:C:103:ILE:HD11	1:D:158:LEU:HD13	1.76	0.67
1:D:46:GLY:H	1:D:176:ALA:HB2	1.59	0.67
1:D:106:ILE:HD11	1:D:124:TYR:C	2.18	0.67
1:A:78:ALA:HA	1:A:81:LYS:HE3	1.75	0.67
1:C:101:ILE:CD1	1:C:128:THR:HB	2.23	0.67
1:B:131:THR:HG21	1:C:232:ILE:O	1.94	0.67
1:C:209:MET:HB2	1:C:211:MET:HE3	1.76	0.67
1:D:63:ARG:NH1	1:D:81:LYS:HZ1	1.83	0.67
1:C:79:MET:CE	1:C:128:THR:HG23	2.24	0.67
1:D:48:MET:HG3	1:D:49:THR:H	1.60	0.67
1:D:140:VAL:HA	1:D:143:ILE:HD12	1.76	0.67
1:C:61:VAL:O	1:C:127:SER:OG	2.08	0.67
1:C:112:ASP:OD1	1:C:112:ASP:C	2.37	0.67
1:D:146:GLU:O	1:D:150:LEU:HG	1.95	0.67
1:B:63:ARG:HH11	1:B:78:ALA:HB2	1.58	0.67
1:D:97:GLN:HG3	1:D:98:THR:N	2.08	0.67
1:C:181:ILE:CG2	1:C:185:LYS:HE3	2.25	0.67
1:D:49:THR:HG21	1:D:232:ILE:HD12	1.77	0.67
1:C:130:LEU:CD2	1:C:132:VAL:HG23	2.25	0.66
1:C:154:GLN:OE1	1:C:155:GLY:N	2.28	0.66
1:A:195:LEU:C	1:A:195:LEU:HD12	2.19	0.66
1:D:219:ARG:O	1:D:222:LEU:N	2.28	0.66
1:A:131:THR:HG23	1:B:233:ALA:CB	2.25	0.66
1:B:59:LEU:HA	1:B:153:ASN:HD21	1.61	0.66
1:C:68:ALA:O	1:C:71:ALA:HB3	1.94	0.66
1:D:41:ALA:HB2	1:D:246:VAL:HG13	1.78	0.66
1:A:218:PHE:H	1:A:218:PHE:HD2	1.44	0.66
1:C:82:VAL:HG23	1:C:150:LEU:CD2	2.25	0.66
1:C:128:THR:OG1	1:C:129:SER:N	2.23	0.66
1:A:243:VAL:HG23	1:A:244:ASN:N	2.11	0.66
1:B:210:PRO:HB3	1:B:239:TYR:CZ	2.30	0.66
1:D:59:LEU:CD1	1:D:130:LEU:HD23	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:O	1:B:118:GLU:HB2	1.95	0.66
1:B:131:THR:HG21	1:C:233:ALA:HA	1.77	0.66
1:A:219:ARG:HA	1:A:222:LEU:HD11	1.77	0.65
1:B:47:MET:HE1	1:B:240:ASN:CG	2.20	0.65
1:B:59:LEU:CA	1:B:153:ASN:HD21	2.09	0.65
1:A:98:THR:HG23	1:A:130:LEU:HD12	1.77	0.65
1:B:61:VAL:HG11	1:B:82:VAL:HG11	1.79	0.65
1:C:82:VAL:O	1:C:85:ALA:HB3	1.97	0.65
1:A:91:ILE:CG1	1:A:96:LEU:HD11	2.26	0.65
1:B:118:GLU:HG3	1:B:119:PRO:CD	2.16	0.65
1:C:131:THR:OG1	1:D:233:ALA:HB2	1.97	0.65
1:C:137:LEU:O	1:C:139:ASN:N	2.30	0.65
1:A:240:ASN:OD1	1:A:240:ASN:N	2.26	0.64
1:C:53:ASP:HB2	1:C:162:ASN:HA	1.79	0.64
1:C:54:MET:CE	1:C:133:ARG:HG2	2.27	0.64
1:D:65:ALA:CB	1:D:67:THR:H	2.09	0.64
1:B:43:THR:HG22	1:B:244:ASN:OD1	1.97	0.64
1:B:171:GLU:OE2	1:B:175:ARG:HD3	1.96	0.64
1:D:48:MET:CE	1:D:171:GLU:HG2	2.21	0.64
1:D:98:THR:HB	1:D:129:SER:O	1.97	0.64
1:D:49:THR:HG21	1:D:232:ILE:CD1	2.27	0.64
1:C:110:PRO:HA	1:C:116:LEU:HD11	1.80	0.64
1:C:184:ALA:HB1	1:C:195:LEU:HD21	1.80	0.64
1:A:49:THR:HG21	1:A:232:ILE:HD11	1.80	0.64
1:C:78:ALA:HA	1:C:81:LYS:HE3	1.80	0.64
1:A:179:ASN:OD1	1:A:179:ASN:C	2.41	0.63
1:C:218:PHE:CD2	1:C:219:ARG:HG2	2.33	0.63
1:B:91:ILE:HG21	1:B:96:LEU:HD11	1.80	0.63
1:B:225:ALA:HB1	1:B:226:PRO:HD2	1.81	0.63
1:D:98:THR:HG22	1:D:130:LEU:CA	2.23	0.63
1:C:110:PRO:HA	1:C:116:LEU:CD1	2.28	0.63
1:C:217:GLN:HB3	1:C:221:MET:HG2	1.79	0.63
1:A:163:ASP:O	1:A:165:PRO:HD3	1.97	0.63
1:B:157:ASP:O	1:B:159:ASN:OD1	2.17	0.63
1:B:140:VAL:HA	1:B:143:ILE:HG22	1.81	0.63
1:B:133:ARG:NH2	1:C:231:PRO:HD3	2.14	0.63
1:C:124:TYR:OH	1:D:148:VAL:HG21	1.99	0.63
1:D:184:ALA:HB2	1:D:247:PHE:HE1	1.63	0.63
1:D:82:VAL:HG23	1:D:150:LEU:HD12	1.79	0.63
1:B:123:GLY:C	1:B:124:TYR:CD1	2.77	0.62
1:D:115:ASN:C	1:D:117:LYS:N	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:O	1:C:61:VAL:HG23	2.00	0.62
1:D:109:TYR:CE2	1:D:119:PRO:CG	2.82	0.62
1:A:173:ARG:HD2	1:B:186:THR:HG21	1.82	0.62
1:A:215:ARG:O	1:A:218:PHE:CD2	2.52	0.62
1:C:60:SER:H	1:C:153:ASN:HD21	1.46	0.62
1:A:86:MET:HA	1:A:89:ALA:HB3	1.82	0.62
1:D:108:VAL:HG12	1:D:120:THR:O	2.00	0.62
1:D:118:GLU:HG3	1:D:119:PRO:O	1.99	0.62
1:B:68:ALA:O	1:B:71:ALA:HB3	2.00	0.61
1:B:168:VAL:HG12	1:B:169:ILE:N	2.14	0.61
1:C:45:GLU:HB3	1:C:242:SER:HA	1.81	0.61
1:C:139:ASN:O	1:C:143:ILE:HG23	2.00	0.61
1:D:103:ILE:HG23	1:D:126:VAL:CG2	2.30	0.61
1:A:59:LEU:HB3	1:A:152:VAL:CG1	2.24	0.61
1:A:63:ARG:HH22	1:A:81:LYS:NZ	1.99	0.61
1:D:150:LEU:N	1:D:150:LEU:HD23	2.15	0.61
1:B:114:ASN:O	1:B:115:ASN:CG	2.43	0.61
1:B:131:THR:HG23	1:C:233:ALA:HA	1.81	0.61
1:C:230:VAL:HG12	1:C:231:PRO:HD2	1.81	0.61
1:D:110:PRO:HA	1:D:114:ASN:HB3	1.82	0.61
1:C:68:ALA:HB3	1:D:145:ASP:OD2	2.00	0.61
1:C:150:LEU:HD12	1:C:151:GLY:N	2.16	0.61
1:A:67:THR:HG22	1:A:70:GLU:CD	2.25	0.61
1:C:199:VAL:HG12	1:C:246:VAL:O	2.00	0.61
1:B:218:PHE:CD1	1:B:219:ARG:N	2.56	0.61
1:C:147:SER:O	1:C:152:VAL:HB	2.00	0.61
1:A:91:ILE:CG2	1:A:143:ILE:HD11	2.31	0.60
1:D:66:LYS:O	1:D:66:LYS:HG2	2.01	0.60
1:D:110:PRO:HG3	1:D:118:GLU:O	2.00	0.60
1:C:45:GLU:N	1:C:45:GLU:OE1	2.35	0.60
1:A:63:ARG:HH12	1:A:81:LYS:HZ1	1.50	0.60
1:A:158:LEU:HD13	1:A:158:LEU:H	1.67	0.60
1:A:173:ARG:NH1	1:A:203:GLU:OE2	2.34	0.60
1:C:130:LEU:HD23	1:C:130:LEU:C	2.26	0.60
1:C:120:THR:OG1	1:C:121:ILE:N	2.35	0.60
1:D:48:MET:HG3	1:D:49:THR:N	2.17	0.60
1:D:61:VAL:HG12	1:D:152:VAL:HG12	1.84	0.60
1:A:85:ALA:O	1:A:88:LYS:HG3	2.02	0.59
1:C:111:ASP:H	1:C:114:ASN:HB2	1.68	0.59
1:C:155:GLY:C	1:C:157:ASP:H	2.10	0.59
1:B:58:ASN:C	1:B:59:LEU:HD23	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HA	1:A:83:LEU:CD1	2.33	0.59
1:A:101:ILE:HG23	1:B:160:LEU:HD21	1.82	0.59
1:A:153:ASN:OD1	1:A:154:GLN:N	2.36	0.59
1:A:160:LEU:H	1:A:160:LEU:HD23	1.67	0.59
1:B:118:GLU:CG	1:B:119:PRO:HD2	2.19	0.59
1:B:163:ASP:C	1:B:165:PRO:HD3	2.27	0.59
1:C:103:ILE:CD1	1:C:103:ILE:N	2.38	0.59
1:C:145:ASP:O	1:C:149:THR:OG1	2.19	0.59
1:D:38:ALA:C	1:D:39:ARG:HG2	2.28	0.59
1:B:57:LEU:HB2	1:B:132:VAL:HG22	1.83	0.59
1:B:67:THR:HG23	1:B:70:GLU:OE1	2.03	0.59
1:D:184:ALA:HB1	1:D:195:LEU:HD11	1.85	0.59
1:D:217:GLN:O	1:D:218:PHE:C	2.45	0.59
1:A:62:LEU:HB3	1:A:127:SER:CB	2.19	0.59
1:B:92:GLU:HG3	1:B:94:ARG:H	1.67	0.59
1:D:46:GLY:H	1:D:176:ALA:CB	2.15	0.59
1:B:53:ASP:OD1	1:B:162:ASN:HA	2.02	0.58
1:C:101:ILE:HD13	1:C:128:THR:CB	2.26	0.58
1:A:109:TYR:HD2	1:A:119:PRO:HG3	1.68	0.58
1:C:91:ILE:CG2	1:C:96:LEU:HD23	2.29	0.58
1:C:152:VAL:HG12	1:C:153:ASN:CG	2.28	0.58
1:D:240:ASN:N	1:D:240:ASN:OD1	2.37	0.58
1:B:59:LEU:HB3	1:B:153:ASN:HD21	1.67	0.58
1:C:101:ILE:HD12	1:C:127:SER:O	2.04	0.58
1:D:184:ALA:CB	1:D:247:PHE:CE1	2.86	0.58
1:A:163:ASP:O	1:A:165:PRO:CD	2.51	0.58
1:B:47:MET:O	1:B:48:MET:HG2	2.03	0.58
1:C:169:ILE:HG22	1:C:170:ASN:N	2.19	0.58
1:A:189:ASP:O	1:A:191:ALA:N	2.36	0.58
1:A:209:MET:HE2	1:A:211:MET:HE2	1.86	0.58
1:B:63:ARG:HH11	1:B:78:ALA:CB	2.17	0.58
1:D:139:ASN:O	1:D:143:ILE:HD11	2.03	0.58
1:D:238:SER:C	1:D:239:TYR:HD1	2.12	0.58
1:A:114:ASN:O	1:A:115:ASN:CB	2.50	0.58
1:D:201:ILE:HD13	1:D:245:VAL:HG13	1.85	0.58
1:C:48:MET:HE3	1:C:171:GLU:CG	2.34	0.58
1:B:116:LEU:HD13	1:B:118:GLU:HB3	1.86	0.57
1:D:61:VAL:HG23	1:D:61:VAL:O	2.03	0.57
1:D:78:ALA:O	1:D:81:LYS:HB2	2.04	0.57
1:A:147:SER:O	1:A:151:GLY:O	2.21	0.57
1:A:158:LEU:HD13	1:A:158:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:CA	1:A:185:LYS:HE2	2.26	0.57
1:B:97:GLN:O	1:B:130:LEU:HD12	2.04	0.57
1:A:131:THR:HG21	1:B:232:ILE:O	2.04	0.57
1:A:121:ILE:HD12	1:A:121:ILE:N	2.07	0.57
1:B:110:PRO:HA	1:B:114:ASN:CG	2.29	0.57
1:C:82:VAL:HG23	1:C:150:LEU:HD22	1.86	0.57
1:A:182:ALA:HA	1:A:185:LYS:CE	2.26	0.57
1:C:108:VAL:CG2	1:C:120:THR:HG23	2.32	0.57
1:D:188:ALA:HB1	1:D:193:VAL:HG23	1.87	0.57
1:A:80:THR:HA	1:A:83:LEU:HD11	1.86	0.57
1:D:109:TYR:HD2	1:D:119:PRO:CG	2.17	0.57
1:A:117:LYS:HG3	1:A:117:LYS:O	2.04	0.57
1:A:198:VAL:HG12	1:A:198:VAL:O	2.05	0.57
1:A:110:PRO:CA	1:A:116:LEU:HD11	2.35	0.57
1:D:63:ARG:NH2	1:D:81:LYS:NZ	2.49	0.57
1:B:250:LYS:O	1:B:250:LYS:HD3	2.05	0.56
1:C:91:ILE:HG23	1:C:96:LEU:CD2	2.29	0.56
1:D:98:THR:CG2	1:D:130:LEU:HA	2.25	0.56
1:A:207:PRO:HG3	1:B:45:GLU:OE2	2.06	0.56
1:A:218:PHE:CD2	1:A:218:PHE:N	2.72	0.56
1:D:114:ASN:ND2	1:D:117:LYS:HG2	2.21	0.56
1:B:91:ILE:HD11	1:B:143:ILE:CD1	2.30	0.56
1:C:184:ALA:HB1	1:C:195:LEU:CD2	2.35	0.56
1:D:43:THR:HG22	1:D:244:ASN:OD1	2.05	0.56
1:C:61:VAL:CG2	1:C:128:THR:H	2.19	0.56
1:C:98:THR:HG22	1:C:130:LEU:HB2	1.87	0.56
1:D:103:ILE:HG23	1:D:126:VAL:HG23	1.88	0.56
1:A:111:ASP:O	1:A:114:ASN:N	2.38	0.56
1:C:48:MET:HE1	1:C:175:ARG:NH1	2.21	0.56
1:D:63:ARG:CZ	1:D:81:LYS:HZ2	2.19	0.56
1:D:202:SER:HB2	1:D:204:LEU:HD11	1.87	0.56
1:D:204:LEU:HD12	1:D:204:LEU:N	2.21	0.56
1:D:123:GLY:C	1:D:124:TYR:CD1	2.84	0.56
1:B:53:ASP:C	1:B:54:MET:HE3	2.30	0.55
1:D:109:TYR:CD2	1:D:119:PRO:HB3	2.40	0.55
1:A:154:GLN:NE2	1:A:157:ASP:OD2	2.40	0.55
1:D:57:LEU:CD2	1:D:132:VAL:O	2.53	0.55
1:D:116:LEU:C	1:D:118:GLU:H	2.14	0.55
1:D:215:ARG:O	1:D:218:PHE:CG	2.60	0.55
1:A:49:THR:HG21	1:A:232:ILE:CD1	2.36	0.55
1:B:134:VAL:HG22	1:B:143:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLY:C	1:A:152:VAL:HG23	2.31	0.55
1:A:109:TYR:CD2	1:A:119:PRO:HG3	2.42	0.55
1:A:133:ARG:CZ	1:B:231:PRO:HG3	2.36	0.55
1:C:82:VAL:HG23	1:C:150:LEU:HD21	1.87	0.55
1:C:111:ASP:O	1:C:114:ASN:HB2	2.06	0.55
1:C:114:ASN:HB3	1:C:116:LEU:HD12	1.85	0.55
1:D:184:ALA:HB2	1:D:247:PHE:CE1	2.40	0.55
1:A:184:ALA:HB1	1:A:195:LEU:HD22	1.89	0.55
1:D:203:GLU:HG3	1:D:203:GLU:O	2.07	0.55
1:A:117:LYS:O	1:A:117:LYS:CG	2.54	0.55
1:C:103:ILE:CD1	1:D:158:LEU:HD13	2.36	0.55
1:B:101:ILE:HD11	1:B:126:VAL:CG1	2.37	0.55
1:B:173:ARG:O	1:B:176:ALA:HB3	2.06	0.55
1:B:216:GLY:C	1:B:218:PHE:H	2.13	0.55
1:A:63:ARG:NH2	1:A:81:LYS:NZ	2.54	0.55
1:A:152:VAL:HG12	1:A:152:VAL:O	2.05	0.55
1:B:161:VAL:HG22	1:B:162:ASN:N	2.22	0.55
1:C:123:GLY:C	1:C:124:TYR:HD1	2.11	0.55
1:C:114:ASN:CB	1:C:116:LEU:HD11	2.33	0.55
1:B:102:ASP:CG	1:C:158:LEU:HD11	2.33	0.54
1:C:95:ASP:OD2	1:C:133:ARG:HD2	2.07	0.54
1:C:45:GLU:CB	1:C:241:VAL:O	2.53	0.54
1:C:82:VAL:HG13	1:C:83:LEU:N	2.22	0.54
1:C:152:VAL:CG1	1:C:153:ASN:N	2.53	0.54
1:D:109:TYR:CD2	1:D:119:PRO:CB	2.90	0.54
1:A:91:ILE:HG23	1:A:143:ILE:HD11	1.89	0.54
1:C:133:ARG:HH21	1:D:231:PRO:HD3	1.72	0.54
1:B:184:ALA:HB2	1:B:247:PHE:CE1	2.43	0.54
1:C:218:PHE:CD2	1:C:218:PHE:N	2.75	0.54
1:B:101:ILE:HD11	1:B:126:VAL:HG13	1.90	0.54
1:C:159:ASN:O	1:C:160:LEU:HD23	2.07	0.54
1:C:172:ALA:O	1:C:173:ARG:C	2.50	0.54
1:D:87:LYS:NZ	1:D:93:ASP:OD1	2.22	0.54
1:D:108:VAL:O	1:D:119:PRO:HB3	2.07	0.54
1:D:147:SER:O	1:D:149:THR:N	2.41	0.54
1:B:108:VAL:HG12	1:B:109:TYR:N	2.22	0.54
1:B:161:VAL:HG13	1:B:162:ASN:N	2.23	0.54
1:D:198:VAL:CG2	1:D:247:PHE:CE2	2.90	0.54
1:A:121:ILE:HD11	1:B:154:GLN:HE22	1.72	0.54
1:C:218:PHE:N	1:C:218:PHE:HD2	2.05	0.54
1:A:63:ARG:HD2	1:A:78:ALA:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLN:CB	1:C:125:SER:HA	2.34	0.54
1:A:110:PRO:CD	1:A:116:LEU:HD11	2.38	0.53
1:B:210:PRO:HD2	1:C:223:ALA:HB1	1.90	0.53
1:D:151:GLY:O	1:D:152:VAL:CG2	2.47	0.53
1:C:48:MET:HE1	1:C:175:ARG:CZ	2.39	0.53
1:C:212:PRO:HA	1:C:237:ASN:OD1	2.08	0.53
1:D:44:GLY:HA3	1:D:180:ALA:HB2	1.89	0.53
1:D:47:MET:HG2	1:D:48:MET:N	2.21	0.53
1:D:137:LEU:O	1:D:139:ASN:N	2.41	0.53
1:A:68:ALA:HB3	1:B:145:ASP:OD1	2.08	0.53
1:A:76:ASN:O	1:A:79:MET:HB3	2.07	0.53
1:A:103:ILE:CG2	1:A:126:VAL:HG22	2.38	0.53
1:B:145:ASP:O	1:B:148:VAL:HG12	2.08	0.53
1:A:68:ALA:HB2	1:B:144:LEU:HD23	1.88	0.53
1:C:58:ASN:C	1:C:59:LEU:HD23	2.34	0.53
1:D:109:TYR:HD2	1:D:119:PRO:HB3	1.74	0.53
1:A:153:ASN:CG	1:A:154:GLN:H	2.16	0.53
1:A:67:THR:O	1:A:70:GLU:HG3	2.09	0.53
1:C:56:ILE:O	1:C:159:ASN:HB2	2.09	0.53
1:C:75:ASN:O	1:C:76:ASN:C	2.52	0.53
1:D:239:TYR:HD1	1:D:239:TYR:N	2.06	0.53
1:B:184:ALA:HB1	1:B:195:LEU:HD21	1.91	0.52
1:A:154:GLN:CD	1:A:157:ASP:OD2	2.52	0.52
1:C:144:LEU:O	1:C:147:SER:N	2.41	0.52
1:C:195:LEU:HD22	1:C:247:PHE:CG	2.44	0.52
1:D:46:GLY:N	1:D:176:ALA:HA	2.24	0.52
1:A:47:MET:HE1	1:A:221:MET:SD	2.50	0.52
1:A:101:ILE:HG22	1:B:160:LEU:CD2	2.39	0.52
1:A:114:ASN:HA	1:A:116:LEU:HD23	1.90	0.52
1:A:116:LEU:HD12	1:A:118:GLU:O	2.09	0.52
1:B:59:LEU:CB	1:B:153:ASN:HD21	2.23	0.52
1:B:68:ALA:HA	1:B:71:ALA:HB2	1.91	0.52
1:C:161:VAL:HG12	1:C:162:ASN:H	1.74	0.52
1:A:100:GLY:HA3	1:B:235:GLY:HA3	1.90	0.52
1:C:135:ARG:O	1:C:136:GLU:HB2	2.09	0.52
1:B:168:VAL:HG12	1:B:169:ILE:HD13	1.92	0.52
1:B:211:MET:HB2	1:B:238:SER:O	2.09	0.52
1:C:43:THR:HB	1:C:244:ASN:OD1	2.10	0.52
1:D:159:ASN:C	1:D:160:LEU:HD23	2.34	0.52
1:D:49:THR:OG1	1:D:236:GLU:OE1	2.26	0.52
1:A:159:ASN:O	1:A:161:VAL:CG1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:PRO:HB3	1:D:160:LEU:HB2	1.91	0.52
1:A:110:PRO:HD3	1:A:116:LEU:CD1	2.40	0.51
1:C:148:VAL:HG12	1:C:149:THR:N	2.25	0.51
1:D:48:MET:HE2	1:D:171:GLU:HB3	1.92	0.51
1:D:213:ILE:CD1	1:D:236:GLU:O	2.58	0.51
1:A:209:MET:HE3	1:A:210:PRO:CD	2.41	0.51
1:D:106:ILE:HD12	1:D:125:SER:HB2	1.92	0.51
1:A:209:MET:HE3	1:A:210:PRO:N	2.26	0.51
1:A:78:ALA:HA	1:A:81:LYS:HG3	1.92	0.51
1:A:207:PRO:CG	1:B:45:GLU:OE2	2.59	0.51
1:D:203:GLU:HB3	1:D:243:VAL:HG23	1.93	0.51
1:B:103:ILE:H	1:C:158:LEU:CD2	2.10	0.51
1:C:57:LEU:HD12	1:C:57:LEU:N	2.24	0.51
1:D:184:ALA:O	1:D:187:LEU:HB2	2.10	0.51
1:A:61:VAL:CG1	1:A:61:VAL:O	2.59	0.51
1:B:49:THR:HG21	1:B:232:ILE:CD1	2.41	0.51
1:C:80:THR:HA	1:C:83:LEU:HD12	1.92	0.51
1:A:165:PRO:O	1:A:166:SER:C	2.54	0.51
1:B:169:ILE:CD1	1:B:239:TYR:CD2	2.92	0.51
1:C:47:MET:HE3	1:C:240:ASN:HD22	1.76	0.51
1:C:147:SER:HA	1:C:152:VAL:HG21	1.93	0.51
1:C:175:ARG:NH1	1:C:175:ARG:CB	2.52	0.51
1:D:209:MET:O	1:D:210:PRO:C	2.53	0.51
1:A:86:MET:HB3	1:A:91:ILE:HD11	1.92	0.51
1:A:49:THR:CG2	1:A:232:ILE:HD11	2.40	0.51
1:A:61:VAL:HG23	1:A:152:VAL:CG2	2.29	0.51
1:A:121:ILE:H	1:A:121:ILE:CD1	1.99	0.51
1:B:82:VAL:HG23	1:B:150:LEU:HD22	1.92	0.51
1:B:68:ALA:O	1:B:71:ALA:CB	2.60	0.50
1:B:215:ARG:O	1:B:218:PHE:HB3	2.11	0.50
1:B:63:ARG:HD3	1:B:78:ALA:HB2	1.93	0.50
1:C:199:VAL:N	1:C:246:VAL:O	2.36	0.50
1:D:239:TYR:N	1:D:239:TYR:CD1	2.77	0.50
1:A:131:THR:CG2	1:B:233:ALA:HB2	2.37	0.50
1:C:64:GLN:HB3	1:C:125:SER:CA	2.36	0.50
1:C:95:ASP:OD1	1:C:135:ARG:HD2	2.12	0.50
1:A:111:ASP:H	1:A:114:ASN:HB3	1.76	0.50
1:A:77:GLU:O	1:A:81:LYS:HG3	2.12	0.50
1:B:124:TYR:OH	1:C:148:VAL:CG2	2.60	0.50
1:B:123:GLY:O	1:B:124:TYR:CD1	2.65	0.50
1:B:249:ILE:HG22	1:B:250:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:NH1	1:C:203:GLU:OE1	2.43	0.50
1:C:178:ALA:HA	1:C:181:ILE:HD12	1.93	0.50
1:D:41:ALA:CB	1:D:246:VAL:HG13	2.41	0.50
1:A:218:PHE:HD2	1:A:218:PHE:N	2.07	0.50
1:C:131:THR:OG1	1:D:233:ALA:CB	2.59	0.50
1:D:213:ILE:N	1:D:213:ILE:HD12	2.26	0.50
1:A:68:ALA:HB3	1:B:145:ASP:CG	2.37	0.49
1:D:116:LEU:O	1:D:118:GLU:N	2.37	0.49
1:D:153:ASN:OD1	1:D:156:GLY:N	2.45	0.49
1:C:56:ILE:HD12	1:D:222:LEU:HD13	1.94	0.49
1:C:117:LYS:O	1:C:118:GLU:HG3	2.12	0.49
1:D:84:ASP:C	1:D:86:MET:N	2.70	0.49
1:A:111:ASP:O	1:A:114:ASN:HB3	2.12	0.49
1:C:193:VAL:HB	1:C:249:ILE:CG2	2.43	0.49
1:C:188:ALA:HB1	1:C:193:VAL:O	2.12	0.49
1:D:62:LEU:HD13	1:D:62:LEU:O	2.12	0.49
1:B:106:ILE:HD11	1:B:125:SER:HB2	1.94	0.49
1:C:39:ARG:HA	1:C:247:PHE:O	2.13	0.49
1:D:147:SER:C	1:D:149:THR:N	2.69	0.49
1:A:86:MET:O	1:A:89:ALA:N	2.45	0.49
1:B:168:VAL:HG11	1:B:239:TYR:CD1	2.46	0.49
1:B:218:PHE:O	1:B:222:LEU:HD13	2.12	0.49
1:D:217:GLN:HB3	1:D:221:MET:HG2	1.94	0.49
1:A:198:VAL:HG22	1:A:247:PHE:CD2	2.48	0.49
1:B:55:ALA:HB3	1:B:134:VAL:HB	1.94	0.49
1:C:217:GLN:O	1:C:218:PHE:C	2.55	0.49
1:A:111:ASP:O	1:A:114:ASN:CB	2.61	0.49
1:A:177:VAL:HG12	1:A:181:ILE:HD12	1.94	0.49
1:B:144:LEU:O	1:B:147:SER:HB2	2.13	0.49
1:B:161:VAL:HG13	1:B:162:ASN:C	2.38	0.49
1:D:59:LEU:HD12	1:D:59:LEU:H	1.77	0.49
1:D:109:TYR:HD2	1:D:119:PRO:CB	2.25	0.49
1:D:122:THR:O	1:D:122:THR:OG1	2.31	0.49
1:A:221:MET:HE3	1:A:238:SER:OG	2.12	0.48
1:C:152:VAL:CG1	1:C:153:ASN:H	2.11	0.48
1:C:164:ASN:HB2	1:D:227:ASP:OD2	2.13	0.48
1:A:101:ILE:CG2	1:B:160:LEU:CD2	2.90	0.48
1:B:48:MET:HA	1:B:48:MET:HE3	1.94	0.48
1:C:121:ILE:N	1:C:121:ILE:HD13	2.28	0.48
1:D:151:GLY:C	1:D:152:VAL:HG13	2.37	0.48
1:B:112:ASP:O	1:B:113:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:CG2	1:A:70:GLU:HG2	2.43	0.48
1:C:54:MET:HE1	1:C:133:ARG:CG	2.41	0.48
1:A:158:LEU:N	1:A:158:LEU:HD22	2.29	0.48
1:A:204:LEU:HA	1:B:43:THR:HG23	1.95	0.48
1:C:204:LEU:HD23	1:D:43:THR:HG23	1.95	0.48
1:A:207:PRO:HB3	1:B:45:GLU:OE2	2.13	0.48
1:B:59:LEU:HB3	1:B:152:VAL:CG1	2.44	0.48
1:B:114:ASN:O	1:B:115:ASN:OD1	2.31	0.48
1:B:206:ARG:HB2	1:B:206:ARG:NH1	2.28	0.48
1:C:152:VAL:CG1	1:C:153:ASN:CG	2.86	0.48
1:B:216:GLY:HA2	1:B:218:PHE:CD2	2.48	0.48
1:C:240:ASN:OD1	1:C:240:ASN:C	2.57	0.48
1:D:100:GLY:C	1:D:101:ILE:HG12	2.38	0.48
1:A:249:ILE:O	1:A:250:LYS:HB2	2.14	0.48
1:B:60:SER:H	1:B:153:ASN:HD22	1.59	0.48
1:C:221:MET:O	1:C:222:LEU:C	2.56	0.48
1:D:82:VAL:CG2	1:D:150:LEU:HD12	2.43	0.48
1:D:166:SER:O	1:D:170:ASN:HB2	2.14	0.48
1:B:61:VAL:HG23	1:B:61:VAL:O	2.14	0.48
1:B:214:ALA:HB3	1:B:217:GLN:CG	2.44	0.48
1:C:72:MET:O	1:C:75:ASN:HB3	2.14	0.48
1:A:57:LEU:N	1:A:57:LEU:CD2	2.72	0.47
1:C:111:ASP:OD1	1:C:112:ASP:N	2.43	0.47
1:C:170:ASN:O	1:C:173:ARG:HB3	2.14	0.47
1:D:49:THR:CB	1:D:232:ILE:HD11	2.44	0.47
1:D:60:SER:O	1:D:152:VAL:HA	2.14	0.47
1:B:159:ASN:O	1:B:160:LEU:HD12	2.14	0.47
1:D:161:VAL:HG22	1:D:162:ASN:H	1.80	0.47
1:C:91:ILE:HG13	1:C:92:GLU:H	1.79	0.47
1:D:46:GLY:N	1:D:176:ALA:HB2	2.29	0.47
1:D:200:GLU:CB	1:D:246:VAL:HG23	2.33	0.47
1:D:225:ALA:O	1:D:226:PRO:C	2.56	0.47
1:C:114:ASN:HD22	1:C:116:LEU:HD11	1.80	0.47
1:D:96:LEU:HD23	1:D:96:LEU:HA	1.63	0.47
1:B:204:LEU:HA	1:C:43:THR:CG2	2.44	0.47
1:C:152:VAL:HG13	1:C:153:ASN:ND2	2.30	0.47
1:D:67:THR:HG23	1:D:70:GLU:CB	2.39	0.47
1:D:79:MET:HE3	1:D:82:VAL:HG13	1.97	0.47
1:A:82:VAL:CG2	1:A:150:LEU:HD13	2.41	0.47
1:C:151:GLY:O	1:C:152:VAL:HB	2.14	0.47
1:C:215:ARG:O	1:C:218:PHE:CG	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD21	1:D:132:VAL:CB	2.35	0.47
1:D:57:LEU:HD23	1:D:57:LEU:H	1.79	0.47
1:D:159:ASN:N	1:D:159:ASN:OD1	2.48	0.47
1:B:162:ASN:O	1:B:165:PRO:HG3	2.15	0.47
1:D:181:ILE:HA	1:D:247:PHE:CZ	2.49	0.47
1:B:48:MET:HE2	1:B:49:THR:H	1.80	0.47
1:C:103:ILE:HD13	1:D:158:LEU:HD12	1.97	0.47
1:B:110:PRO:HG3	1:B:118:GLU:CA	2.44	0.47
1:D:87:LYS:C	1:D:90:GLY:H	2.23	0.47
1:A:75:ASN:O	1:A:76:ASN:C	2.57	0.46
1:A:110:PRO:HD3	1:A:116:LEU:HD11	1.98	0.46
1:C:162:ASN:OD1	1:C:162:ASN:N	2.48	0.46
1:C:111:ASP:H	1:C:114:ASN:CB	2.28	0.46
1:C:137:LEU:O	1:C:138:ALA:C	2.57	0.46
1:D:185:LYS:HD2	1:D:189:ASP:OD1	2.15	0.46
1:C:48:MET:HE1	1:C:175:ARG:NH2	2.30	0.46
1:C:139:ASN:O	1:C:143:ILE:CG2	2.63	0.46
1:A:111:ASP:N	1:A:114:ASN:HB3	2.29	0.46
1:A:121:ILE:N	1:A:121:ILE:CD1	2.70	0.46
1:C:137:LEU:C	1:C:139:ASN:N	2.72	0.46
1:D:46:GLY:N	1:D:176:ALA:CB	2.78	0.46
1:A:72:MET:O	1:A:75:ASN:HB3	2.15	0.46
1:A:102:ASP:OD1	1:A:102:ASP:C	2.58	0.46
1:D:195:LEU:HD21	1:D:247:PHE:CG	2.51	0.46
1:C:105:PRO:HG3	1:D:155:GLY:CA	2.40	0.46
1:A:232:ILE:HD12	1:A:236:GLU:OE1	2.16	0.46
1:C:103:ILE:CD1	1:D:158:LEU:CD1	2.94	0.46
1:C:144:LEU:O	1:C:147:SER:HB2	2.15	0.46
1:D:67:THR:OG1	1:D:68:ALA:N	2.49	0.46
1:B:59:LEU:HB3	1:B:152:VAL:HG11	1.98	0.46
1:B:68:ALA:O	1:B:71:ALA:N	2.48	0.46
1:C:57:LEU:N	1:C:57:LEU:CD1	2.79	0.46
1:C:60:SER:O	1:C:152:VAL:HA	2.16	0.46
1:C:157:ASP:CB	1:D:218:PHE:CZ	2.92	0.46
1:D:128:THR:HG22	1:D:129:SER:N	2.30	0.46
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.41	0.46
1:A:185:LYS:O	1:A:186:THR:C	2.58	0.46
1:B:62:LEU:HB3	1:B:127:SER:HB3	1.97	0.46
1:A:113:LYS:O	1:A:113:LYS:HG3	2.16	0.46
1:A:184:ALA:HB3	1:A:195:LEU:HD21	1.98	0.46
1:C:75:ASN:C	1:C:77:GLU:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ARG:CZ	1:D:81:LYS:NZ	2.77	0.46
1:D:106:ILE:CD1	1:D:125:SER:HB2	2.46	0.46
1:A:243:VAL:CG2	1:A:244:ASN:N	2.78	0.45
1:C:79:MET:O	1:C:82:VAL:N	2.50	0.45
1:A:140:VAL:HG12	1:A:141:GLY:N	2.31	0.45
1:B:49:THR:HG22	1:B:238:SER:HB3	1.98	0.45
1:D:106:ILE:HD11	1:D:124:TYR:O	2.15	0.45
1:A:67:THR:CG2	1:A:70:GLU:OE1	2.57	0.45
1:B:98:THR:HG22	1:B:130:LEU:HB2	1.98	0.45
1:B:175:ARG:O	1:B:179:ASN:N	2.44	0.45
1:B:204:LEU:HA	1:B:204:LEU:HD23	1.58	0.45
1:C:67:THR:CG2	1:C:70:GLU:OE1	2.49	0.45
1:A:198:VAL:CG2	1:A:247:PHE:CD2	2.99	0.45
1:C:47:MET:HE2	1:C:47:MET:HB2	1.84	0.45
1:C:59:LEU:HD11	1:C:147:SER:OG	2.17	0.45
1:D:57:LEU:HD23	1:D:57:LEU:N	2.31	0.45
1:A:117:LYS:O	1:A:118:GLU:C	2.57	0.45
1:C:220:THR:O	1:C:223:ALA:HB3	2.16	0.45
1:D:114:ASN:O	1:D:115:ASN:CB	2.64	0.45
1:A:158:LEU:HA	1:A:160:LEU:HD21	1.99	0.45
1:A:173:ARG:NH1	1:A:203:GLU:OE1	2.50	0.45
1:B:110:PRO:HG3	1:B:118:GLU:N	2.32	0.45
1:C:103:ILE:CG2	1:C:126:VAL:HG23	2.39	0.45
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.67	0.45
1:B:215:ARG:O	1:B:218:PHE:CD2	2.70	0.45
1:C:67:THR:OG1	1:D:145:ASP:OD1	2.34	0.45
1:C:98:THR:HG22	1:C:130:LEU:CB	2.47	0.45
1:A:204:LEU:HD23	1:B:43:THR:HG23	1.98	0.45
1:C:48:MET:CG	1:C:168:VAL:HG13	2.47	0.45
1:B:101:ILE:CG2	1:C:160:LEU:HD11	2.47	0.45
1:C:45:GLU:HA	1:C:176:ALA:HB1	1.98	0.45
1:C:97:GLN:HG3	1:C:98:THR:N	2.31	0.45
1:D:48:MET:CE	1:D:171:GLU:CB	2.94	0.45
1:D:217:GLN:HB3	1:D:221:MET:CG	2.47	0.45
1:A:86:MET:HE3	1:A:146:GLU:HG2	1.99	0.44
1:B:72:MET:O	1:B:75:ASN:N	2.50	0.44
1:B:169:ILE:O	1:B:172:ALA:N	2.49	0.44
1:C:94:ARG:O	1:D:231:PRO:HD3	2.16	0.44
1:C:165:PRO:CD	1:C:166:SER:H	2.29	0.44
1:A:48:MET:HE3	1:A:175:ARG:NH2	2.32	0.44
1:B:62:LEU:HD12	1:B:125:SER:OG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:MET:O	1:B:212:PRO:C	2.58	0.44
1:B:219:ARG:O	1:B:220:THR:C	2.61	0.44
1:D:98:THR:HG21	1:D:130:LEU:HB2	1.99	0.44
1:A:88:LYS:HG3	1:A:89:ALA:N	2.31	0.44
1:B:44:GLY:C	1:B:45:GLU:OE1	2.60	0.44
1:D:149:THR:HB	1:D:150:LEU:HD23	1.99	0.44
1:A:173:ARG:NH1	1:A:203:GLU:CD	2.75	0.44
1:B:146:GLU:OE1	1:B:150:LEU:CD1	2.66	0.44
1:C:148:VAL:O	1:C:149:THR:C	2.58	0.44
1:D:114:ASN:O	1:D:115:ASN:HB2	2.17	0.44
1:A:144:LEU:O	1:A:147:SER:OG	2.31	0.44
1:C:213:ILE:HG12	1:C:221:MET:HG3	1.98	0.44
1:A:91:ILE:CD1	1:A:96:LEU:HD11	2.48	0.44
1:A:209:MET:HG2	1:A:210:PRO:HD2	1.99	0.44
1:A:230:VAL:CG1	1:A:231:PRO:HD2	2.33	0.44
1:D:57:LEU:CD2	1:D:57:LEU:N	2.80	0.44
1:D:219:ARG:O	1:D:221:MET:N	2.51	0.44
1:A:171:GLU:O	1:A:175:ARG:HG2	2.16	0.44
1:B:102:ASP:OD2	1:C:158:LEU:CD1	2.60	0.44
1:B:205:SER:O	1:B:207:PRO:HD3	2.17	0.44
1:D:136:GLU:O	1:D:137:LEU:C	2.61	0.44
1:B:177:VAL:HG11	1:C:190:ALA:CB	2.48	0.44
1:C:48:MET:HE3	1:C:171:GLU:HG3	1.98	0.44
1:A:159:ASN:O	1:A:161:VAL:HG12	2.18	0.43
1:A:152:VAL:O	1:A:153:ASN:C	2.61	0.43
1:A:189:ASP:C	1:A:191:ALA:N	2.74	0.43
1:C:143:ILE:HD12	1:C:143:ILE:C	2.42	0.43
1:D:109:TYR:HD2	1:D:119:PRO:HG3	1.83	0.43
1:A:161:VAL:HG23	1:A:162:ASN:O	2.19	0.43
1:A:184:ALA:CB	1:A:195:LEU:CD2	2.96	0.43
1:B:115:ASN:HB3	1:B:116:LEU:H	1.66	0.43
1:B:221:MET:O	1:B:222:LEU:C	2.61	0.43
1:A:38:ALA:C	1:A:39:ARG:HG2	2.43	0.43
1:A:103:ILE:H	1:B:158:LEU:HG	1.83	0.43
1:C:83:LEU:O	1:C:86:MET:N	2.49	0.43
1:A:98:THR:CG2	1:A:130:LEU:HD12	2.45	0.43
1:B:64:GLN:N	1:B:64:GLN:CD	2.77	0.43
1:B:186:THR:HG22	1:B:187:LEU:N	2.33	0.43
1:C:48:MET:CE	1:C:175:ARG:NH1	2.81	0.43
1:D:230:VAL:HG12	1:D:231:PRO:HD2	2.00	0.43
1:A:175:ARG:HH21	1:A:226:PRO:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:MET:O	1:A:224:ALA:N	2.51	0.43
1:B:82:VAL:HG23	1:B:150:LEU:CD2	2.49	0.43
1:C:104:GLN:OE1	1:C:105:PRO:HD2	2.19	0.43
1:C:201:ILE:O	1:D:40:ILE:HA	2.18	0.43
1:D:62:LEU:HD12	1:D:62:LEU:H	1.83	0.43
1:A:117:LYS:C	1:A:118:GLU:O	2.60	0.43
1:A:118:GLU:HA	1:A:118:GLU:OE1	2.19	0.43
1:B:63:ARG:HD2	1:B:78:ALA:HB1	2.00	0.43
1:C:169:ILE:O	1:C:172:ALA:HB3	2.18	0.43
1:B:62:LEU:HA	1:B:126:VAL:O	2.18	0.43
1:B:88:LYS:C	1:B:90:GLY:N	2.75	0.43
1:C:75:ASN:O	1:C:77:GLU:N	2.51	0.43
1:C:94:ARG:HB2	1:C:94:ARG:NH1	2.34	0.43
1:D:84:ASP:C	1:D:86:MET:H	2.27	0.43
1:A:91:ILE:HG21	1:A:143:ILE:CD1	2.48	0.43
1:A:165:PRO:HD2	1:B:227:ASP:OD1	2.19	0.43
1:B:54:MET:HG3	1:B:55:ALA:H	1.84	0.43
1:B:104:GLN:HA	1:B:105:PRO:HD2	1.89	0.43
1:B:213:ILE:HG13	1:B:236:GLU:O	2.19	0.43
1:C:93:ASP:OD1	1:C:94:ARG:N	2.52	0.43
1:D:41:ALA:HB2	1:D:246:VAL:CG1	2.47	0.43
1:D:109:TYR:HA	1:D:110:PRO:HD2	1.77	0.43
1:A:131:THR:CG2	1:B:233:ALA:CB	2.97	0.43
1:A:133:ARG:NH2	1:B:231:PRO:HG3	2.34	0.43
1:A:172:ALA:O	1:A:175:ARG:HB2	2.19	0.43
1:A:209:MET:CE	1:A:211:MET:HE2	2.48	0.43
1:B:54:MET:CE	1:B:135:ARG:HA	2.35	0.43
1:A:164:ASN:HA	1:A:165:PRO:HD2	1.84	0.42
1:B:157:ASP:O	1:B:158:LEU:C	2.62	0.42
1:C:57:LEU:HB3	1:C:59:LEU:HD21	2.00	0.42
1:C:165:PRO:O	1:C:166:SER:C	2.61	0.42
1:D:61:VAL:O	1:D:75:ASN:ND2	2.52	0.42
1:A:156:GLY:O	1:A:159:ASN:OD1	2.36	0.42
1:B:45:GLU:HA	1:B:241:VAL:O	2.19	0.42
1:B:91:ILE:HG22	1:B:92:GLU:O	2.20	0.42
1:B:174:LYS:O	1:B:178:ALA:CB	2.67	0.42
1:C:63:ARG:C	1:C:64:GLN:HG3	2.44	0.42
1:C:184:ALA:CB	1:C:195:LEU:HD21	2.47	0.42
1:D:218:PHE:HB3	1:D:219:ARG:H	1.27	0.42
1:A:122:THR:O	1:A:122:THR:HG23	2.19	0.42
1:C:84:ASP:HB3	1:C:88:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:SER:O	1:D:148:VAL:C	2.62	0.42
1:A:100:GLY:CA	1:B:235:GLY:HA3	2.49	0.42
1:B:83:LEU:HA	1:B:83:LEU:HD23	1.71	0.42
1:B:88:LYS:C	1:B:90:GLY:H	2.26	0.42
1:B:199:VAL:HG23	1:B:246:VAL:HG12	2.01	0.42
1:C:92:GLU:O	1:C:96:LEU:HG	2.20	0.42
1:C:120:THR:C	1:C:121:ILE:HD13	2.44	0.42
1:C:140:VAL:CG1	1:C:141:GLY:N	2.81	0.42
1:D:59:LEU:O	1:D:130:LEU:O	2.37	0.42
1:C:62:LEU:HA	1:C:127:SER:OG	2.19	0.42
1:D:63:ARG:HD2	1:D:78:ALA:CB	2.50	0.42
1:A:209:MET:HE2	1:A:209:MET:HB3	1.83	0.42
1:C:103:ILE:HD13	1:D:158:LEU:CD1	2.49	0.42
1:C:118:GLU:HA	1:C:119:PRO:HD3	1.66	0.42
1:C:133:ARG:NH2	1:D:231:PRO:HD3	2.34	0.42
1:D:104:GLN:HA	1:D:105:PRO:HD2	1.80	0.42
1:A:218:PHE:O	1:A:222:LEU:HG	2.20	0.42
1:B:108:VAL:CG1	1:B:109:TYR:N	2.82	0.42
1:C:121:ILE:N	1:C:121:ILE:CD1	2.80	0.42
1:D:140:VAL:O	1:D:143:ILE:HD12	2.20	0.42
1:A:204:LEU:CD2	1:B:43:THR:HG23	2.49	0.42
1:B:169:ILE:N	1:B:169:ILE:HD13	2.34	0.42
1:C:111:ASP:CG	1:C:112:ASP:H	2.27	0.42
1:C:150:LEU:CD1	1:C:152:VAL:HG23	2.50	0.42
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.85	0.42
1:A:56:ILE:C	1:A:57:LEU:HD23	2.44	0.42
1:A:59:LEU:HD13	1:A:147:SER:HB2	2.01	0.42
1:A:154:GLN:C	1:A:155:GLY:O	2.59	0.42
1:A:210:PRO:O	1:A:212:PRO:CD	2.63	0.42
1:B:72:MET:O	1:B:73:THR:C	2.62	0.42
1:C:58:ASN:C	1:C:58:ASN:ND2	2.77	0.42
1:A:78:ALA:O	1:A:81:LYS:HB2	2.19	0.42
1:C:82:VAL:CG1	1:C:83:LEU:N	2.81	0.42
1:B:57:LEU:HD13	1:B:57:LEU:HA	1.88	0.41
1:B:204:LEU:HA	1:C:43:THR:HG23	2.01	0.41
1:C:156:GLY:O	1:C:158:LEU:N	2.53	0.41
1:D:63:ARG:NH1	1:D:81:LYS:HZ2	2.13	0.41
1:D:124:TYR:CD1	1:D:124:TYR:N	2.88	0.41
1:D:198:VAL:CG2	1:D:247:PHE:CD2	2.98	0.41
1:D:208:PRO:HB3	1:D:240:ASN:O	2.20	0.41
1:A:106:ILE:HD11	1:A:125:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB1	1:A:193:VAL:O	2.20	0.41
1:C:135:ARG:O	1:C:136:GLU:CB	2.66	0.41
1:D:96:LEU:HD23	1:D:131:THR:O	2.19	0.41
1:A:161:VAL:HG23	1:A:162:ASN:C	2.45	0.41
1:A:38:ALA:HB1	1:A:249:ILE:HB	2.02	0.41
1:C:48:MET:HE3	1:C:171:GLU:HG2	2.02	0.41
1:D:137:LEU:C	1:D:139:ASN:N	2.77	0.41
1:A:148:VAL:C	1:A:150:LEU:N	2.78	0.41
1:A:189:ASP:O	1:A:190:ALA:C	2.63	0.41
1:A:201:ILE:HB	1:B:40:ILE:HG23	2.02	0.41
1:A:173:ARG:HH11	1:A:203:GLU:CD	2.28	0.41
1:C:154:GLN:CD	1:C:155:GLY:N	2.77	0.41
1:D:165:PRO:O	1:D:166:SER:C	2.62	0.41
1:A:123:GLY:C	1:A:124:TYR:CD1	2.99	0.41
1:A:159:ASN:O	1:A:161:VAL:HG13	2.21	0.41
1:B:48:MET:O	1:B:238:SER:HA	2.21	0.41
1:B:98:THR:HB	1:B:99:GLY:H	1.77	0.41
1:D:153:ASN:OD1	1:D:156:GLY:HA2	2.21	0.41
1:B:47:MET:CE	1:B:240:ASN:CG	2.90	0.41
1:B:49:THR:O	1:B:50:ALA:HB2	2.21	0.41
1:D:46:GLY:HA3	1:D:176:ALA:N	2.36	0.41
1:D:57:LEU:HD21	1:D:132:VAL:CG1	2.49	0.41
1:D:110:PRO:CA	1:D:114:ASN:HB3	2.51	0.41
1:D:137:LEU:C	1:D:139:ASN:H	2.28	0.41
1:D:173:ARG:HA	1:D:241:VAL:HG11	2.02	0.41
1:A:154:GLN:NE2	1:A:154:GLN:HA	2.35	0.41
1:B:54:MET:O	1:B:137:LEU:HD13	2.21	0.41
1:B:71:ALA:HB1	1:B:126:VAL:CG2	2.51	0.41
1:B:91:ILE:HG22	1:B:96:LEU:HD11	2.02	0.41
1:B:184:ALA:CB	1:B:247:PHE:CE1	3.04	0.41
1:C:65:ALA:O	1:C:67:THR:N	2.54	0.41
1:C:72:MET:CE	1:D:140:VAL:HG12	2.51	0.41
1:A:85:ALA:O	1:A:89:ALA:HB2	2.21	0.41
1:A:184:ALA:CB	1:A:195:LEU:HD22	2.51	0.41
1:A:201:ILE:O	1:B:40:ILE:HA	2.21	0.41
1:A:230:VAL:CG1	1:A:231:PRO:CD	2.96	0.41
1:C:131:THR:HG1	1:D:233:ALA:HB2	1.86	0.41
1:D:49:THR:HG21	1:D:232:ILE:HD11	2.03	0.41
1:D:110:PRO:HA	1:D:114:ASN:CB	2.49	0.41
1:B:121:ILE:HD11	1:B:124:TYR:CZ	2.56	0.40
1:C:62:LEU:O	1:C:63:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PRO:CG	1:B:223:ALA:HB1	2.52	0.40
1:B:140:VAL:HA	1:B:143:ILE:CG2	2.50	0.40
1:D:169:ILE:HG12	1:D:239:TYR:HD2	1.87	0.40
1:A:112:ASP:O	1:A:113:LYS:CB	2.69	0.40
1:A:209:MET:O	1:A:211:MET:N	2.54	0.40
1:A:241:VAL:HG12	1:A:242:SER:N	2.35	0.40
1:D:160:LEU:H	1:D:160:LEU:HG	1.70	0.40
1:A:239:TYR:CD1	1:A:239:TYR:N	2.89	0.40
1:C:219:ARG:HG3	1:C:220:THR:H	1.87	0.40
1:D:228:ASN:C	1:D:229:SER:O	2.63	0.40

All (4) 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:113:LYS:NZ	1:D:127:SER:O[8_554]	1.85	0.35
1:C:102:ASP:O	1:D:113:LYS:NZ[8_554]	1.88	0.32
1:B:114:ASN:OD1	1:B:215:ARG:NH2[10_555]	2.05	0.15
1:C:127:SER:O	1:D:113:LYS:NZ[8_554]	2.09	0.11

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	212/224 (95%)	182 (86%)	26 (12%)	4 (2%)	6	33
1	B	212/224 (95%)	191 (90%)	21 (10%)	0	100	100
1	C	212/224 (95%)	186 (88%)	21 (10%)	5 (2%)	4	29
1	D	212/224 (95%)	181 (85%)	26 (12%)	5 (2%)	4	29
All	All	848/896 (95%)	740 (87%)	94 (11%)	14 (2%)	7	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	VAL
1	D	114	ASN
1	D	152	VAL
1	C	152	VAL
1	D	115	ASN
1	D	117	LYS
1	A	114	ASN
1	A	115	ASN
1	A	118	GLU
1	C	157	ASP
1	C	149	THR
1	D	116	LEU
1	C	148	VAL
1	C	161	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/180 (95%)	124 (72%)	47 (28%)	0	3
1	B	171/180 (95%)	123 (72%)	48 (28%)	0	3
1	C	171/180 (95%)	118 (69%)	53 (31%)	0	2
1	D	171/180 (95%)	126 (74%)	45 (26%)	0	3
All	All	684/720 (95%)	491 (72%)	193 (28%)	0	3

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	42	VAL
1	A	48	MET
1	A	56	ILE
1	A	57	LEU
1	A	61	VAL
1	A	64	GLN
1	A	67	THR

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Mol	Chain	Res	Type
1	A	70	GLU
1	A	73	THR
1	A	79	MET
1	A	82	VAL
1	A	83	LEU
1	A	92	GLU
1	A	98	THR
1	A	113	LYS
1	A	116	LEU
1	A	117	LYS
1	A	121	ILE
1	A	122	THR
1	A	128	THR
1	A	130	LEU
1	A	135	ARG
1	A	143	ILE
1	A	158	LEU
1	A	159	ASN
1	A	160	LEU
1	A	161	VAL
1	A	162	ASN
1	A	174	LYS
1	A	179	ASN
1	A	181	ILE
1	A	195	LEU
1	A	198	VAL
1	A	199	VAL
1	A	205	SER
1	A	209	MET
1	A	215	ARG
1	A	218	PHE
1	A	221	MET
1	A	222	LEU
1	A	230	VAL
1	A	232	ILE
1	A	240	ASN
1	A	243	VAL
1	A	245	VAL
1	A	246	VAL
1	B	39	ARG
1	B	45	GLU
1	B	47	MET

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Mol	Chain	Res	Type
1	B	48	MET
1	B	51	SER
1	B	54	MET
1	B	56	ILE
1	B	59	LEU
1	B	67	THR
1	B	69	ARG
1	B	75	ASN
1	B	76	ASN
1	B	77	GLU
1	B	80	THR
1	B	84	ASP
1	B	97	GLN
1	B	103	ILE
1	B	113	LYS
1	B	116	LEU
1	B	120	THR
1	B	122	THR
1	B	128	THR
1	B	130	LEU
1	B	132	VAL
1	B	135	ARG
1	B	136	GLU
1	B	139	ASN
1	B	146	GLU
1	B	150	LEU
1	B	158	LEU
1	B	159	ASN
1	B	160	LEU
1	B	162	ASN
1	B	163	ASP
1	B	168	VAL
1	B	175	ARG
1	B	177	VAL
1	B	181	ILE
1	B	186	THR
1	B	193	VAL
1	B	195	LEU
1	B	198	VAL
1	B	199	VAL
1	B	202	SER
1	B	230	VAL

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Mol	Chain	Res	Type
1	B	240	ASN
1	B	245	VAL
1	B	249	ILE
1	C	40	ILE
1	C	43	THR
1	C	45	GLU
1	C	47	MET
1	C	51	SER
1	C	64	GLN
1	C	66	LYS
1	C	67	THR
1	C	77	GLU
1	C	96	LEU
1	C	102	ASP
1	C	103	ILE
1	C	108	VAL
1	C	112	ASP
1	C	115	ASN
1	C	116	LEU
1	C	120	THR
1	C	121	ILE
1	C	128	THR
1	C	130	LEU
1	C	132	VAL
1	C	137	LEU
1	C	140	VAL
1	C	143	ILE
1	C	149	THR
1	C	150	LEU
1	C	158	LEU
1	C	161	VAL
1	C	162	ASN
1	C	169	ILE
1	C	175	ARG
1	C	183	LYS
1	C	189	ASP
1	C	193	VAL
1	C	195	LEU
1	C	197	ARG
1	C	198	VAL
1	C	200	GLU
1	C	201	ILE

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Mol	Chain	Res	Type
1	C	218	PHE
1	C	219	ARG
1	C	220	THR
1	C	222	LEU
1	C	228	ASN
1	C	230	VAL
1	C	232	ILE
1	C	238	SER
1	C	241	VAL
1	C	242	SER
1	C	243	VAL
1	C	245	VAL
1	C	249	ILE
1	C	250	LYS
1	D	39	ARG
1	D	49	THR
1	D	57	LEU
1	D	59	LEU
1	D	62	LEU
1	D	67	THR
1	D	73	THR
1	D	77	GLU
1	D	101	ILE
1	D	103	ILE
1	D	106	ILE
1	D	108	VAL
1	D	112	ASP
1	D	116	LEU
1	D	120	THR
1	D	121	ILE
1	D	122	THR
1	D	130	LEU
1	D	140	VAL
1	D	143	ILE
1	D	144	LEU
1	D	150	LEU
1	D	152	VAL
1	D	153	ASN
1	D	159	ASN
1	D	160	LEU
1	D	162	ASN
1	D	163	ASP

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Mol	Chain	Res	Type
1	D	166	SER
1	D	171	GLU
1	D	173	ARG
1	D	183	LYS
1	D	195	LEU
1	D	201	ILE
1	D	205	SER
1	D	218	PHE
1	D	219	ARG
1	D	230	VAL
1	D	232	ILE
1	D	239	TYR
1	D	240	ASN
1	D	241	VAL
1	D	245	VAL
1	D	246	VAL
1	D	249	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	154	GLN
1	B	58	ASN
1	B	75	ASN
1	B	114	ASN
1	B	153	ASN
1	B	154	GLN
1	C	75	ASN
1	C	114	ASN
1	C	153	ASN
1	C	170	ASN
1	C	179	ASN
1	D	164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	214/224 (95%)	-0.18	0 100 100	83, 122, 157, 173	0
1	B	214/224 (95%)	-0.19	2 (0%) 81 58	79, 122, 163, 187	0
1	C	214/224 (95%)	-0.21	0 100 100	78, 118, 157, 176	0
1	D	214/224 (95%)	-0.13	1 (0%) 87 68	77, 120, 155, 166	0
All	All	856/896 (95%)	-0.18	3 (0%) 88 72	77, 121, 158, 187	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	ASP	2.6
1	B	113	LYS	2.4
1	D	109	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.