



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:03 AM EDT

PDB ID : 6II2 / pdb_00006ii2
Title : Crystal structure of alpha-beta hydrolase (ABH) and Makes Caterpillars Floppy (MCF)-Like effectors of *Vibrio vulnificus* MO6-24/O
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Deposited on : 2018-10-03
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

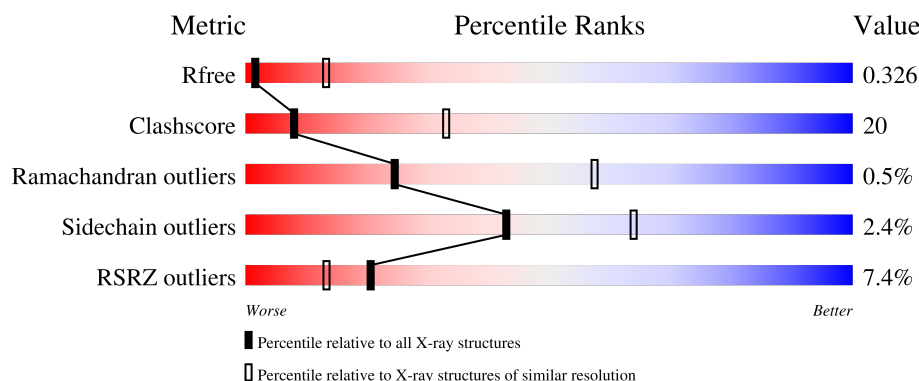
1 Overall quality at a glance

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	694	
1	B	694	
1	C	694	
1	D	694	

2 Entry composition

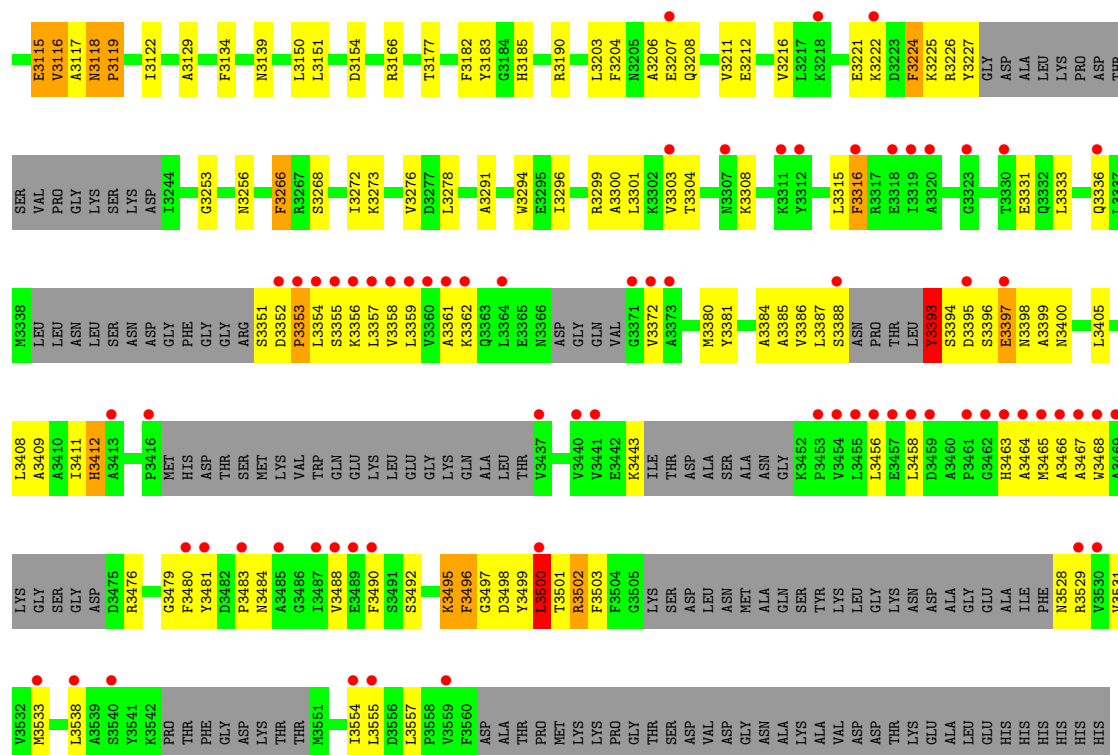
There is only 1 type of molecule in this entry. The entry contains 17825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative RTX-toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4681	2938	808	920	15			
1	B	612	Total	C	N	O	S	0	0	0
			4673	2932	808	918	15			
1	C	568	Total	C	N	O	S	0	0	0
			4338	2732	748	847	11			
1	D	539	Total	C	N	O	S	0	0	0
			4133	2604	717	800	12			





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.22Å 108.59Å 334.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.50 49.60 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.5 (49.60-3.50) 77.5 (49.60-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0158, REFMAC	Depositor
R, R_{free}	0.285 , 0.327 0.284 , 0.326	Depositor DCC
R_{free} test set	1514 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	17825	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.75	0/4756	0.92	18/6412 (0.3%)
1	B	0.74	3/4746 (0.1%)	0.89	17/6394 (0.3%)
1	C	0.72	0/4402	0.96	25/5928 (0.4%)
1	D	0.77	1/4194 (0.0%)	0.99	18/5643 (0.3%)
All	All	0.75	4/18098 (0.0%)	0.94	78/24377 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	3
1	D	0	6
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2926	LEU	CA-C	6.77	1.59	1.53
1	B	2911	VAL	CA-C	5.63	1.59	1.52
1	D	2919	PRO	CA-C	5.25	1.57	1.52
1	B	3071	ILE	C-O	-5.09	1.18	1.24

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3071	ILE	N-CA-C	13.11	125.29	111.00
1	C	3065	ASP	N-CA-C	10.90	133.90	109.81
1	D	3396	SER	N-CA-C	-9.74	95.00	109.62
1	B	3516	LYS	N-CA-C	9.50	124.65	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3226	ARG	N-CA-C	-8.83	95.34	109.39
1	D	3064	ILE	N-CA-C	-8.83	94.70	107.77
1	A	3338	MET	N-CA-C	-8.81	92.03	110.80
1	C	3516	LYS	N-CA-C	-8.34	87.65	111.00
1	B	2912	ALA	N-CA-C	8.21	123.02	111.52
1	A	2926	LEU	N-CA-C	8.18	128.22	110.80
1	C	3526	ILE	N-CA-C	-8.13	98.90	108.82
1	A	3000	LEU	N-CA-C	-8.09	98.05	110.10
1	D	3068	ASN	CA-C-N	7.79	135.07	122.69
1	D	3068	ASN	C-N-CA	7.79	135.07	122.69
1	C	3016	ILE	CB-CA-C	-7.77	100.69	111.65
1	C	3115	GLU	CB-CA-C	-7.63	97.24	110.45
1	B	3064	ILE	N-CA-C	-7.51	98.79	108.93
1	D	3386	VAL	CB-CA-C	-7.38	102.44	111.88
1	D	3386	VAL	N-CA-C	7.37	118.09	110.36
1	A	3224	PHE	CB-CA-C	-7.26	99.38	110.92
1	C	2926	LEU	N-CA-C	7.18	120.21	108.08
1	D	3496	PHE	N-CA-C	-7.12	103.52	111.28
1	C	3353	PRO	N-CA-C	7.12	122.94	113.40
1	C	3120	ALA	N-CA-C	-6.99	98.88	109.79
1	B	3017	ARG	CB-CA-C	-6.94	96.61	110.42
1	B	3060	ASN	N-CA-C	6.66	119.53	111.40
1	A	2945	ARG	CB-CA-C	-6.59	97.70	109.24
1	C	3515	TYR	N-CA-C	6.55	124.76	110.80
1	A	3073	GLY	N-CA-C	-6.53	94.36	113.30
1	D	3071	ILE	N-CA-C	-6.53	102.94	110.05
1	D	3072	HIS	N-CA-C	-6.50	97.65	108.32
1	A	3305	PHE	N-CA-C	6.47	119.30	111.40
1	B	2923	LYS	N-CA-C	6.41	117.96	108.60
1	A	3449	ALA	N-CA-C	-6.30	98.12	108.76
1	C	3017	ARG	N-CA-C	6.24	120.45	112.34
1	C	3513	GLN	N-CA-C	-6.21	104.62	111.82
1	C	2912	ALA	N-CA-C	6.19	119.64	111.28
1	B	3338	MET	N-CA-C	6.09	118.00	111.36
1	B	3064	ILE	CB-CA-C	6.03	121.09	111.69
1	B	3305	PHE	N-CA-C	5.98	118.96	111.24
1	B	3339	LEU	CB-CA-C	-5.91	109.78	116.63
1	C	3305	PHE	N-CA-C	5.83	118.76	111.24
1	C	3355	SER	N-CA-C	5.82	118.09	111.11
1	D	3066	PRO	CA-N-CD	-5.81	103.36	111.50
1	A	3000	LEU	CB-CA-C	5.79	118.93	109.90
1	D	3102	ARG	NE-CZ-NH2	5.78	124.40	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2911	VAL	CA-C-N	5.77	130.36	122.34
1	B	2911	VAL	C-N-CA	5.77	130.36	122.34
1	D	3065	ASP	C-N-CD	5.77	133.30	120.60
1	D	3078	GLY	N-CA-C	-5.74	100.62	112.34
1	C	3121	GLY	CA-C-N	-5.74	112.44	120.53
1	C	3121	GLY	C-N-CA	-5.74	112.44	120.53
1	D	3102	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	B	3017	ARG	N-CA-C	5.64	122.81	110.80
1	A	3224	PHE	N-CA-C	5.61	117.86	111.02
1	A	3074	TYR	CB-CA-C	5.57	123.39	111.91
1	B	2911	VAL	CB-CA-C	5.55	120.40	111.29
1	C	3069	ILE	N-CA-C	5.52	116.68	108.46
1	C	2945	ARG	CB-CA-C	-5.44	99.71	109.24
1	D	3397	GLU	N-CA-C	-5.43	106.71	113.55
1	B	3360	VAL	CB-CA-C	-5.35	105.03	111.88
1	B	3217	LEU	CB-CA-C	-5.35	99.77	110.42
1	A	2923	LYS	N-CA-C	5.32	116.37	108.60
1	C	3069	ILE	CB-CA-C	-5.32	102.30	110.50
1	A	3389	ASN	N-CA-C	-5.26	98.17	109.81
1	D	3119	PRO	N-CA-C	5.25	123.28	112.47
1	A	3074	TYR	N-CA-C	5.20	115.39	108.38
1	C	3358	VAL	CB-CA-C	-5.18	105.34	111.97
1	C	3355	SER	CB-CA-C	-5.17	102.54	110.81
1	C	3360	VAL	CB-CA-C	-5.17	105.35	111.81
1	D	2925	SER	N-CA-C	-5.14	100.64	108.76
1	A	3122	ILE	N-CA-C	5.13	115.86	110.62
1	C	3115	GLU	CA-C-N	5.11	131.17	121.97
1	C	3115	GLU	C-N-CA	5.11	131.17	121.97
1	A	3338	MET	CB-CA-C	5.10	120.56	110.42
1	B	3217	LEU	N-CA-C	5.06	121.58	110.80
1	C	2923	LYS	N-CA-C	5.05	116.49	108.96
1	A	3072	HIS	N-CA-C	5.04	121.54	110.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3283	SER	Peptide
1	B	2927	SER	Peptide
1	B	3201	SER	Peptide
1	B	3337	LEU	Peptide
1	B	3338	MET	Peptide

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Mol	Chain	Res	Type	Group
1	C	2927	SER	Peptide
1	C	3115	GLU	Peptide
1	C	3204	PHE	Peptide
1	D	2927	SER	Peptide
1	D	3077	GLY	Peptide
1	D	3102	ARG	Sidechain
1	D	3115	GLU	Peptide
1	D	3393	TYR	Peptide
1	D	3500	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	4681	0	4639	148	0
1	B	4673	0	4633	152	0
1	C	4338	0	4314	154	0
1	D	4133	0	4104	260	0
All	All	17825	0	17690	697	0

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 20.

All (697) 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:C:3354:LEU:CD1	1:C:3380:MET:HE1	1.50	1.40
1:B:3304:THR:HG21	1:B:3337:LEU:HD23	1.31	1.13
1:C:2911:VAL:HA	1:C:3060:ASN:ND2	1.65	1.10
1:C:3354:LEU:HD12	1:C:3380:MET:HE1	1.13	1.09
1:D:3315:LEU:HD21	1:D:3502:ARG:CB	1.82	1.09
1:A:3266:PHE:HB2	1:A:3278:LEU:CD2	1.84	1.06
1:A:3072:HIS:HD2	1:A:3099:LEU:HD23	1.18	1.06
1:D:3066:PRO:HD2	1:D:3068:ASN:H	1.21	1.06
1:A:3122:ILE:CD1	1:D:3122:ILE:HG21	1.85	1.05
1:C:3517:LEU:HD13	1:C:3518:GLY:N	1.71	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3355:SER:O	1:C:3359:LEU:HD12	1.57	1.05
1:D:3315:LEU:HD21	1:D:3502:ARG:HB3	1.33	1.03
1:D:3315:LEU:HD23	1:D:3499:TYR:CE1	1.92	1.03
1:A:3440:VAL:HG21	1:A:3527:PHE:HE2	1.24	1.01
1:B:3017:ARG:O	1:B:3021:GLN:HG2	1.59	1.01
1:C:3516:LYS:HB2	1:C:3517:LEU:HB2	1.38	1.01
1:D:3315:LEU:HD23	1:D:3499:TYR:HE1	1.20	1.01
1:D:2923:LYS:HE3	1:D:2941:LYS:HE3	1.43	1.00
1:B:3203:LEU:O	1:B:3203:LEU:HD22	1.60	1.00
1:B:3301:LEU:HD22	1:B:3384:ALA:HB2	1.39	1.00
1:C:3120:ALA:HB1	1:C:3121:GLY:HA2	1.42	0.99
1:C:3354:LEU:HD11	1:C:3380:MET:HE1	1.40	0.99
1:B:2921:ARG:HE	1:B:2945:ARG:HD2	1.26	0.99
1:C:3221:GLU:OE2	1:C:3276:VAL:HB	1.63	0.97
1:A:3074:TYR:CD1	1:A:3075:SER:N	2.32	0.97
1:C:3070:ILE:HG21	1:C:3203:LEU:HG	1.46	0.97
1:C:3509:LEU:HD11	1:C:3511:MET:HE2	1.46	0.97
1:D:3315:LEU:CD2	1:D:3499:TYR:HE1	1.77	0.96
1:A:3509:LEU:HD11	1:A:3511:MET:HE2	1.48	0.96
1:C:3354:LEU:CD1	1:C:3380:MET:CE	2.44	0.95
1:A:3204:PHE:O	1:A:3207:GLU:HG2	1.66	0.95
1:C:3362:LYS:HA	1:C:3362:LYS:HE2	1.49	0.93
1:A:3509:LEU:HD12	1:A:3511:MET:HB2	1.50	0.93
1:D:3528:ASN:HA	1:D:3529:ARG:HG3	1.49	0.92
1:A:3017:ARG:O	1:A:3021:GLN:HG2	1.68	0.92
1:B:2998:VAL:HG22	1:B:3026:ASP:HB2	1.51	0.91
1:B:3304:THR:HG21	1:B:3337:LEU:CD2	2.00	0.91
1:A:3217:LEU:HD21	1:A:3273:LYS:HE3	1.50	0.91
1:C:3509:LEU:HD12	1:C:3511:MET:HB2	1.53	0.91
1:B:2923:LYS:HD2	1:B:2941:LYS:HD2	1.52	0.90
1:D:3352:ASP:N	1:D:3353:PRO:HD3	1.86	0.90
1:C:2911:VAL:HA	1:C:3060:ASN:HD22	1.26	0.90
1:D:3183:TYR:CE1	1:D:3190:ARG:HG3	2.05	0.90
1:B:3065:ASP:HB3	1:B:3066:PRO:HD2	1.54	0.90
1:C:3064:ILE:HG22	1:C:3065:ASP:H	1.37	0.89
1:D:3315:LEU:CD2	1:D:3499:TYR:CE1	2.54	0.88
1:C:3116:VAL:HG23	1:C:3119:PRO:HG3	1.53	0.88
1:A:3072:HIS:CD2	1:A:3099:LEU:HD23	2.08	0.88
1:A:3440:VAL:HG21	1:A:3527:PHE:CE2	2.10	0.87
1:C:2956:ASP:O	1:C:2958:ALA:HB3	1.74	0.87
1:B:3301:LEU:CD2	1:B:3384:ALA:HB2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2956:ASP:O	1:C:2958:ALA:CB	2.23	0.87
1:D:3352:ASP:N	1:D:3353:PRO:CD	2.36	0.87
1:D:3499:TYR:CD1	1:D:3502:ARG:HG2	2.10	0.87
1:A:3266:PHE:HB2	1:A:3278:LEU:HD22	1.54	0.87
1:C:3354:LEU:HD12	1:C:3380:MET:CE	2.02	0.87
1:D:3117:ALA:O	1:D:3118:ASN:HB2	1.73	0.87
1:D:3076:MET:O	1:D:3080:ILE:HG12	1.74	0.86
1:C:3513:GLN:O	1:C:3516:LYS:HD3	1.73	0.86
1:C:3516:LYS:CB	1:C:3517:LEU:HB2	2.05	0.86
1:D:3208:GLN:HA	1:D:3211:VAL:CG2	2.05	0.86
1:B:3182:PHE:CE2	1:B:3392:LEU:CD1	2.58	0.86
1:D:3316:PHE:CZ	1:D:3488:VAL:HG12	2.11	0.85
1:A:3206:ALA:N	1:A:3207:GLU:HB3	1.92	0.85
1:A:2997:LYS:HE3	1:A:3203:LEU:HD22	1.56	0.85
1:A:3001:PHE:HD1	1:A:3072:HIS:HD1	1.19	0.85
1:B:3509:LEU:HD11	1:B:3511:MET:HE2	1.57	0.84
1:A:3122:ILE:CD1	1:D:3122:ILE:CG2	2.55	0.84
1:C:3017:ARG:O	1:C:3021:GLN:HG2	1.78	0.84
1:B:3509:LEU:HD12	1:B:3511:MET:HB2	1.58	0.83
1:A:3354:LEU:HD21	1:A:3358:VAL:CG2	2.07	0.83
1:B:3463:HIS:NE2	1:B:3483:PRO:HB2	1.94	0.82
1:B:3182:PHE:CE2	1:B:3392:LEU:HD12	2.15	0.82
1:B:3520:ASN:HB3	1:B:3526:ILE:HG21	1.60	0.82
1:C:3202:GLY:C	1:C:3203:LEU:HD12	2.05	0.82
1:C:3304:THR:O	1:C:3336:GLN:HG2	1.79	0.82
1:A:3074:TYR:HD1	1:A:3075:SER:H	1.27	0.81
1:A:3072:HIS:HD2	1:A:3099:LEU:CD2	1.91	0.81
1:B:3338:MET:HG3	1:B:3351:SER:HA	1.62	0.81
1:C:3354:LEU:HD11	1:C:3380:MET:CE	2.09	0.81
1:D:3221:GLU:O	1:D:3224:PHE:HB3	1.80	0.81
1:A:2997:LYS:CE	1:A:3203:LEU:HD22	2.10	0.80
1:B:3517:LEU:HD13	1:B:3517:LEU:H	1.45	0.80
1:A:3065:ASP:HB3	1:A:3066:PRO:HD2	1.62	0.80
1:C:2957:HIS:HA	1:C:2958:ALA:HB3	1.62	0.80
1:D:3315:LEU:HD21	1:D:3502:ARG:CG	2.12	0.80
1:D:3354:LEU:O	1:D:3358:VAL:HG23	1.82	0.80
1:C:3070:ILE:CG2	1:C:3203:LEU:HG	2.11	0.80
1:D:3115:GLU:HB3	1:D:3116:VAL:HG13	1.64	0.79
1:D:3017:ARG:O	1:D:3021:GLN:HG2	1.81	0.79
1:D:3074:TYR:O	1:D:3077:GLY:HA3	1.83	0.79
1:D:2997:LYS:NZ	1:D:3203:LEU:HD21	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3227:TYR:O	1:D:3227:TYR:CD1	2.36	0.79
1:D:2923:LYS:CE	1:D:2941:LYS:HE3	2.14	0.78
1:B:2998:VAL:CG2	1:B:3064:ILE:CD1	2.62	0.77
1:B:3304:THR:CG2	1:B:3337:LEU:HD23	2.11	0.77
1:D:3315:LEU:HD11	1:D:3502:ARG:HG3	1.64	0.77
1:B:3196:ALA:O	1:B:3200:VAL:HG23	1.85	0.77
1:D:3356:LYS:HA	1:D:3359:LEU:HD12	1.67	0.77
1:A:3509:LEU:CD1	1:A:3511:MET:HB2	2.15	0.76
1:D:3458:LEU:HB2	1:D:3465:MET:O	1.84	0.76
1:B:3182:PHE:CE2	1:B:3392:LEU:HD11	2.21	0.76
1:C:3509:LEU:CD1	1:C:3511:MET:HB2	2.15	0.76
1:D:3353:PRO:C	1:D:3357:LEU:HD12	2.09	0.76
1:B:2923:LYS:CD	1:B:2941:LYS:HD2	2.16	0.76
1:D:3316:PHE:CE2	1:D:3331:GLU:HB2	2.21	0.76
1:A:3389:ASN:OD1	1:A:3392:LEU:HD13	1.85	0.75
1:B:3301:LEU:HD22	1:B:3384:ALA:CB	2.16	0.75
1:A:2997:LYS:HE3	1:A:3203:LEU:CD2	2.17	0.75
1:A:3266:PHE:HB2	1:A:3278:LEU:HD21	1.68	0.75
1:D:2911:VAL:O	1:D:3060:ASN:HB3	1.86	0.74
1:B:2965:GLN:OE1	1:B:2982:GLN:HG2	1.88	0.74
1:B:2998:VAL:CG2	1:B:3064:ILE:HD11	2.17	0.74
1:A:3354:LEU:CD2	1:A:3358:VAL:HG23	2.16	0.74
1:A:3122:ILE:HD13	1:D:3122:ILE:CG2	2.18	0.73
1:D:3004:GLY:HA2	1:D:3075:SER:O	1.88	0.73
1:D:3395:ASP:HB3	1:D:3397:GLU:HG3	1.70	0.73
1:B:2997:LYS:NZ	1:B:3203:LEU:CD2	2.52	0.73
1:C:3355:SER:O	1:C:3359:LEU:CD1	2.35	0.73
1:A:3509:LEU:HD13	1:A:3509:LEU:C	2.14	0.73
1:B:3017:ARG:O	1:B:3021:GLN:CG	2.36	0.73
1:C:3354:LEU:HD23	1:C:3358:VAL:CG2	2.18	0.73
1:D:3076:MET:O	1:D:3080:ILE:CG1	2.36	0.73
1:D:3222:LYS:HZ2	1:D:3303:VAL:CG1	2.02	0.72
1:B:3182:PHE:HE2	1:B:3392:LEU:HD12	1.53	0.72
1:C:2933:LEU:CD1	1:C:3126:ILE:HG23	2.20	0.72
1:C:3064:ILE:HG22	1:C:3065:ASP:N	2.00	0.72
1:B:2997:LYS:CD	1:B:3203:LEU:HD21	2.19	0.72
1:D:3208:GLN:HA	1:D:3211:VAL:HG21	1.72	0.72
1:D:3351:SER:N	1:D:3353:PRO:HD3	2.06	0.71
1:D:3077:GLY:O	1:D:3081:ALA:CB	2.38	0.71
1:A:3207:GLU:HG3	1:A:3208:GLN:N	2.03	0.71
1:A:3122:ILE:HD13	1:D:3122:ILE:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2998:VAL:HG21	1:B:3064:ILE:CD1	2.20	0.71
1:D:2997:LYS:CD	1:D:3203:LEU:HD21	2.21	0.71
1:D:3077:GLY:O	1:D:3081:ALA:HB2	1.91	0.71
1:D:3351:SER:C	1:D:3353:PRO:CD	2.63	0.71
1:A:3354:LEU:HD21	1:A:3358:VAL:HG23	1.71	0.71
1:B:3304:THR:CG2	1:B:3337:LEU:HB3	2.21	0.71
1:A:3074:TYR:HD1	1:A:3075:SER:N	1.84	0.70
1:C:3354:LEU:HD23	1:C:3358:VAL:HG23	1.73	0.70
1:C:3362:LYS:HZ3	1:C:3365:GLU:CD	1.99	0.70
1:D:3183:TYR:CD1	1:D:3190:ARG:HG3	2.27	0.70
1:D:3208:GLN:O	1:D:3211:VAL:HB	1.91	0.70
1:D:3351:SER:C	1:D:3353:PRO:HD2	2.16	0.70
1:D:3492:SER:HB3	1:D:3495:LYS:CG	2.21	0.70
1:A:3217:LEU:C	1:A:3217:LEU:HD13	2.17	0.70
1:D:3118:ASN:N	1:D:3119:PRO:HD3	2.07	0.70
1:C:3362:LYS:NZ	1:C:3365:GLU:CD	2.50	0.69
1:B:3304:THR:HG21	1:B:3337:LEU:HB3	1.74	0.69
1:C:2954:LEU:O	1:C:2957:HIS:HB2	1.92	0.69
1:B:2921:ARG:HH21	1:B:2945:ARG:HB3	1.58	0.69
1:D:3078:GLY:HA2	1:D:3079:PRO:C	2.18	0.69
1:A:2973:VAL:HG12	1:A:2973:VAL:O	1.92	0.68
1:D:3351:SER:N	1:D:3353:PRO:CD	2.56	0.68
1:B:3509:LEU:C	1:B:3509:LEU:HD13	2.18	0.68
1:A:3065:ASP:O	1:A:3066:PRO:C	2.36	0.68
1:A:3204:PHE:O	1:A:3207:GLU:CG	2.41	0.68
1:D:3079:PRO:HG3	1:D:3134:PHE:HB3	1.74	0.68
1:B:3463:HIS:CD2	1:B:3483:PRO:HG2	2.28	0.68
1:D:3057:TYR:CZ	1:D:3062:LYS:HE2	2.29	0.68
1:D:3385:ALA:O	1:D:3388:SER:HB3	1.94	0.68
1:D:2997:LYS:CE	1:D:3203:LEU:HD21	2.24	0.68
1:D:3253:GLY:O	1:D:3291:ALA:HA	1.94	0.68
1:B:3354:LEU:HD21	1:B:3358:VAL:HG23	1.74	0.67
1:C:3070:ILE:HG21	1:C:3203:LEU:CG	2.22	0.67
1:C:3509:LEU:C	1:C:3509:LEU:HD13	2.19	0.67
1:D:3498:ASP:O	1:D:3501:THR:HB	1.92	0.67
1:D:3492:SER:HB3	1:D:3495:LYS:HG3	1.76	0.67
1:B:3122:ILE:HB	1:C:3122:ILE:HD12	1.76	0.67
1:D:3066:PRO:CG	1:D:3067:SER:H	2.07	0.67
1:D:3183:TYR:CE1	1:D:3190:ARG:CG	2.76	0.67
1:D:3304:THR:O	1:D:3336:GLN:HG2	1.95	0.67
1:D:3315:LEU:HD21	1:D:3502:ARG:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3065:ASP:N	1:D:3066:PRO:HA	2.09	0.66
1:C:3120:ALA:HB1	1:C:3121:GLY:CA	2.23	0.66
1:A:3542:LYS:HZ2	1:A:3548:LYS:HA	1.60	0.66
1:A:3266:PHE:CB	1:A:3278:LEU:CD2	2.70	0.66
1:B:2921:ARG:CD	1:B:3037:GLU:HA	2.26	0.66
1:B:3354:LEU:CD2	1:B:3358:VAL:HG23	2.26	0.66
1:C:2957:HIS:CA	1:C:2958:ALA:HB3	2.24	0.66
1:A:3073:GLY:HA3	1:A:3099:LEU:O	1.95	0.66
1:D:3057:TYR:OH	1:D:3062:LYS:HE2	1.95	0.66
1:B:3509:LEU:CD1	1:B:3511:MET:HB2	2.25	0.66
1:D:3463:HIS:CE1	1:D:3484:ASN:HB2	2.31	0.66
1:B:2933:LEU:HD13	1:B:3126:ILE:CG2	2.26	0.66
1:C:2954:LEU:HD23	1:C:3017:ARG:HH22	1.61	0.66
1:C:3311:LYS:HE2	1:C:3509:LEU:HD21	1.77	0.65
1:B:3076:MET:HA	1:B:3104:MET:HE2	1.78	0.65
1:D:3315:LEU:CG	1:D:3499:TYR:HE1	2.09	0.65
1:B:2998:VAL:HG21	1:B:3064:ILE:HD11	1.78	0.65
1:C:3517:LEU:HD12	1:C:3519:LYS:HG3	1.78	0.65
1:A:3544:THR:OG1	1:A:3547:ASP:HB3	1.97	0.65
1:C:3544:THR:OG1	1:C:3547:ASP:HB3	1.96	0.65
1:D:3351:SER:CA	1:D:3353:PRO:HD2	2.26	0.65
1:B:3351:SER:O	1:B:3355:SER:HB3	1.97	0.65
1:D:3057:TYR:OH	1:D:3062:LYS:CE	2.44	0.65
1:D:3381:TYR:O	1:D:3384:ALA:HB3	1.97	0.65
1:B:3517:LEU:H	1:B:3517:LEU:CD1	2.09	0.65
1:C:2912:ALA:HA	1:C:3061:ASP:OD1	1.97	0.65
1:B:2911:VAL:HG23	1:B:3060:ASN:CG	2.22	0.64
1:C:3221:GLU:CD	1:C:3273:LYS:HA	2.21	0.64
1:D:3204:PHE:O	1:D:3207:GLU:HG2	1.97	0.64
1:D:3409:ALA:O	1:D:3412:HIS:HB2	1.97	0.64
1:D:3315:LEU:CD1	1:D:3502:ARG:HG3	2.27	0.64
1:B:3311:LYS:HE2	1:B:3509:LEU:HD21	1.79	0.64
1:C:2997:LYS:HZ3	1:C:3200:VAL:HG13	1.61	0.64
1:D:3206:ALA:N	1:D:3207:GLU:HB3	2.12	0.64
1:D:3315:LEU:CG	1:D:3502:ARG:HG3	2.28	0.64
1:D:3316:PHE:HE2	1:D:3331:GLU:HB2	1.63	0.64
1:D:3116:VAL:HG22	1:D:3116:VAL:O	1.97	0.64
1:D:3222:LYS:NZ	1:D:3303:VAL:CG1	2.60	0.64
1:D:3496:PHE:CE2	1:D:3500:LEU:HD23	2.32	0.64
1:A:3122:ILE:HD11	1:D:3122:ILE:HG21	1.79	0.64
1:D:3074:TYR:HE1	1:D:3102:ARG:NH1	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3001:PHE:CD1	1:A:3072:HIS:ND1	2.64	0.64
1:A:3354:LEU:HD12	1:A:3380:MET:HE1	1.79	0.64
1:C:2933:LEU:HD11	1:C:3126:ILE:HG23	1.79	0.64
1:C:3120:ALA:CB	1:C:3121:GLY:HA2	2.14	0.64
1:D:3458:LEU:H	1:D:3466:ALA:HB2	1.62	0.63
1:B:3520:ASN:HB3	1:B:3526:ILE:CG2	2.28	0.63
1:D:2998:VAL:HG21	1:D:3064:ILE:HD11	1.80	0.63
1:D:3102:ARG:HD2	1:D:3185:HIS:HA	1.80	0.63
1:A:2959:VAL:O	1:A:2960:GLU:HG3	1.99	0.63
1:D:3225:LYS:HB2	1:D:3276:VAL:HG13	1.79	0.63
1:B:2997:LYS:HZ3	1:B:3203:LEU:CD2	2.12	0.63
1:D:3355:SER:O	1:D:3359:LEU:HG	1.98	0.63
1:C:3465:MET:CE	1:C:3515:TYR:CE2	2.82	0.63
1:D:3393:TYR:CD1	1:D:3394:SER:HA	2.34	0.63
1:B:3337:LEU:HD12	1:B:3337:LEU:C	2.24	0.62
1:C:3518:GLY:O	1:C:3525:ALA:HA	1.99	0.62
1:D:3352:ASP:O	1:D:3355:SER:HB3	1.99	0.62
1:B:3338:MET:SD	1:B:3351:SER:N	2.72	0.62
1:B:3278:LEU:HD22	1:B:3292:LEU:HD21	1.82	0.62
1:A:3001:PHE:HD1	1:A:3072:HIS:ND1	1.93	0.62
1:B:3354:LEU:HA	1:B:3357:LEU:HD12	1.82	0.62
1:C:3465:MET:HE1	1:C:3515:TYR:CE2	2.34	0.62
1:A:3354:LEU:CD2	1:A:3358:VAL:CG2	2.77	0.62
1:A:3440:VAL:CG2	1:A:3527:PHE:HE2	2.05	0.62
1:D:3352:ASP:H	1:D:3353:PRO:HD3	1.65	0.62
1:D:3354:LEU:HD12	1:D:3354:LEU:H	1.65	0.62
1:D:3393:TYR:CG	1:D:3394:SER:HA	2.35	0.61
1:B:2998:VAL:HG23	1:B:3064:ILE:HD11	1.82	0.61
1:B:3338:MET:CG	1:B:3351:SER:HA	2.30	0.61
1:B:2998:VAL:HG23	1:B:3064:ILE:CD1	2.31	0.61
1:C:3513:GLN:O	1:C:3516:LYS:HB3	2.00	0.61
1:D:3358:VAL:O	1:D:3362:LYS:HG2	2.00	0.61
1:B:3195:TYR:O	1:B:3199:ILE:HG13	2.01	0.61
1:C:3017:ARG:O	1:C:3021:GLN:CG	2.48	0.61
1:C:3463:HIS:CD2	1:C:3483:PRO:HB2	2.35	0.61
1:A:3122:ILE:HD12	1:D:3122:ILE:HG21	1.81	0.61
1:A:3059:VAL:O	1:A:3063:GLY:HA2	2.00	0.61
1:D:2997:LYS:HD2	1:D:3203:LEU:HD21	1.81	0.60
1:D:3458:LEU:N	1:D:3466:ALA:HB2	2.15	0.60
1:D:3222:LYS:HG2	1:D:3272:ILE:HG21	1.83	0.60
1:B:3278:LEU:HD22	1:B:3292:LEU:CD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2997:LYS:NZ	1:C:3200:VAL:HG13	2.17	0.60
1:D:3079:PRO:HG3	1:D:3134:PHE:CA	2.32	0.60
1:D:3221:GLU:HG3	1:D:3273:LYS:HE3	1.84	0.60
1:C:3066:PRO:C	1:C:3068:ASN:H	2.10	0.60
1:C:3216:VAL:O	1:C:3220:LEU:HD13	2.01	0.60
1:D:3059:VAL:HA	1:D:3064:ILE:O	2.02	0.60
1:C:3301:LEU:HD23	1:C:3384:ALA:HA	1.83	0.60
1:D:3005:SER:HB3	1:D:3076:MET:SD	2.42	0.60
1:D:3058:LEU:O	1:D:3064:ILE:HB	2.02	0.60
1:D:3074:TYR:O	1:D:3077:GLY:CA	2.50	0.60
1:D:3079:PRO:HG3	1:D:3134:PHE:CB	2.31	0.60
1:A:2927:SER:OG	1:A:2928:PRO:HD2	2.02	0.59
1:A:3116:VAL:O	1:A:3119:PRO:HD3	2.01	0.59
1:A:3074:TYR:O	1:A:3078:GLY:N	2.33	0.59
1:B:3203:LEU:H	1:B:3203:LEU:CD1	2.15	0.59
1:B:3517:LEU:CD1	1:B:3517:LEU:N	2.64	0.59
1:D:3316:PHE:HE1	1:D:3490:PHE:CZ	2.20	0.59
1:A:3509:LEU:HD13	1:A:3509:LEU:O	2.03	0.59
1:D:3066:PRO:HD2	1:D:3068:ASN:N	2.05	0.59
1:C:2997:LYS:HB2	1:C:3068:ASN:O	2.02	0.59
1:D:3066:PRO:HG2	1:D:3067:SER:H	1.66	0.59
1:D:3336:GLN:O	1:D:3336:GLN:HG3	2.03	0.59
1:A:3266:PHE:CB	1:A:3278:LEU:HD21	2.31	0.59
1:D:3048:TYR:CE1	1:D:3080:ILE:HD13	2.37	0.59
1:C:3517:LEU:HD13	1:C:3518:GLY:H	1.65	0.59
1:A:3354:LEU:HD21	1:A:3358:VAL:HG21	1.84	0.59
1:B:3206:ALA:N	1:B:3207:GLU:HB3	2.18	0.59
1:D:3316:PHE:CD2	1:D:3331:GLU:HB2	2.37	0.59
1:D:3499:TYR:CD1	1:D:3502:ARG:CG	2.85	0.59
1:A:3417:MET:CE	1:A:3424:VAL:CG2	2.80	0.58
1:D:3116:VAL:O	1:D:3119:PRO:HG3	2.03	0.58
1:D:3395:ASP:C	1:D:3397:GLU:H	2.11	0.58
1:D:3393:TYR:CB	1:D:3394:SER:HA	2.33	0.58
1:C:3465:MET:HE1	1:C:3515:TYR:CD2	2.37	0.58
1:A:3220:LEU:HD13	1:A:3220:LEU:C	2.28	0.58
1:B:3071:ILE:HD12	1:B:3095:VAL:HG11	1.84	0.58
1:C:3248:LYS:O	1:C:3248:LYS:HG2	2.03	0.58
1:C:3357:LEU:HD22	1:C:3555:LEU:HD23	1.84	0.58
1:C:2956:ASP:O	1:C:2958:ALA:HB2	2.04	0.58
1:C:3206:ALA:N	1:C:3207:GLU:HB3	2.19	0.58
1:D:3500:LEU:O	1:D:3500:LEU:HD12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3324:VAL:HG13	1:B:2973:VAL:HG12	1.86	0.58
1:B:3354:LEU:CD1	1:B:3380:MET:HE1	2.35	0.57
1:C:3517:LEU:HD13	1:C:3518:GLY:C	2.30	0.57
1:A:2914:GLU:N	1:A:3061:ASP:OD2	2.37	0.57
1:A:3354:LEU:HD22	1:A:3481:TYR:CZ	2.39	0.57
1:D:3315:LEU:CD2	1:D:3502:ARG:HB3	2.21	0.57
1:C:3517:LEU:HD13	1:C:3517:LEU:C	2.30	0.57
1:A:3214:GLY:O	1:A:3217:LEU:HB3	2.04	0.57
1:D:3358:VAL:HG11	1:D:3468:TRP:CH2	2.40	0.57
1:D:2997:LYS:HZ2	1:D:3203:LEU:HD21	1.70	0.57
1:B:3207:GLU:O	1:B:3210:ALA:N	2.36	0.57
1:D:2923:LYS:HE3	1:D:2941:LYS:CE	2.26	0.57
1:B:2921:ARG:HD2	1:B:3037:GLU:HA	1.86	0.56
1:A:3207:GLU:HG3	1:A:3208:GLN:H	1.70	0.56
1:D:3316:PHE:CE1	1:D:3488:VAL:CG1	2.88	0.56
1:C:3177:THR:HG22	1:C:3178:GLY:N	2.20	0.56
1:B:3203:LEU:O	1:B:3203:LEU:CD2	2.43	0.56
1:D:3224:PHE:CD1	1:D:3224:PHE:C	2.83	0.56
1:D:3492:SER:HB3	1:D:3495:LYS:HG2	1.87	0.56
1:A:3072:HIS:CD2	1:A:3099:LEU:CD2	2.80	0.56
1:A:3354:LEU:C	1:A:3354:LEU:HD23	2.30	0.56
1:D:3185:HIS:O	1:D:3185:HIS:CG	2.57	0.56
1:A:3001:PHE:HE1	1:A:3072:HIS:CE1	2.24	0.56
1:C:3137:GLU:HG2	1:C:3141:LYS:HE3	1.88	0.56
1:C:3357:LEU:HD22	1:C:3555:LEU:CD2	2.34	0.56
1:D:3315:LEU:CD2	1:D:3502:ARG:HG3	2.35	0.56
1:D:3528:ASN:CA	1:D:3529:ARG:HG3	2.30	0.56
1:A:2997:LYS:CE	1:A:3203:LEU:CD2	2.79	0.56
1:D:3316:PHE:CE1	1:D:3488:VAL:HG12	2.41	0.56
1:D:3353:PRO:O	1:D:3357:LEU:HD12	2.05	0.56
1:A:3122:ILE:HD11	1:D:3122:ILE:CG2	2.35	0.56
1:A:3270:MET:HE3	1:A:3275:LEU:HD12	1.88	0.56
1:D:3056:ASN:O	1:D:3060:ASN:HB2	2.05	0.56
1:D:3499:TYR:HD1	1:D:3502:ARG:HG2	1.63	0.56
1:A:3366:ASN:ND2	1:A:3453:PRO:HD3	2.21	0.55
1:C:3517:LEU:CD1	1:C:3519:LYS:HG3	2.35	0.55
1:C:3362:LYS:HE2	1:C:3362:LYS:CA	2.30	0.55
1:A:3517:LEU:HD21	1:A:3525:ALA:HB1	1.87	0.55
1:B:2997:LYS:HD3	1:B:3203:LEU:CD2	2.36	0.55
1:B:3203:LEU:CD1	1:B:3203:LEU:N	2.69	0.55
1:D:3351:SER:CA	1:D:3353:PRO:CD	2.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2911:VAL:HG23	1:B:3060:ASN:HB3	1.89	0.55
1:C:3064:ILE:CG2	1:C:3065:ASP:H	2.13	0.55
1:A:3220:LEU:HD11	1:A:3224:PHE:HE1	1.72	0.55
1:B:3337:LEU:HD12	1:B:3337:LEU:O	2.07	0.55
1:B:3542:LYS:HD2	1:B:3547:ASP:O	2.07	0.55
1:C:2923:LYS:HZ3	1:C:2945:ARG:NE	2.05	0.55
1:D:3316:PHE:CE2	1:D:3488:VAL:HG12	2.42	0.55
1:A:3221:GLU:O	1:A:3224:PHE:HB2	2.07	0.55
1:B:3203:LEU:H	1:B:3203:LEU:HD13	1.71	0.55
1:D:3183:TYR:CD1	1:D:3190:ARG:CG	2.90	0.55
1:C:2973:VAL:HG22	1:C:2973:VAL:O	2.08	0.54
1:D:3316:PHE:CZ	1:D:3488:VAL:CG1	2.89	0.54
1:C:3220:LEU:N	1:C:3220:LEU:HD12	2.22	0.54
1:B:2997:LYS:HD2	1:B:3203:LEU:HD21	1.90	0.54
1:D:2997:LYS:HD2	1:D:3203:LEU:CD2	2.37	0.54
1:D:3118:ASN:N	1:D:3119:PRO:CD	2.71	0.54
1:D:3492:SER:CB	1:D:3495:LYS:HG2	2.38	0.54
1:C:3218:LYS:HA	1:C:3221:GLU:HB3	1.90	0.54
1:D:3071:ILE:HG21	1:D:3081:ALA:HB1	1.89	0.54
1:D:3356:LYS:HG2	1:D:3533:MET:HE1	1.89	0.54
1:A:3001:PHE:CE1	1:A:3072:HIS:CE1	2.96	0.54
1:A:3163:GLU:OE2	1:A:3166:ARG:NH1	2.40	0.54
1:A:3417:MET:HE1	1:A:3424:VAL:HG23	1.89	0.54
1:A:3307:ASN:O	1:A:3336:GLN:NE2	2.41	0.53
1:C:3311:LYS:CE	1:C:3509:LEU:HD21	2.38	0.53
1:C:3352:ASP:N	1:C:3353:PRO:CD	2.72	0.53
1:D:3497:GLY:O	1:D:3501:THR:N	2.40	0.53
1:A:3220:LEU:CD1	1:A:3224:PHE:CE1	2.91	0.53
1:A:3253:GLY:O	1:A:3291:ALA:HA	2.08	0.53
1:A:3111:ILE:O	1:A:3115:GLU:HG2	2.08	0.53
1:B:2998:VAL:HG21	1:B:3064:ILE:HD12	1.89	0.53
1:C:3207:GLU:O	1:C:3210:ALA:N	2.40	0.53
1:B:3359:LEU:HD12	1:B:3533:MET:HE3	1.90	0.53
1:C:3463:HIS:NE2	1:C:3483:PRO:HB2	2.24	0.53
1:A:3205:ASN:C	1:A:3207:GLU:HB3	2.34	0.53
1:C:3516:LYS:CG	1:C:3517:LEU:HB2	2.38	0.53
1:D:3066:PRO:CD	1:D:3067:SER:N	2.72	0.53
1:B:3212:GLU:O	1:B:3216:VAL:HG23	2.09	0.53
1:D:3395:ASP:C	1:D:3397:GLU:N	2.66	0.53
1:A:2911:VAL:HG12	1:A:2912:ALA:N	2.24	0.53
1:A:3073:GLY:O	1:A:3074:TYR:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3217:LEU:C	1:C:3217:LEU:HD23	2.33	0.53
1:A:3542:LYS:CD	1:A:3548:LYS:HA	2.39	0.52
1:D:2997:LYS:NZ	1:D:3203:LEU:CD2	2.69	0.52
1:D:3207:GLU:HG3	1:D:3208:GLN:N	2.25	0.52
1:D:3499:TYR:O	1:D:3502:ARG:N	2.34	0.52
1:B:3509:LEU:HD13	1:B:3509:LEU:O	2.09	0.52
1:B:3096:SER:OG	1:B:3203:LEU:HB2	2.09	0.52
1:D:3183:TYR:HE1	1:D:3190:ARG:HE	1.56	0.52
1:A:2911:VAL:HG12	1:A:2912:ALA:H	1.75	0.52
1:A:3386:VAL:O	1:A:3389:ASN:O	2.28	0.52
1:D:3073:GLY:HA3	1:D:3077:GLY:C	2.34	0.52
1:A:3017:ARG:O	1:A:3021:GLN:CG	2.49	0.52
1:A:3074:TYR:H	1:A:3077:GLY:C	2.18	0.52
1:B:3463:HIS:CD2	1:B:3483:PRO:HB2	2.45	0.52
1:C:3362:LYS:HD3	1:C:3470:LYS:HD3	1.91	0.52
1:B:2997:LYS:HD3	1:B:3203:LEU:HD21	1.92	0.52
1:D:3117:ALA:O	1:D:3118:ASN:CB	2.46	0.52
1:B:3463:HIS:NE2	1:B:3483:PRO:CB	2.70	0.52
1:D:3222:LYS:NZ	1:D:3303:VAL:HG13	2.25	0.52
1:D:2965:GLN:OE1	1:D:2982:GLN:HG3	2.11	0.51
1:B:3177:THR:HG22	1:B:3178:GLY:N	2.26	0.51
1:D:3479:GLY:O	1:D:3496:PHE:CE1	2.63	0.51
1:D:3224:PHE:C	1:D:3224:PHE:HD1	2.19	0.51
1:D:3315:LEU:HG	1:D:3499:TYR:CE1	2.46	0.51
1:A:2913:ILE:H	1:A:3061:ASP:CG	2.18	0.51
1:A:2929:LEU:HD11	1:D:2933:LEU:HD22	1.91	0.51
1:A:3217:LEU:C	1:A:3217:LEU:CD1	2.84	0.51
1:A:3509:LEU:CD1	1:A:3509:LEU:C	2.84	0.51
1:B:2913:ILE:CG2	1:B:2913:ILE:O	2.58	0.51
1:D:3004:GLY:CA	1:D:3075:SER:O	2.57	0.51
1:D:3398:ASN:OD1	1:D:3399:ALA:N	2.44	0.51
1:C:3069:ILE:O	1:C:3095:VAL:HG22	2.11	0.51
1:C:3463:HIS:CD2	1:C:3483:PRO:HG2	2.45	0.51
1:C:3465:MET:HE2	1:C:3515:TYR:CE2	2.46	0.51
1:B:2997:LYS:CD	1:B:3203:LEU:CD2	2.89	0.51
1:C:3351:SER:N	1:C:3412:HIS:CE1	2.79	0.50
1:D:3102:ARG:HD2	1:D:3154:ASP:HB3	1.92	0.50
1:D:3301:LEU:HD23	1:D:3384:ALA:HA	1.93	0.50
1:A:2973:VAL:O	1:A:2973:VAL:CG1	2.60	0.50
1:C:3112:THR:O	1:C:3115:GLU:O	2.30	0.50
1:B:3268:SER:O	1:B:3299:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3032:LEU:HD13	1:C:3047:LEU:HD22	1.93	0.50
1:D:3212:GLU:O	1:D:3216:VAL:HG23	2.10	0.50
1:B:2997:LYS:HZ2	1:B:3203:LEU:CD2	2.24	0.50
1:C:2910:ASN:O	1:C:2911:VAL:HG23	2.11	0.50
1:C:2923:LYS:HE3	1:C:2941:LYS:HD3	1.94	0.50
1:D:2916:ASP:OD1	1:D:2917:GLY:N	2.44	0.50
1:A:3351:SER:HB3	1:A:3483:PRO:HB3	1.93	0.50
1:D:3079:PRO:CB	1:D:3139:ASN:ND2	2.75	0.50
1:D:3225:LYS:HD2	1:D:3296:ILE:HG21	1.92	0.50
1:B:3151:LEU:O	1:B:3166:ARG:NH2	2.35	0.49
1:B:3206:ALA:HA	1:B:3207:GLU:C	2.37	0.49
1:D:3405:LEU:C	1:D:3405:LEU:HD13	2.37	0.49
1:D:3502:ARG:HA	1:D:3502:ARG:NE	2.27	0.49
1:B:3207:GLU:HG3	1:B:3208:GLN:N	2.27	0.49
1:D:3071:ILE:CG2	1:D:3081:ALA:HB1	2.42	0.49
1:B:3354:LEU:HD12	1:B:3380:MET:HE1	1.94	0.49
1:D:3080:ILE:HD11	1:D:3134:PHE:HE1	1.76	0.49
1:D:3465:MET:O	1:D:3465:MET:CG	2.61	0.49
1:A:3351:SER:OG	1:A:3352:ASP:N	2.40	0.49
1:B:2997:LYS:HE2	1:B:3068:ASN:HB2	1.95	0.49
1:B:3069:ILE:O	1:B:3095:VAL:HG22	2.12	0.49
1:C:2923:LYS:NZ	1:C:2945:ARG:HE	2.10	0.49
1:D:3528:ASN:HA	1:D:3529:ARG:CG	2.33	0.49
1:B:3463:HIS:CD2	1:B:3483:PRO:CG	2.94	0.49
1:D:3533:MET:SD	1:D:3538:LEU:HD22	2.53	0.49
1:A:3542:LYS:HD2	1:A:3548:LYS:HA	1.95	0.49
1:C:3374:ARG:NH1	1:C:3378:GLU:OE2	2.46	0.49
1:D:3222:LYS:HZ2	1:D:3303:VAL:HG11	1.75	0.49
1:B:2933:LEU:HD13	1:B:3126:ILE:HG21	1.94	0.49
1:D:3315:LEU:CG	1:D:3499:TYR:CE1	2.92	0.49
1:B:3111:ILE:HD13	1:B:3126:ILE:HD13	1.93	0.49
1:D:3066:PRO:HD2	1:D:3067:SER:N	2.28	0.49
1:A:3001:PHE:HB2	1:A:3027:MET:HE2	1.95	0.48
1:A:3122:ILE:HD13	1:D:3122:ILE:CG1	2.43	0.48
1:A:3220:LEU:HD11	1:A:3224:PHE:CE1	2.48	0.48
1:D:3086:ARG:HD3	1:D:3139:ASN:O	2.12	0.48
1:B:2911:VAL:HG23	1:B:3060:ASN:CB	2.43	0.48
1:B:3311:LYS:CE	1:B:3509:LEU:HD21	2.43	0.48
1:A:3354:LEU:HD22	1:A:3481:TYR:CE2	2.48	0.48
1:D:3495:LYS:O	1:D:3498:ASP:N	2.46	0.48
1:A:3417:MET:HE1	1:A:3424:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2921:ARG:NH2	1:B:2945:ARG:HB3	2.27	0.48
1:B:3517:LEU:C	1:B:3517:LEU:HD22	2.38	0.48
1:C:2923:LYS:NZ	1:C:2945:ARG:NE	2.62	0.48
1:C:3513:GLN:O	1:C:3516:LYS:CD	2.56	0.48
1:B:3200:VAL:HG12	1:B:3200:VAL:O	2.14	0.48
1:B:3353:PRO:O	1:B:3357:LEU:HD12	2.14	0.48
1:B:3354:LEU:HD23	1:B:3354:LEU:O	2.14	0.48
1:D:3076:MET:HG3	1:D:3104:MET:HE1	1.96	0.48
1:A:3151:LEU:O	1:A:3166:ARG:NH2	2.40	0.48
1:B:3256:ASN:HB3	1:B:3294:TRP:CZ2	2.49	0.48
1:D:3064:ILE:CA	1:D:3065:ASP:HB2	2.44	0.48
1:A:3474:ASP:OD2	1:B:2926:LEU:HB3	2.14	0.48
1:C:2998:VAL:HG21	1:C:3064:ILE:HD11	1.96	0.47
1:D:3554:ILE:HA	1:D:3557:LEU:HD12	1.96	0.47
1:C:3151:LEU:O	1:C:3166:ARG:NH2	2.39	0.47
1:C:3397:GLU:O	1:C:3400:ASN:HB2	2.14	0.47
1:A:3000:LEU:O	1:A:3071:ILE:O	2.32	0.47
1:B:2910:ASN:O	1:B:2911:VAL:HB	2.13	0.47
1:D:3225:LYS:C	1:D:3227:TYR:N	2.72	0.47
1:D:3256:ASN:HB3	1:D:3294:TRP:CZ2	2.50	0.47
1:D:3266:PHE:HB2	1:D:3278:LEU:CD2	2.44	0.47
1:B:3074:TYR:CD1	1:B:3075:SER:N	2.82	0.47
1:D:3222:LYS:HZ1	1:D:3300:ALA:HB1	1.80	0.47
1:B:2997:LYS:NZ	1:B:3203:LEU:HD21	2.29	0.47
1:C:3177:THR:HG22	1:C:3178:GLY:H	1.79	0.47
1:C:3509:LEU:HD13	1:C:3509:LEU:O	2.15	0.47
1:D:3151:LEU:O	1:D:3166:ARG:NH2	2.37	0.47
1:D:3206:ALA:HA	1:D:3207:GLU:C	2.39	0.47
1:D:3357:LEU:HD23	1:D:3555:LEU:HD21	1.95	0.47
1:B:2944:ARG:HG2	1:B:3035:TYR:CE1	2.50	0.47
1:B:2998:VAL:CG2	1:B:3064:ILE:HD12	2.44	0.47
1:B:3204:PHE:CE1	1:B:3207:GLU:HB2	2.49	0.47
1:C:2982:GLN:O	1:C:3021:GLN:NE2	2.48	0.47
1:C:3001:PHE:HB2	1:C:3027:MET:HE2	1.96	0.47
1:C:3121:GLY:O	1:C:3122:ILE:C	2.50	0.47
1:D:3150:LEU:HD13	1:D:3177:THR:HG23	1.97	0.47
1:A:3217:LEU:HD21	1:A:3273:LYS:CE	2.34	0.47
1:A:3222:LYS:HZ2	1:A:3338:MET:HB2	1.80	0.47
1:C:3253:GLY:O	1:C:3291:ALA:HA	2.15	0.47
1:A:3218:LYS:HD3	1:A:3272:ILE:HD12	1.97	0.47
1:A:3301:LEU:HD23	1:A:3384:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3517:LEU:HD21	1:B:3525:ALA:HB1	1.97	0.46
1:A:3122:ILE:HG21	1:D:3122:ILE:CD1	2.45	0.46
1:C:3301:LEU:HG	1:C:3384:ALA:HB2	1.97	0.46
1:B:3339:LEU:O	1:B:3340:LEU:C	2.57	0.46
1:D:3208:GLN:C	1:D:3211:VAL:HB	2.39	0.46
1:A:3512:ALA:O	1:A:3517:LEU:CD1	2.64	0.46
1:B:3517:LEU:HD22	1:B:3517:LEU:O	2.16	0.46
1:D:3227:TYR:O	1:D:3227:TYR:CG	2.65	0.46
1:A:3533:MET:SD	1:A:3538:LEU:HD22	2.55	0.46
1:B:2912:ALA:HA	1:B:3061:ASP:OD1	2.15	0.46
1:C:2953:THR:O	1:C:2957:HIS:ND1	2.46	0.46
1:C:2957:HIS:CA	1:C:2958:ALA:CB	2.93	0.46
1:D:2923:LYS:HZ2	1:D:2941:LYS:HG2	1.79	0.46
1:A:3326:ASP:HB3	1:A:3329:ALA:HB2	1.98	0.46
1:B:3019:HIS:HA	1:B:3022:LYS:NZ	2.30	0.46
1:C:2956:ASP:C	1:C:2958:ALA:HB3	2.40	0.46
1:D:3224:PHE:HD1	1:D:3224:PHE:O	1.98	0.46
1:A:3511:MET:SD	1:A:3514:SER:OG	2.68	0.46
1:D:3357:LEU:HD22	1:D:3555:LEU:CD2	2.45	0.46
1:D:3479:GLY:C	1:D:3496:PHE:HE1	2.24	0.46
1:D:3492:SER:OG	1:D:3495:LYS:HG2	2.15	0.46
1:A:3354:LEU:O	1:A:3357:LEU:N	2.46	0.46
1:B:2911:VAL:HG22	1:B:2912:ALA:N	2.30	0.46
1:D:3074:TYR:O	1:D:3077:GLY:N	2.48	0.46
1:C:3118:ASN:N	1:C:3119:PRO:HD3	2.31	0.46
1:C:3215:GLU:OE2	1:C:3306:GLN:HB3	2.16	0.46
1:C:3396:SER:O	1:C:3399:ALA:HB3	2.16	0.46
1:A:3436:THR:HG22	1:A:3526:ILE:HG22	1.98	0.46
1:C:3354:LEU:O	1:C:3358:VAL:HG23	2.17	0.46
1:B:3351:SER:O	1:B:3355:SER:CB	2.63	0.45
1:B:3509:LEU:C	1:B:3509:LEU:CD1	2.88	0.45
1:C:2981:HIS:CE1	1:C:3017:ARG:HD3	2.51	0.45
1:D:3077:GLY:O	1:D:3081:ALA:N	2.40	0.45
1:D:3063:GLY:C	1:D:3065:ASP:HB2	2.41	0.45
1:D:3076:MET:HG3	1:D:3104:MET:CE	2.46	0.45
1:A:3004:GLY:HA2	1:A:3075:SER:O	2.16	0.45
1:D:3354:LEU:HD21	1:D:3380:MET:HE1	1.98	0.45
1:D:3479:GLY:O	1:D:3496:PHE:HE1	1.99	0.45
1:A:3065:ASP:HB3	1:A:3066:PRO:CD	2.41	0.45
1:C:3076:MET:HA	1:C:3104:MET:HE2	1.99	0.45
1:C:3301:LEU:HD23	1:C:3384:ALA:CA	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3057:TYR:CZ	1:D:3062:LYS:CE	2.97	0.45
1:D:3294:TRP:CZ2	1:D:3387:LEU:HD22	2.51	0.45
1:D:3465:MET:HA	1:D:3481:TYR:O	2.17	0.45
1:A:3352:ASP:N	1:A:3353:PRO:CD	2.80	0.45
1:C:3354:LEU:CD2	1:C:3358:VAL:CG2	2.92	0.45
1:D:3116:VAL:O	1:D:3116:VAL:CG2	2.65	0.45
1:A:2912:ALA:HA	1:A:3061:ASP:OD1	2.17	0.45
1:B:3071:ILE:CG2	1:B:3081:ALA:HB1	2.46	0.45
1:D:3465:MET:O	1:D:3465:MET:HG3	2.17	0.45
1:A:3308:LYS:HE2	1:A:3333:LEU:CD2	2.47	0.45
1:A:3311:LYS:HE2	1:A:3509:LEU:HD21	1.98	0.45
1:D:3361:ALA:CB	1:D:3372:VAL:HG23	2.47	0.45
1:C:3352:ASP:H	1:C:3353:PRO:CD	2.29	0.45
1:D:2923:LYS:NZ	1:D:2945:ARG:HE	2.14	0.45
1:B:2913:ILE:O	1:B:2913:ILE:HG22	2.16	0.45
1:C:2923:LYS:CD	1:C:2941:LYS:HD3	2.47	0.45
1:C:3016:ILE:O	1:C:3016:ILE:HG22	2.15	0.45
1:C:3220:LEU:N	1:C:3220:LEU:CD1	2.80	0.45
1:D:3225:LYS:O	1:D:3227:TYR:N	2.45	0.45
1:D:3354:LEU:HA	1:D:3357:LEU:HB2	1.97	0.45
1:D:3465:MET:HB2	1:D:3480:PHE:CE1	2.52	0.45
1:A:3074:TYR:O	1:A:3075:SER:C	2.58	0.44
1:B:3221:GLU:HA	1:B:3224:PHE:HB2	1.99	0.44
1:C:3517:LEU:HD13	1:C:3518:GLY:CA	2.45	0.44
1:A:3354:LEU:HD23	1:A:3358:VAL:HG23	1.95	0.44
1:C:3256:ASN:HB3	1:C:3294:TRP:CZ2	2.52	0.44
1:D:3115:GLU:HB3	1:D:3116:VAL:CG1	2.43	0.44
1:A:2928:PRO:HG2	1:D:3129:ALA:HB2	1.99	0.44
1:A:3222:LYS:NZ	1:A:3338:MET:HB2	2.32	0.44
1:C:3516:LYS:HB2	1:C:3517:LEU:CB	2.28	0.44
1:D:3074:TYR:O	1:D:3075:SER:C	2.61	0.44
1:C:2924:GLU:HG2	1:C:2926:LEU:CD1	2.46	0.44
1:D:2945:ARG:HD3	1:D:3036:GLY:O	2.17	0.44
1:D:2964:SER:O	1:D:2980:TYR:HB3	2.17	0.44
1:D:3064:ILE:CA	1:D:3065:ASP:CB	2.95	0.44
1:A:3032:LEU:HD13	1:A:3047:LEU:HD22	1.99	0.44
1:A:3300:ALA:O	1:A:3303:VAL:HG12	2.17	0.44
1:C:3070:ILE:HD13	1:C:3203:LEU:HD21	1.99	0.44
1:D:3001:PHE:HB2	1:D:3027:MET:HE2	1.98	0.44
1:D:3395:ASP:HB3	1:D:3397:GLU:CG	2.45	0.44
1:A:3212:GLU:O	1:A:3215:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3266:PHE:HB2	1:B:3278:LEU:CD1	2.48	0.44
1:B:3459:ASP:O	1:B:3528:ASN:HB2	2.18	0.44
1:D:3076:MET:CG	1:D:3104:MET:HE1	2.47	0.44
1:A:3122:ILE:CD1	1:D:3122:ILE:HD13	2.48	0.44
1:A:3337:LEU:HD22	1:A:3351:SER:N	2.32	0.44
1:B:3071:ILE:CD1	1:B:3095:VAL:HG11	2.48	0.44
1:B:3207:GLU:HG3	1:B:3208:GLN:H	1.82	0.44
1:C:2998:VAL:HG22	1:C:3026:ASP:HB2	2.00	0.44
1:C:3066:PRO:C	1:C:3068:ASN:N	2.73	0.44
1:C:3509:LEU:CD1	1:C:3509:LEU:C	2.89	0.44
1:A:3224:PHE:O	1:A:3225:LYS:C	2.60	0.44
1:B:2997:LYS:HZ3	1:B:3203:LEU:HD23	1.83	0.44
1:B:3032:LEU:HD13	1:B:3047:LEU:HD22	2.00	0.44
1:C:3513:GLN:C	1:C:3516:LYS:HB3	2.43	0.44
1:D:3503:PHE:CD1	1:D:3503:PHE:C	2.95	0.44
1:A:3459:ASP:O	1:A:3528:ASN:HB2	2.17	0.43
1:B:3201:SER:N	1:B:3202:GLY:HA3	2.32	0.43
1:D:3208:GLN:HA	1:D:3211:VAL:CB	2.47	0.43
1:B:3071:ILE:HG22	1:B:3081:ALA:HB1	2.00	0.43
1:D:3359:LEU:HD21	1:D:3456:LEU:O	2.18	0.43
1:D:3463:HIS:HB3	1:D:3483:PRO:HD2	2.00	0.43
1:A:2958:ALA:HB1	1:A:2965:GLN:HB2	2.00	0.43
1:C:3116:VAL:CG2	1:C:3119:PRO:HG3	2.38	0.43
1:D:3221:GLU:C	1:D:3224:PHE:HB3	2.43	0.43
1:B:3203:LEU:O	1:B:3204:PHE:HB3	2.18	0.43
1:C:3356:LYS:HE3	1:C:3457:GLU:OE2	2.18	0.43
1:C:3362:LYS:HZ1	1:C:3365:GLU:CD	2.25	0.43
1:D:3351:SER:C	1:D:3353:PRO:HD3	2.39	0.43
1:B:2921:ARG:HD3	1:B:3037:GLU:HA	1.99	0.43
1:C:3362:LYS:HA	1:C:3362:LYS:CE	2.33	0.43
1:D:2913:ILE:HB	1:D:3061:ASP:CG	2.43	0.43
1:D:3073:GLY:HA3	1:D:3077:GLY:O	2.18	0.43
1:D:3495:LYS:HE2	1:D:3495:LYS:HB3	1.83	0.43
1:D:3064:ILE:HA	1:D:3065:ASP:CB	2.48	0.43
1:C:3065:ASP:N	1:C:3066:PRO:HA	2.33	0.43
1:A:3074:TYR:H	1:A:3078:GLY:N	2.16	0.43
1:D:2923:LYS:NZ	1:D:2945:ARG:NE	2.67	0.43
1:D:3032:LEU:HD13	1:D:3047:LEU:HD22	1.99	0.43
1:A:3356:LYS:HA	1:A:3356:LYS:HD3	1.83	0.43
1:D:3357:LEU:CD2	1:D:3555:LEU:HD21	2.49	0.43
1:D:3397:GLU:O	1:D:3400:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3463:HIS:ND1	1:D:3483:PRO:HB2	2.34	0.43
1:D:2998:VAL:HG22	1:D:3026:ASP:HB2	2.01	0.43
1:D:3268:SER:O	1:D:3299:ARG:NH1	2.52	0.43
1:B:3280:VAL:HG23	1:B:3281:LYS:HG3	2.01	0.42
1:C:3202:GLY:O	1:C:3203:LEU:HD12	2.16	0.42
1:D:3203:LEU:C	1:D:3203:LEU:HD12	2.44	0.42
1:A:3266:PHE:CB	1:A:3278:LEU:HD22	2.38	0.42
1:A:3517:LEU:HD13	1:A:3517:LEU:H	1.84	0.42
1:D:3048:TYR:HE1	1:D:3080:ILE:HD13	1.80	0.42
1:C:2955:LEU:C	1:C:2957:HIS:H	2.27	0.42
1:A:3311:LYS:CE	1:A:3509:LEU:HD21	2.50	0.42
1:B:3204:PHE:HD1	1:B:3206:ALA:H	1.67	0.42
1:B:3517:LEU:HD13	1:B:3517:LEU:N	2.15	0.42
1:C:2923:LYS:HZ3	1:C:2945:ARG:CZ	2.32	0.42
1:D:3358:VAL:HG11	1:D:3468:TRP:CZ3	2.54	0.42
1:D:3496:PHE:O	1:D:3500:LEU:HB3	2.19	0.42
1:C:3249:ASP:CB	1:C:3286:ALA:HB3	2.50	0.42
1:C:3359:LEU:HD11	1:C:3466:ALA:CB	2.49	0.42
1:C:3511:MET:SD	1:C:3514:SER:CB	3.07	0.42
1:B:3526:ILE:O	1:B:3526:ILE:HG13	2.19	0.42
1:D:3079:PRO:HG3	1:D:3134:PHE:HA	2.02	0.42
1:D:3079:PRO:HB2	1:D:3139:ASN:ND2	2.33	0.42
1:A:2964:SER:O	1:A:2980:TYR:HB3	2.20	0.42
1:A:3104:MET:SD	1:A:3107:MET:HA	2.60	0.42
1:C:3104:MET:SD	1:C:3107:MET:HA	2.60	0.42
1:D:3185:HIS:O	1:D:3185:HIS:ND1	2.52	0.42
1:D:3464:ALA:H	1:D:3483:PRO:HG2	1.85	0.42
1:A:3204:PHE:O	1:A:3207:GLU:CB	2.68	0.41
1:A:3353:PRO:HD2	1:A:3354:LEU:H	1.85	0.41
1:B:3303:VAL:O	1:B:3303:VAL:HG22	2.20	0.41
1:D:3117:ALA:C	1:D:3119:PRO:HD3	2.46	0.41
1:A:3122:ILE:HD13	1:D:3122:ILE:HD13	2.02	0.41
1:A:3310:GLU:O	1:A:3314:ARG:HG2	2.20	0.41
1:B:3359:LEU:HD12	1:B:3533:MET:CE	2.50	0.41
1:A:3221:GLU:C	1:A:3224:PHE:HB2	2.45	0.41
1:B:3359:LEU:HD11	1:B:3456:LEU:O	2.21	0.41
1:D:3467:ALA:CB	1:D:3496:PHE:HZ	2.34	0.41
1:C:2923:LYS:CE	1:C:2941:LYS:HD3	2.50	0.41
1:C:3206:ALA:HA	1:C:3207:GLU:C	2.46	0.41
1:A:2926:LEU:HD22	1:B:3474:ASP:OD1	2.20	0.41
1:B:3074:TYR:OH	1:B:3185:HIS:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3511:MET:HG3	1:B:3515:TYR:CD2	2.55	0.41
1:C:3204:PHE:O	1:C:3207:GLU:HG2	2.21	0.41
1:D:2944:ARG:HG2	1:D:3035:TYR:CE2	2.55	0.41
1:C:3362:LYS:NZ	1:C:3365:GLU:OE1	2.51	0.41
1:C:3517:LEU:C	1:C:3517:LEU:CD1	2.93	0.41
1:B:3278:LEU:CD2	1:B:3292:LEU:HD11	2.49	0.41
1:C:3511:MET:HA	1:C:3514:SER:HB2	2.03	0.41
1:D:3225:LYS:CD	1:D:3296:ILE:HG21	2.50	0.41
1:B:2933:LEU:HD13	1:B:3126:ILE:HG22	2.00	0.41
1:B:3007:SER:OG	1:B:3012:GLN:HG3	2.21	0.41
1:B:3337:LEU:HB2	1:B:3338:MET:C	2.46	0.41
1:C:2955:LEU:C	1:C:2957:HIS:N	2.78	0.41
1:C:2956:ASP:C	1:C:2958:ALA:CB	2.94	0.41
1:D:3357:LEU:CD2	1:D:3555:LEU:CD2	2.99	0.41
1:B:2911:VAL:CG2	1:B:2912:ALA:N	2.84	0.41
1:B:3196:ALA:HA	1:B:3199:ILE:HD12	2.03	0.41
1:B:3334:ALA:HA	1:B:3377:LEU:HD22	2.03	0.41
1:D:3115:GLU:CB	1:D:3116:VAL:HG13	2.41	0.40
1:D:3225:LYS:HB2	1:D:3276:VAL:CG1	2.47	0.40
1:C:3458:LEU:HB3	1:C:3527:PHE:CE2	2.56	0.40
1:D:2918:THR:N	1:D:2919:PRO:CD	2.84	0.40
1:D:3221:GLU:HA	1:D:3224:PHE:HB3	2.03	0.40
1:A:3417:MET:CE	1:A:3424:VAL:HG23	2.49	0.40
1:D:3076:MET:CG	1:D:3104:MET:CE	3.00	0.40
1:A:3542:LYS:HD2	1:A:3547:ASP:O	2.22	0.40
1:D:3308:LYS:NZ	1:D:3333:LEU:CD2	2.85	0.40
1:B:3056:ASN:O	1:B:3060:ASN:HB2	2.20	0.40
1:B:3365:GLU:HA	1:B:3369:GLN:O	2.22	0.40
1:D:3007:SER:HB2	1:D:3012:GLN:HG3	2.03	0.40
1:D:3066:PRO:CD	1:D:3067:SER:H	2.35	0.40
1:D:3408:LEU:O	1:D:3411:ILE:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	604/694 (87%)	572 (95%)	29 (5%)	3 (0%)	24	57
1	B	600/694 (86%)	563 (94%)	34 (6%)	3 (0%)	24	57
1	C	546/694 (79%)	510 (93%)	34 (6%)	2 (0%)	30	62
1	D	515/694 (74%)	478 (93%)	34 (7%)	3 (1%)	21	54
All	All	2265/2776 (82%)	2123 (94%)	131 (6%)	11 (0%)	24	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3066	PRO
1	D	3066	PRO
1	A	3353	PRO
1	C	3118	ASN
1	C	3352	ASP
1	B	3353	PRO
1	D	3118	ASN
1	B	2911	VAL
1	A	3066	PRO
1	D	3353	PRO
1	A	3390	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/555 (88%)	481 (98%)	9 (2%)	51	69
1	B	490/555 (88%)	479 (98%)	11 (2%)	45	65
1	C	453/555 (82%)	445 (98%)	8 (2%)	51	69
1	D	431/555 (78%)	415 (96%)	16 (4%)	30	56
All	All	1864/2220 (84%)	1820 (98%)	44 (2%)	43	64

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2921	ARG
1	A	2923	LYS
1	A	2941	LYS
1	A	2997	LYS
1	A	3220	LEU
1	A	3266	PHE
1	A	3275	LEU
1	A	3474	ASP
1	A	3517	LEU
1	B	3064	ILE
1	B	3066	PRO
1	B	3090	GLN
1	B	3131	ASN
1	B	3203	LEU
1	B	3266	PHE
1	B	3275	LEU
1	B	3379	LYS
1	B	3405	LEU
1	B	3463	HIS
1	B	3517	LEU
1	C	2921	ARG
1	C	3122	ILE
1	C	3405	LEU
1	C	3463	HIS
1	C	3509	LEU
1	C	3517	LEU
1	C	3526	ILE
1	C	3545	PHE
1	D	2921	ARG
1	D	2941	LYS
1	D	3064	ILE
1	D	3116	VAL
1	D	3182	PHE
1	D	3224	PHE
1	D	3266	PHE
1	D	3316	PHE
1	D	3393	TYR
1	D	3412	HIS
1	D	3443	LYS
1	D	3476	ARG
1	D	3495	LYS
1	D	3500	LEU

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Mol	Chain	Res	Type
1	D	3502	ARG
1	D	3531	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2910	ASN
1	A	2981	HIS
1	A	2982	GLN
1	A	3021	GLN
1	A	3274	GLN
1	A	3313	ASN
1	A	3484	ASN
1	B	3021	GLN
1	B	3274	GLN
1	B	3313	ASN
1	B	3336	GLN
1	C	3021	GLN
1	C	3415	ASN
1	C	3510	ASN
1	D	2965	GLN
1	D	3049	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	614/694 (88%)	0.36	26 (4%)	40	22	6, 33, 114, 159	0
1	B	612/694 (88%)	0.63	22 (3%)	46	25	22, 58, 99, 133	0
1	C	568/694 (81%)	0.77	50 (8%)	15	10	26, 74, 144, 172	0
1	D	539/694 (77%)	0.87	75 (13%)	6	5	17, 48, 145, 213	0
All	All	2333/2776 (84%)	0.65	173 (7%)	20	13	6, 54, 131, 213	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3457	GLU	6.9
1	D	3312	TYR	5.2
1	D	3465	MET	5.0
1	D	3356	LYS	4.8
1	B	2959	VAL	4.6
1	C	3527	PHE	4.4
1	D	3065	ASP	4.2
1	D	3466	ALA	4.1
1	D	3490	PHE	4.1
1	D	3361	ALA	3.9
1	D	3481	TYR	3.9
1	D	3463	HIS	3.8
1	D	3455	LEU	3.8
1	B	3463	HIS	3.7
1	C	3004	GLY	3.7
1	D	3357	LEU	3.6
1	D	3554	ILE	3.6
1	D	3485	ALA	3.6
1	D	3487	ILE	3.5
1	D	3358	VAL	3.4
1	D	3462	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	3483	PRO	3.3
1	D	3456	LEU	3.3
1	D	3371	GLY	3.3
1	D	3437	VAL	3.3
1	B	3207	GLU	3.3
1	D	3360	VAL	3.2
1	D	3459	ASP	3.2
1	D	3440	VAL	3.2
1	B	2948	GLY	3.2
1	A	3339	LEU	3.1
1	D	3454	VAL	3.1
1	D	3311	LYS	3.1
1	C	3203	LEU	3.1
1	D	3469	ALA	3.1
1	B	3303	VAL	3.0
1	D	3359	LEU	3.0
1	A	3368	GLY	3.0
1	B	3474	ASP	3.0
1	B	2915	ASN	3.0
1	D	3468	TRP	3.0
1	B	3290	GLY	3.0
1	C	2951	THR	3.0
1	C	3530	VAL	2.9
1	D	3355	SER	2.9
1	D	3207	GLU	2.9
1	D	3500	LEU	2.9
1	D	3388	SER	2.9
1	D	3538	LEU	2.9
1	D	3316	PHE	2.9
1	D	3441	VAL	2.9
1	D	3372	VAL	2.8
1	C	2911	VAL	2.8
1	C	3275	LEU	2.8
1	A	3337	LEU	2.8
1	D	3461	PRO	2.8
1	C	3531	VAL	2.8
1	D	3354	LEU	2.8
1	D	3480	PHE	2.7
1	A	3276	VAL	2.7
1	D	3540	SER	2.7
1	C	3077	GLY	2.7
1	C	3499	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	3338	MET	2.7
1	D	3336	GLN	2.7
1	C	3272	ILE	2.7
1	A	3218	LYS	2.7
1	C	3336	GLN	2.7
1	A	2960	GLU	2.7
1	D	3222	LYS	2.7
1	D	3530	VAL	2.7
1	D	3529	ARG	2.7
1	D	3559	VAL	2.6
1	A	3284	TRP	2.6
1	B	3336	GLN	2.6
1	D	3352	ASP	2.6
1	D	3416	PRO	2.6
1	A	3207	GLU	2.6
1	D	3364	LEU	2.6
1	A	3289	LYS	2.6
1	C	3337	LEU	2.6
1	D	3458	LEU	2.6
1	C	3427	GLU	2.6
1	D	3395	ASP	2.6
1	A	3325	VAL	2.5
1	C	3459	ASP	2.5
1	D	3307	ASN	2.5
1	C	2912	ALA	2.5
1	C	3440	VAL	2.5
1	D	3489	GLU	2.5
1	C	3292	LEU	2.5
1	A	3279	PHE	2.5
1	A	3286	ALA	2.5
1	C	3413	ALA	2.5
1	C	3066	PRO	2.5
1	A	3065	ASP	2.5
1	A	3291	ALA	2.5
1	D	3218	LYS	2.5
1	C	3436	THR	2.5
1	A	3463	HIS	2.5
1	B	3215	GLU	2.5
1	B	3222	LYS	2.5
1	D	3353	PRO	2.5
1	B	3464	ALA	2.4
1	D	3464	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	2996	GLY	2.4
1	C	2973	VAL	2.4
1	C	3289	LYS	2.4
1	D	3467	ALA	2.4
1	B	3460	ALA	2.4
1	C	3257	ASP	2.4
1	C	3504	PHE	2.3
1	D	3095	VAL	2.3
1	A	3203	LEU	2.3
1	C	3216	VAL	2.3
1	A	3351	SER	2.3
1	C	3320	ALA	2.3
1	B	3340	LEU	2.3
1	C	3254	TYR	2.3
1	B	3208	GLN	2.3
1	A	3066	PRO	2.3
1	C	3301	LEU	2.3
1	D	3318	GLU	2.3
1	D	3533	MET	2.3
1	D	3362	LYS	2.2
1	A	3265	GLY	2.2
1	A	3278	LEU	2.2
1	C	2910	ASN	2.2
1	C	3312	TYR	2.2
1	C	3215	GLU	2.2
1	B	2958	ALA	2.2
1	C	3333	LEU	2.2
1	D	3330	THR	2.2
1	C	3327	ALA	2.2
1	B	2964	SER	2.2
1	D	3303	VAL	2.2
1	D	3488	VAL	2.2
1	D	3063	GLY	2.2
1	D	3319	ILE	2.2
1	D	3373	ALA	2.2
1	A	3280	VAL	2.2
1	C	3276	VAL	2.2
1	A	2914	GLU	2.2
1	C	2918	THR	2.2
1	B	3315	LEU	2.2
1	C	3014	SER	2.1
1	C	3207	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	2914	GLU	2.1
1	D	3397	GLU	2.1
1	D	3555	LEU	2.1
1	D	2964	SER	2.1
1	B	3301	LEU	2.1
1	C	3435	LEU	2.1
1	C	3409	ALA	2.1
1	D	3320	ALA	2.1
1	C	2916	ASP	2.1
1	C	3352	ASP	2.1
1	C	3367	ASP	2.1
1	A	3219	GLY	2.1
1	C	3204	PHE	2.1
1	D	3453	PRO	2.1
1	B	3317	ARG	2.1
1	B	2979	TYR	2.1
1	A	2916	ASP	2.1
1	D	3323	GLY	2.1
1	D	3413	ALA	2.1
1	C	3458	LEU	2.1
1	C	2942	ASP	2.0
1	C	3075	SER	2.0
1	C	3123	VAL	2.0
1	A	3064	ILE	2.0
1	C	3083	ASP	2.0
1	B	3160	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.