



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:03 PM UTC

PDB ID : 4BP9 / pdb_00004bp9
Title : Oligopeptidase B from Trypanosoma brucei with covalently bound antipain - closed form
Authors : Canning, P.; Rea, D.; Morty, R.; Fulop, V.
Deposited on : 2013-05-23
Resolution : 2.85 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

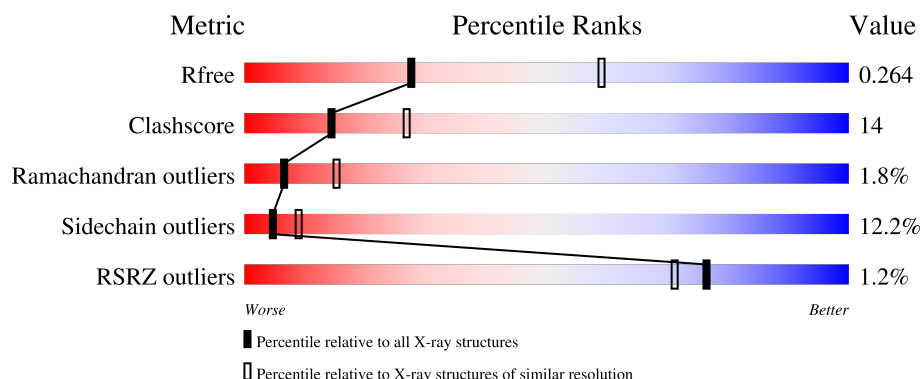
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	715	% 64% 29% 5% ..
1	B	715	% 63% 31%
1	C	715	% 63% 31% 5% ..
1	D	715	64% 30%
1	E	715	% 63% 31% 5% ..

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Mol	Chain	Length	Quality of chain
1	F	715	
2	G	4	
2	H	4	
2	I	4	
2	J	4	
2	K	4	
2	L	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OAR	G	4	X	-	-	-
2	OAR	H	4	X	-	-	-
2	OAR	I	4	X	-	-	-
2	OAR	J	4	X	-	-	-
2	OAR	K	4	X	-	-	-
2	OAR	L	4	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34406 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 OLIGOPEPTIDASSE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	B	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	C	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	D	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	E	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	F	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			

- Molecule 2 is a protein called ANTIPAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	H	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	I	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	J	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	K	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	L	4	Total	C	N	O	0	0	0
			43	27	10	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	4	OAR	RGL	conflict	NOR NOR00664

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Chain	Residue	Modelled	Actual	Comment	Reference
H	4	OAR	RGL	conflict	NOR NOR00664
I	4	OAR	RGL	conflict	NOR NOR00664
J	4	OAR	RGL	conflict	NOR NOR00664
K	4	OAR	RGL	conflict	NOR NOR00664
L	4	OAR	RGL	conflict	NOR NOR00664

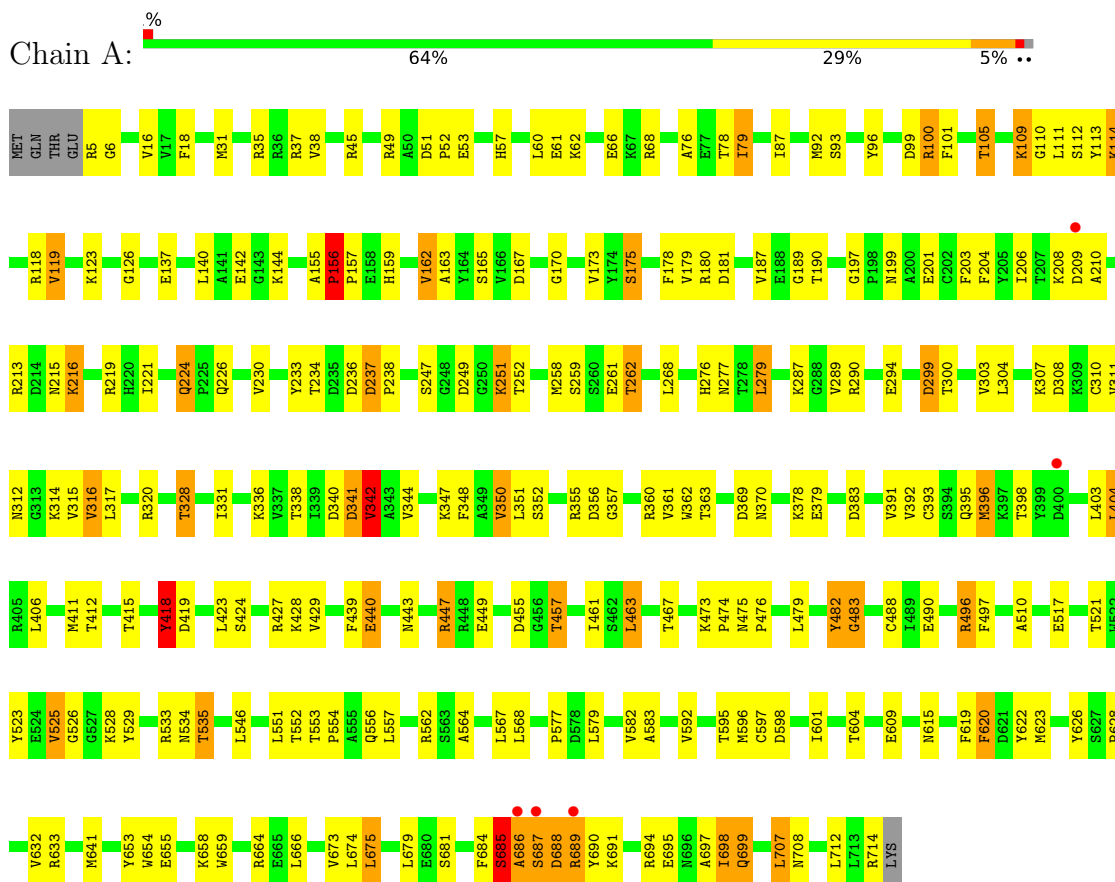
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	75	Total	O	0	0
			75	75		
3	C	36	Total	O	0	0
			36	36		
3	D	39	Total	O	0	0
			39	39		
3	E	37	Total	O	0	0
			37	37		
3	F	48	Total	O	0	0
			48	48		

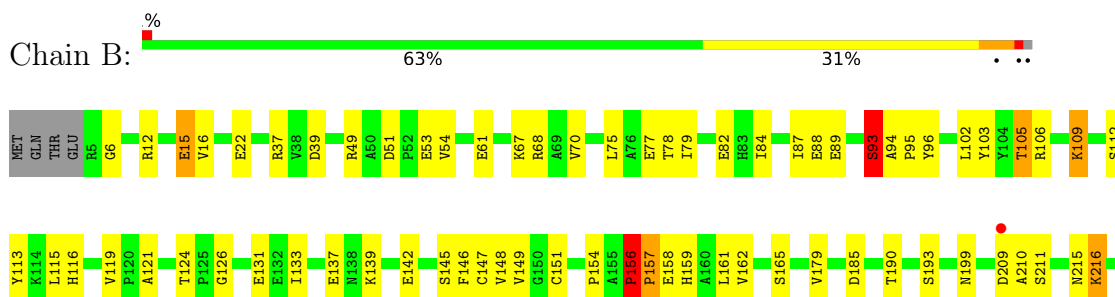
3 Residue-property plots

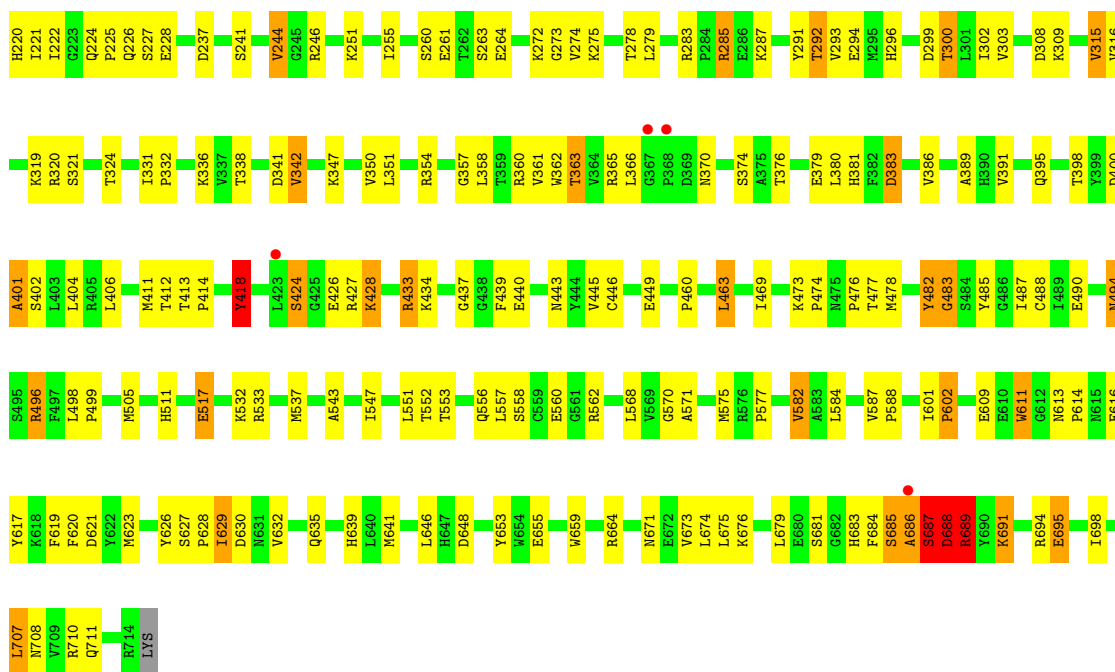
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: OLIGOPEPTIDASSE B

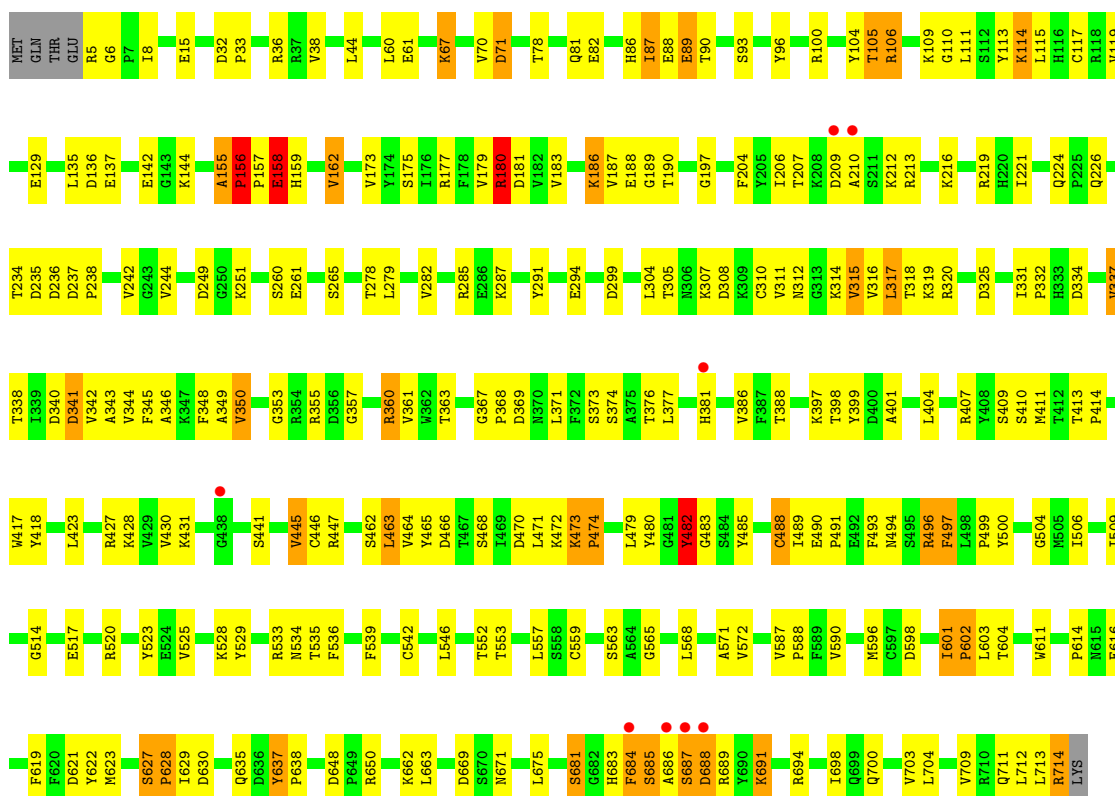


• Molecule 1: OLIGOPEPTIDASSE B



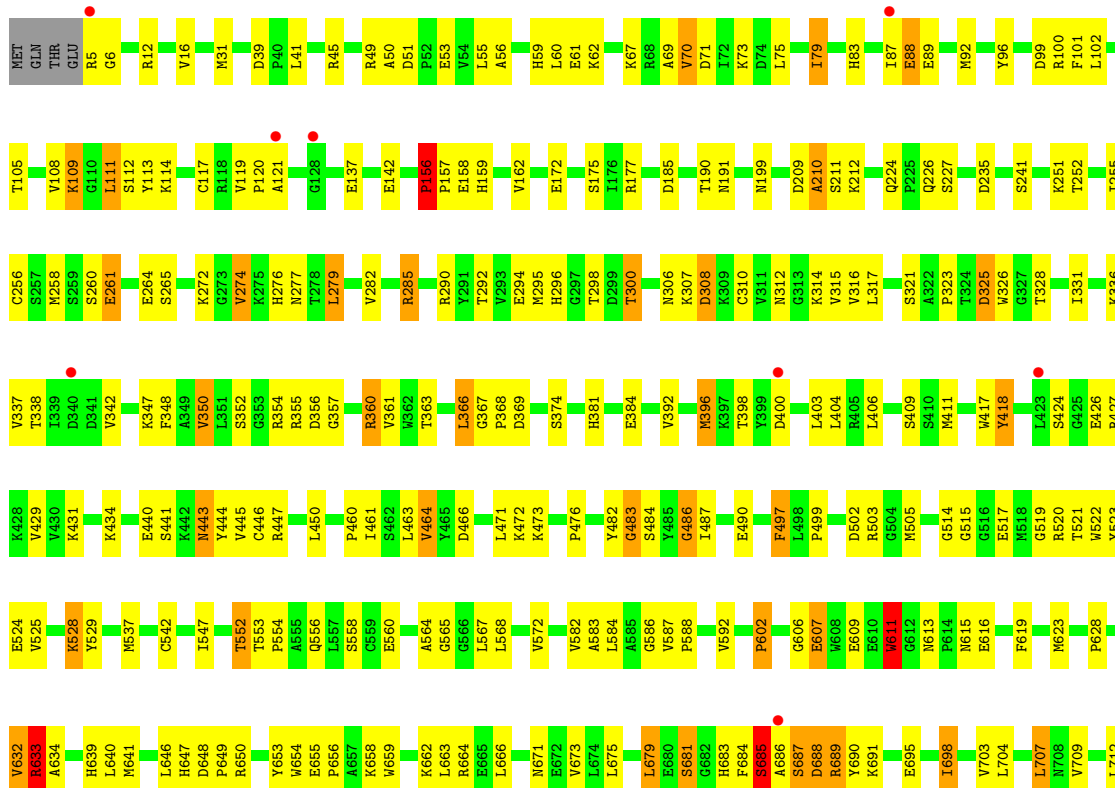


• Molecule 1: OLIGOPEPTIDASSE B



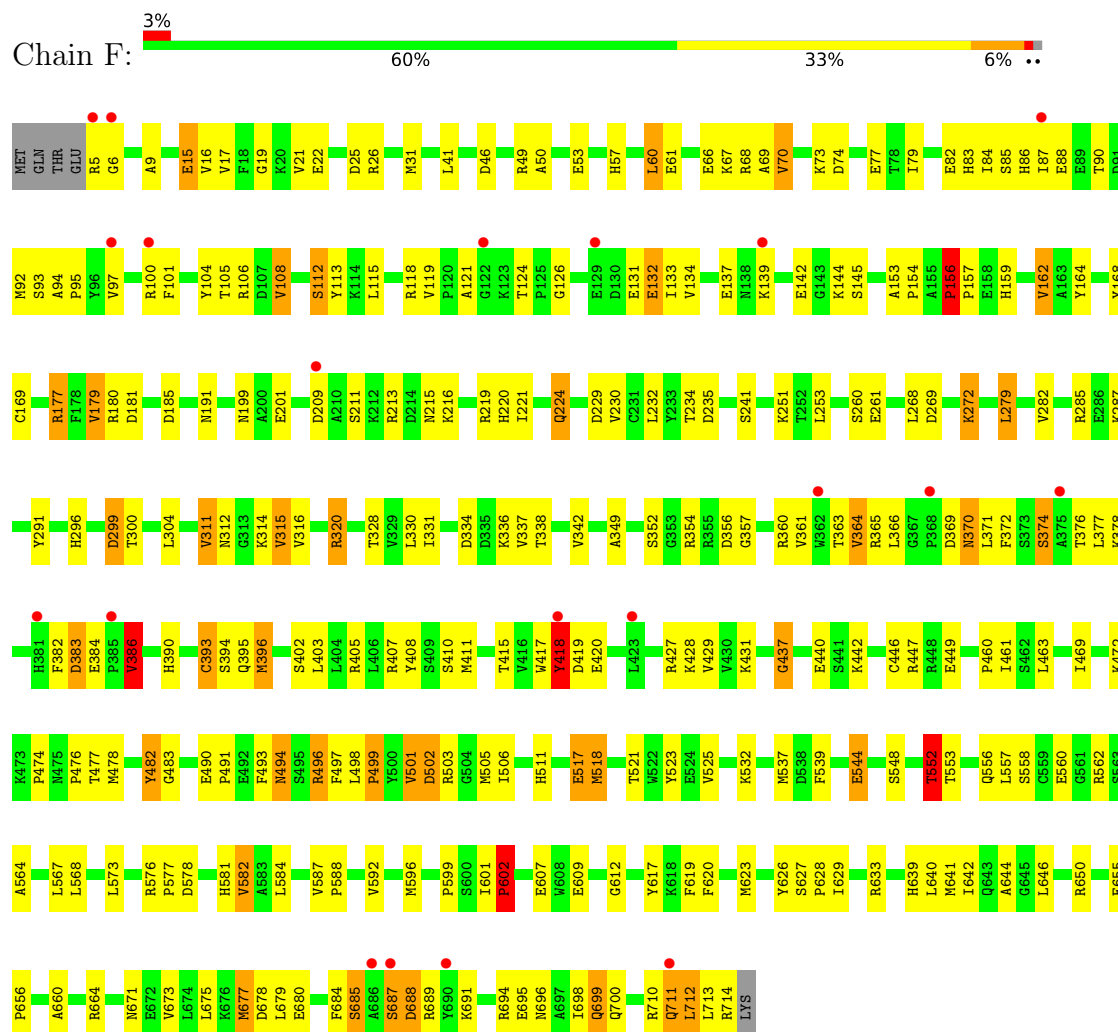
• Molecule 1: OLIGOPEPTIDASSE B





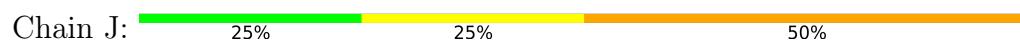
L713
R714
LYS

• Molecule 1: OLIGOPEPTIDASSE B





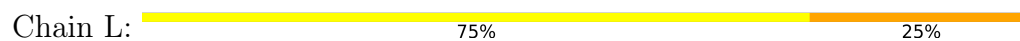
- Molecule 2: ANTIPAIN



- Molecule 2: ANTIPAIN



- Molecule 2: ANTIPAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.80Å 148.80Å 268.00Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	58.59 – 2.85 58.59 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (58.59-2.85) 96.7 (58.59-2.85)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.281 (Not available) , 0.264	Depositor DCC
R_{free} test set	5162 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34406	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2588e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FC0, OAR

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	0.95	1/5772 (0.0%)	1.18	37/7832 (0.5%)
1	B	0.93	3/5772 (0.1%)	1.16	26/7832 (0.3%)
1	C	0.81	0/5772	1.11	22/7832 (0.3%)
1	D	0.84	0/5772	1.12	25/7832 (0.3%)
1	E	0.81	0/5772	1.10	29/7832 (0.4%)
1	F	0.85	1/5772 (0.0%)	1.11	20/7832 (0.3%)
2	G	1.24	0/17	1.67	0/21
2	H	1.54	0/17	1.86	1/21 (4.8%)
2	I	1.33	0/17	2.06	0/21
2	J	1.32	0/17	1.69	0/21
2	K	1.21	0/17	1.53	0/21
2	L	1.49	0/17	1.84	0/21
All	All	0.87	5/34734 (0.0%)	1.13	160/47118 (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	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	2
1	F	0	2
2	G	1	3
2	H	1	2
2	I	1	1
2	J	1	1
2	K	1	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	1	3
All	All	6	30

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	684	PHE	CA-C	-6.58	1.43	1.52
1	B	88	GLU	CA-C	6.29	1.61	1.52
1	F	469	ILE	CA-CB	5.28	1.59	1.54
1	B	244	VAL	CA-CB	5.24	1.62	1.54
1	A	38	VAL	CA-CB	5.14	1.60	1.54

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	418	TYR	N-CA-C	10.04	124.81	108.55
1	D	155	ALA	CA-C-N	9.50	130.17	120.38
1	D	155	ALA	C-N-CA	9.50	130.17	120.38
1	A	350	VAL	CB-CA-C	-9.36	99.30	110.91
1	B	156	PRO	CA-C-N	9.32	131.49	119.84
1	B	156	PRO	C-N-CA	9.32	131.49	119.84
1	C	601	ILE	N-CA-C	8.55	116.39	107.76
1	F	211	SER	N-CA-C	-8.35	103.04	113.23
1	C	156	PRO	CA-C-N	8.11	129.98	119.84
1	C	156	PRO	C-N-CA	8.11	129.98	119.84
1	B	613	ASN	CA-C-N	-7.43	113.25	120.83
1	B	613	ASN	C-N-CA	-7.43	113.25	120.83
1	F	581	HIS	N-CA-C	-7.33	104.47	113.41
1	A	687	SER	N-CA-C	7.31	117.53	107.73
1	A	482	TYR	CA-C-N	7.28	134.80	121.70
1	A	482	TYR	C-N-CA	7.28	134.80	121.70
1	B	517	GLU	N-CA-C	7.27	119.83	111.11
1	D	604	THR	N-CA-C	7.20	118.77	111.07
1	E	224	GLN	N-CA-C	7.18	120.98	110.14
1	D	87	ILE	N-CA-C	7.12	117.93	111.81
1	D	418	TYR	N-CA-C	7.05	120.98	109.85
1	A	109	LYS	N-CA-C	7.04	120.77	111.75
1	E	606	GLY	N-CA-C	-7.00	104.02	112.49
1	E	158	GLU	N-CA-C	6.95	120.24	111.69
1	E	514	GLY	N-CA-C	-6.90	105.72	113.79
1	A	482	TYR	CA-C-O	-6.87	114.80	119.68
1	C	687	SER	N-CA-C	6.87	116.94	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	PRO	N-CA-C	6.84	119.04	110.70
1	A	655	GLU	CA-C-N	-6.82	112.67	119.56
1	A	655	GLU	C-N-CA	-6.82	112.67	119.56
1	D	441	SER	N-CA-C	6.77	121.15	112.34
1	A	224	GLN	N-CA-C	6.77	120.61	109.58
1	D	602	PRO	CA-C-N	-6.76	111.38	122.54
1	D	602	PRO	C-N-CA	-6.76	111.38	122.54
1	A	155	ALA	CA-C-N	6.76	127.34	120.38
1	A	155	ALA	C-N-CA	6.76	127.34	120.38
1	A	690	TYR	N-CA-C	-6.70	105.11	113.28
1	F	185	ASP	N-CA-C	6.70	120.55	110.64
1	F	126	GLY	N-CA-C	-6.68	103.94	111.63
1	D	156	PRO	CA-C-N	6.63	128.13	119.84
1	D	156	PRO	C-N-CA	6.63	128.13	119.84
1	D	261	GLU	N-CA-C	6.62	121.30	112.30
1	A	237	ASP	CA-C-N	6.62	128.11	119.84
1	A	237	ASP	C-N-CA	6.62	128.11	119.84
1	F	602	PRO	N-CA-C	6.59	123.57	113.75
1	B	156	PRO	N-CA-C	6.56	118.70	110.70
1	B	185	ASP	N-CA-C	6.55	119.86	110.24
1	B	418	TYR	N-CA-C	6.45	119.23	109.23
1	B	483	GLY	N-CA-C	-6.41	97.99	113.18
1	C	158	GLU	N-CA-C	6.39	118.32	111.36
1	C	197	GLY	CA-C-N	-6.31	114.12	120.31
1	C	197	GLY	C-N-CA	-6.31	114.12	120.31
1	C	334	ASP	N-CA-C	6.29	118.56	107.61
1	A	659	TRP	N-CA-C	-6.27	103.97	111.69
1	C	155	ALA	CA-C-N	6.24	126.81	120.38
1	C	155	ALA	C-N-CA	6.24	126.81	120.38
1	C	681	SER	N-CA-C	6.23	118.66	109.69
1	E	112	SER	N-CA-C	6.20	118.84	111.33
1	E	602	PRO	N-CA-C	6.19	122.79	113.81
1	A	156	PRO	N-CA-C	6.06	118.10	110.70
1	E	655	GLU	CA-C-N	-6.05	113.45	119.56
1	E	655	GLU	C-N-CA	-6.05	113.45	119.56
1	B	94	ALA	CA-C-N	6.04	125.98	119.76
1	B	94	ALA	C-N-CA	6.04	125.98	119.76
1	B	389	ALA	N-CA-C	5.99	118.20	108.26
1	C	337	VAL	N-CA-C	5.94	116.42	107.75
1	C	6	GLY	CA-C-N	5.94	127.26	119.84
1	C	6	GLY	C-N-CA	5.94	127.26	119.84
1	F	311	VAL	N-CA-C	5.91	118.44	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	GLU	N-CA-C	5.91	121.27	112.94
1	E	681	SER	N-CA-C	5.91	117.56	109.18
1	F	124	THR	CA-C-N	5.90	125.86	119.78
1	F	124	THR	C-N-CA	5.90	125.86	119.78
1	A	311	VAL	N-CA-C	5.88	116.62	110.62
2	H	2	ARG	CA-CB-CG	-5.88	102.34	114.10
1	A	342	VAL	CB-CA-C	-5.87	102.44	111.31
1	B	87	ILE	N-CA-C	5.83	119.26	111.44
1	A	197	GLY	N-CA-C	-5.81	105.20	112.23
1	D	211	SER	N-CA-C	-5.75	105.85	112.86
1	A	483	GLY	N-CA-C	-5.73	96.67	113.30
1	A	156	PRO	CA-C-N	5.73	127.00	119.84
1	A	156	PRO	C-N-CA	5.73	127.00	119.84
1	B	689	ARG	N-CA-C	5.71	116.62	108.74
1	C	637	TYR	CA-C-N	-5.71	112.71	119.84
1	C	637	TYR	C-N-CA	-5.71	112.71	119.84
1	F	112	SER	N-CA-C	5.71	119.76	112.34
1	E	210	ALA	N-CA-C	-5.71	102.96	110.43
1	B	602	PRO	N-CA-C	5.69	124.20	112.47
1	D	418	TYR	CA-CB-CG	5.69	124.14	113.90
1	F	418	TYR	CA-CB-CG	5.68	124.12	113.90
1	B	211	SER	N-CA-C	-5.68	105.93	112.86
1	E	354	ARG	N-CA-C	5.68	118.71	109.06
1	F	687	SER	N-CA-C	5.66	115.31	107.73
1	E	687	SER	N-CA-C	5.65	115.84	107.88
1	F	517	GLU	N-CA-C	5.62	117.08	111.07
1	C	684	PHE	N-CA-C	-5.62	106.38	113.18
1	D	690	TYR	N-CA-C	-5.62	104.55	111.40
1	B	655	GLU	N-CA-C	-5.58	105.02	112.55
1	E	633	ARG	N-CA-C	5.55	117.51	109.07
1	D	182	VAL	N-CA-C	-5.53	105.11	110.42
1	A	525	VAL	N-CA-C	-5.50	107.08	111.81
1	A	344	VAL	N-CA-C	5.49	115.79	108.11
1	B	686	ALA	N-CA-C	-5.48	99.12	110.80
1	E	441	SER	N-CA-C	5.48	118.76	111.75
1	A	259	SER	N-CA-C	-5.47	101.91	110.17
1	E	274	VAL	N-CA-C	5.47	120.72	109.34
1	E	109	LYS	N-CA-C	5.46	117.94	111.33
1	A	99	ASP	CB-CA-C	-5.46	110.30	116.63
1	F	386	VAL	N-CA-C	5.45	114.21	106.53
1	A	415	THR	N-CA-C	5.43	117.90	110.24
1	E	409	SER	N-CA-C	5.43	116.24	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	N-CA-C	5.42	119.05	111.90
1	F	482	TYR	CA-C-N	5.39	131.40	121.70
1	F	482	TYR	C-N-CA	5.39	131.40	121.70
1	D	342	VAL	N-CA-C	5.38	116.48	108.46
1	C	490	GLU	N-CA-C	5.36	116.58	109.93
1	E	111	LEU	N-CA-C	5.35	117.46	107.99
1	A	475	ASN	CA-C-N	-5.34	114.42	119.76
1	A	475	ASN	C-N-CA	-5.34	114.42	119.76
1	A	216	LYS	N-CA-C	5.33	118.12	109.06
1	E	418	TYR	N-CA-C	5.33	118.43	109.95
1	D	109	LYS	N-CA-C	5.32	117.08	111.28
1	E	611	TRP	N-CA-C	-5.31	106.93	113.41
1	B	687	SER	N-CA-C	5.31	114.84	107.73
1	A	87	ILE	CB-CA-C	5.27	115.69	111.06
1	B	147	CYS	N-CA-C	5.25	116.12	107.20
1	E	483	GLY	N-CA-C	-5.24	98.12	113.30
1	C	482	TYR	CA-C-N	5.23	131.12	121.70
1	C	482	TYR	C-N-CA	5.23	131.12	121.70
1	F	17	VAL	N-CA-C	5.21	115.40	108.11
1	E	486	GLY	N-CA-C	-5.21	107.06	115.08
1	B	601	ILE	N-CA-C	5.21	114.19	108.05
1	A	686	ALA	N-CA-C	-5.20	99.72	110.80
1	D	51	ASP	CA-C-N	5.20	125.25	119.32
1	D	51	ASP	C-N-CA	5.20	125.25	119.32
1	A	535	THR	N-CA-C	-5.17	104.90	111.11
1	B	237	ASP	CA-C-N	-5.17	114.34	119.56
1	B	237	ASP	C-N-CA	-5.17	114.34	119.56
1	E	156	PRO	N-CA-C	5.16	117.00	110.70
1	E	440	GLU	N-CA-C	5.16	116.92	108.76
1	D	339	ILE	N-CA-C	5.11	115.13	107.51
1	E	525	VAL	N-CA-C	-5.10	107.86	112.96
1	F	544	GLU	N-CA-C	-5.09	105.73	111.28
1	E	261	GLU	N-CA-C	5.08	120.11	112.94
1	F	552	THR	N-CA-C	5.08	116.03	108.86
1	A	440	GLU	N-CA-C	5.07	117.60	108.48
1	B	12	ARG	CA-C-N	-5.07	114.40	120.13
1	B	12	ARG	C-N-CA	-5.07	114.40	120.13
1	C	111	LEU	N-CA-C	5.06	117.82	109.72
1	E	592	VAL	N-CA-C	5.06	115.29	110.53
1	A	418	TYR	N-CA-C	5.06	116.53	108.79
1	D	197	GLY	CA-C-N	-5.06	114.13	120.51
1	D	197	GLY	C-N-CA	-5.06	114.13	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	602	PRO	CA-C-N	-5.06	114.58	122.37
1	E	602	PRO	C-N-CA	-5.06	114.58	122.37
1	D	603	LEU	N-CA-C	5.04	119.51	113.17
1	D	162	VAL	N-CA-C	5.03	115.28	107.78
1	F	108	VAL	N-CA-C	5.03	115.36	108.12
1	A	526	GLY	N-CA-C	5.01	120.09	113.37
1	B	341	ASP	N-CA-C	5.00	115.90	108.60

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	4	OAR	CA
2	H	4	OAR	CA
2	I	4	OAR	CA
2	J	4	OAR	CA
2	K	4	OAR	CA
2	L	4	OAR	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	PRO	Peptide
1	A	685	SER	Peptide
1	B	156	PRO	Peptide
1	B	482	TYR	Peptide
1	B	685	SER	Peptide
1	B	688	ASP	Peptide
1	C	110	GLY	Peptide
1	C	156	PRO	Peptide
1	C	482	TYR	Peptide
1	C	685	SER	Peptide
1	D	156	PRO	Peptide
1	D	482	TYR	Peptide
1	D	684	PHE	Peptide
1	D	685	SER	Peptide
1	E	156	PRO	Peptide
1	E	685	SER	Peptide
1	F	156	PRO	Peptide
1	F	685	SER	Peptide
2	G	2	ARG	Peptide,Sidechain
2	G	3	VAL	Peptide
2	H	2	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	H	3	VAL	Peptide
2	I	2	ARG	Sidechain
2	J	2	ARG	Sidechain
2	K	2	ARG	Sidechain
2	K	3	VAL	Peptide
2	L	2	ARG	Peptide,Sidechain
2	L	3	VAL	Peptide

5.2 Too-close contacts [i](#)

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	5634	0	5522	160	0
1	B	5634	0	5522	144	0
1	C	5634	0	5522	162	0
1	D	5634	0	5522	140	0
1	E	5634	0	5522	161	0
1	F	5634	0	5522	178	0
2	G	43	0	40	1	0
2	H	43	0	39	1	0
2	I	43	0	40	1	0
2	J	43	0	41	4	0
2	K	43	0	40	2	0
2	L	43	0	39	0	0
3	A	109	0	0	12	0
3	B	75	0	0	15	0
3	C	36	0	0	7	0
3	D	39	0	0	8	0
3	E	37	0	0	5	0
3	F	48	0	0	3	0
All	All	34406	0	33371	949	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 14.

All (949) 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:61:GLU:HG2	1:C:675:LEU:HD23	1.13	1.12
1:A:496:ARG:HG2	1:A:496:ARG:HH11	1.19	1.05
1:E:61:GLU:HG2	1:E:675:LEU:HD23	1.34	1.05
1:D:681:SER:HB2	1:D:685:SER:CB	1.87	1.02
1:D:619:PHE:HB3	1:D:623:MET:HE2	1.37	1.01
1:F:87:ILE:HG13	1:F:88:GLU:H	1.24	1.01
1:A:681:SER:HB2	1:A:685:SER:HB2	1.44	0.98
1:D:681:SER:HB2	1:D:685:SER:HB2	1.43	0.97
1:F:494:ASN:HD21	1:F:496:ARG:HD3	1.29	0.97
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.29	0.96
1:E:315:VAL:HG12	1:E:331:ILE:HB	1.47	0.96
1:C:619:PHE:HB3	1:C:623:MET:HE2	1.46	0.96
1:A:418:TYR:HB2	1:A:428:LYS:O	1.66	0.95
1:E:619:PHE:HB3	1:E:623:MET:HE2	1.50	0.91
1:A:61:GLU:HG2	1:A:675:LEU:HD23	1.53	0.91
1:D:340:ASP:O	1:D:341:ASP:HB3	1.68	0.91
1:C:494:ASN:ND2	1:C:496:ARG:HB2	1.86	0.91
1:F:612:GLY:C	1:F:623:MET:HE1	1.97	0.90
1:D:619:PHE:HB3	1:D:623:MET:CE	2.02	0.89
1:B:61:GLU:HG2	1:B:675:LEU:HD23	1.53	0.89
1:F:87:ILE:HG13	1:F:88:GLU:N	1.88	0.89
1:A:688:ASP:OD1	1:A:688:ASP:N	2.06	0.89
1:B:552:THR:HG22	1:B:553:THR:N	1.84	0.89
1:E:366:LEU:H	1:E:366:LEU:HD12	1.39	0.87
1:B:93:SER:O	1:B:95:PRO:HD3	1.74	0.87
1:E:632:VAL:HG12	1:E:666:LEU:HD12	1.55	0.85
1:F:418:TYR:HB2	1:F:428:LYS:O	1.76	0.85
1:F:482:TYR:HB3	1:F:483:GLY:HA2	1.59	0.85
1:C:340:ASP:O	1:C:341:ASP:HB3	1.75	0.85
1:B:93:SER:HB3	1:B:105:THR:HG22	1.58	0.84
1:E:5:ARG:HG2	1:E:6:GLY:H	1.44	0.83
1:D:154:PRO:O	1:D:156:PRO:HD3	1.78	0.83
1:E:619:PHE:HB3	1:E:623:MET:CE	2.10	0.82
1:A:496:ARG:HG2	1:A:496:ARG:NH1	1.93	0.82
1:D:488:CYS:HB3	1:D:517:GLU:HG3	1.62	0.82
1:A:619:PHE:HB3	1:A:623:MET:CE	2.11	0.81
1:A:496:ARG:HH11	1:A:496:ARG:CG	1.92	0.81
1:A:315:VAL:HG12	1:A:331:ILE:HB	1.62	0.81
1:D:496:ARG:HG2	1:D:496:ARG:HH11	1.44	0.81
1:A:641:MET:HE2	1:A:699:GLN:HE21	1.47	0.80
1:B:552:THR:CG2	1:B:553:THR:N	2.44	0.80
1:C:367:GLY:O	1:C:369:ASP:N	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:HIS:O	1:B:427:ARG:NH2	2.15	0.79
1:B:688:ASP:N	1:B:688:ASP:OD1	2.15	0.79
1:F:104:TYR:OH	1:F:131:GLU:HG3	1.82	0.79
1:B:246:ARG:HD2	3:B:2027:HOH:O	1.81	0.79
1:E:681:SER:HB2	1:E:685:SER:CB	2.10	0.79
1:A:418:TYR:HB3	1:A:429:VAL:HA	1.64	0.79
1:E:482:TYR:HB3	1:E:483:GLY:HA2	1.64	0.79
1:E:537:MET:HE2	3:E:2028:HOH:O	1.81	0.79
1:F:688:ASP:OD1	1:F:688:ASP:N	2.14	0.78
1:C:315:VAL:HG13	1:C:331:ILE:HB	1.64	0.78
1:D:363:THR:HG22	1:D:378:LYS:HB3	1.64	0.78
1:D:618:LYS:HE2	3:D:2038:HOH:O	1.82	0.78
1:C:312:ASN:ND2	1:C:338:THR:OG1	2.15	0.77
1:E:357:GLY:HA2	1:E:517:GLU:O	1.85	0.77
1:E:490:GLU:OE1	1:E:490:GLU:HA	1.83	0.77
1:A:112:SER:HB3	1:A:689:ARG:HG2	1.66	0.77
1:C:175:SER:HB3	1:C:188:GLU:OE1	1.84	0.77
1:B:619:PHE:HB3	1:B:623:MET:HE2	1.66	0.77
1:A:689:ARG:HB3	1:A:691:LYS:H	1.47	0.76
1:E:400:ASP:HB2	3:E:2023:HOH:O	1.84	0.76
1:C:681:SER:HB2	1:C:685:SER:CB	2.16	0.76
1:B:209:ASP:OD1	1:B:210:ALA:N	2.15	0.76
1:A:681:SER:HB2	1:A:685:SER:CB	2.15	0.75
1:F:83:HIS:CE1	1:F:499:PRO:HG2	2.21	0.75
1:A:439:PHE:HA	3:A:2065:HOH:O	1.84	0.75
1:B:293:VAL:HG22	1:B:303:VAL:HG22	1.67	0.75
1:C:210:ALA:HA	3:C:2012:HOH:O	1.85	0.75
1:F:279:LEU:HD22	1:F:279:LEU:H	1.52	0.75
1:F:711:GLN:HE21	1:F:711:GLN:HA	1.49	0.75
1:F:677:MET:O	1:F:677:MET:HG3	1.86	0.75
1:F:664:ARG:NH2	1:F:673:VAL:O	2.14	0.74
1:D:5:ARG:HG3	1:D:6:GLY:H	1.52	0.74
1:D:648:ASP:OD1	1:D:683:HIS:HB2	1.87	0.74
1:F:213:ARG:NH2	1:F:235:ASP:O	2.20	0.74
1:C:598:ASP:HB3	1:C:601:ILE:HD12	1.69	0.74
1:D:641:MET:HE2	1:D:699:GLN:HG2	1.69	0.73
1:F:168:TYR:HE2	1:F:177:ARG:NH2	1.84	0.73
1:C:648:ASP:OD1	1:C:683:HIS:HB2	1.89	0.73
1:E:681:SER:HB2	1:E:685:SER:HB2	1.70	0.73
1:F:494:ASN:ND2	1:F:496:ARG:H	1.85	0.73
1:F:582:VAL:HG23	1:F:639:HIS:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:ASP:HB3	1:F:337:VAL:HB	1.70	0.73
2:J:1:FC0:HE2	2:J:2:ARG:NH2	2.03	0.73
1:A:310:CYS:SG	1:A:314:LYS:HD3	2.29	0.73
1:C:411:MET:HE2	1:C:491:PRO:HB3	1.70	0.73
1:C:93:SER:HB3	1:C:105:THR:HG22	1.69	0.73
1:E:444:TYR:OH	1:E:502:ASP:OD1	2.06	0.72
1:C:482:TYR:HB3	1:C:483:GLY:HA2	1.69	0.72
1:C:621:ASP:OD2	1:D:575:MET:HG2	1.90	0.72
1:A:45:ARG:HD2	1:A:654:TRP:CZ2	2.24	0.71
1:B:209:ASP:CG	1:B:210:ALA:H	1.97	0.71
1:D:689:ARG:NH1	1:D:691:LYS:HG2	2.06	0.71
1:F:279:LEU:HD22	1:F:279:LEU:N	2.06	0.71
1:E:588:PRO:HD2	1:E:656:PRO:HG3	1.73	0.71
1:C:106:ARG:HH11	1:C:106:ARG:HB3	1.56	0.71
1:B:413:THR:HG22	1:B:414:PRO:O	1.91	0.70
1:C:681:SER:HB2	1:C:685:SER:HB2	1.71	0.70
1:B:22:GLU:HG3	3:B:2002:HOH:O	1.90	0.70
1:B:426:GLU:HA	3:B:2043:HOH:O	1.91	0.70
1:B:552:THR:CG2	1:B:553:THR:H	2.04	0.70
1:D:681:SER:CB	1:D:685:SER:HB2	2.19	0.70
1:C:209:ASP:OD1	1:C:210:ALA:N	2.23	0.70
1:B:315:VAL:CG1	1:B:331:ILE:HB	2.22	0.70
1:C:588:PRO:O	1:C:590:VAL:HG22	1.92	0.70
1:F:655:GLU:HB2	1:F:656:PRO:HD3	1.72	0.69
1:A:113:TYR:HB3	1:A:137:GLU:HB2	1.75	0.69
1:F:619:PHE:HB3	1:F:623:MET:HE3	1.75	0.68
1:E:381:HIS:O	1:E:427:ARG:NH2	2.26	0.68
1:B:418:TYR:HB3	1:B:428:LYS:O	1.94	0.68
1:A:632:VAL:HG12	1:A:666:LEU:HD12	1.75	0.68
1:F:494:ASN:HD22	1:F:496:ARG:H	1.38	0.68
1:B:358:LEU:HB2	1:B:360:ARG:NH1	2.08	0.68
1:A:93:SER:HB3	1:A:105:THR:HG22	1.75	0.68
1:D:482:TYR:HB3	1:D:483:GLY:HA2	1.75	0.68
1:A:221:ILE:HB	1:A:224:GLN:HE21	1.58	0.68
1:A:447:ARG:NH1	1:A:449:GLU:OE2	2.27	0.68
1:B:112:SER:HB3	1:B:689:ARG:HE	1.58	0.67
1:C:346:ALA:HB2	1:C:399:TYR:CE2	2.29	0.67
1:B:474:PRO:HB2	1:B:556:GLN:HE22	1.59	0.67
1:B:331:ILE:HD13	1:B:351:LEU:HD21	1.75	0.67
2:G:1:FC0:HA	2:G:2:ARG:HB2	1.76	0.67
1:A:619:PHE:HB3	1:A:623:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:THR:OG1	1:D:556:GLN:HG3	1.95	0.67
1:F:209:ASP:HB2	1:F:215:ASN:CG	2.20	0.67
1:E:12:ARG:NH2	1:E:53:GLU:OE1	2.27	0.67
1:F:15:GLU:O	1:F:15:GLU:HG3	1.94	0.67
1:A:664:ARG:NH2	1:A:673:VAL:O	2.28	0.67
1:A:483:GLY:HA2	3:A:2074:HOH:O	1.94	0.66
1:C:113:TYR:HB3	1:C:137:GLU:HB2	1.77	0.66
1:D:650:ARG:NH2	1:D:684:PHE:HE2	1.93	0.66
1:B:400:ASP:O	1:B:401:ALA:O	2.13	0.66
1:C:319:LYS:HB3	3:C:2016:HOH:O	1.96	0.66
1:C:221:ILE:HB	1:C:224:GLN:NE2	2.09	0.66
1:F:269:ASP:OD2	1:F:272:LYS:HE2	1.96	0.66
1:F:420:GLU:OE1	1:F:427:ARG:NE	2.28	0.66
1:A:304:LEU:CD2	1:A:341:ASP:HA	2.25	0.66
1:D:455:ASP:OD1	1:D:457:THR:OG1	2.11	0.66
1:A:546:LEU:CD2	1:A:551:LEU:HD12	2.25	0.65
1:E:607:GLU:HG2	1:E:611:TRP:NE1	2.10	0.65
1:D:496:ARG:HG2	1:D:496:ARG:NH1	2.10	0.65
1:A:53:GLU:HG3	3:A:2016:HOH:O	1.95	0.65
1:E:476:PRO:HB2	1:E:505:MET:HG2	1.78	0.65
1:F:477:THR:HB	1:F:557:LEU:HD12	1.78	0.65
1:F:70:VAL:O	1:F:73:LYS:HG2	1.97	0.65
1:F:474:PRO:HB2	1:F:556:GLN:HE22	1.62	0.65
1:F:696:ASN:HA	1:F:699:GLN:HB2	1.78	0.65
1:C:650:ARG:NH2	1:C:684:PHE:HE2	1.93	0.65
1:E:315:VAL:CG1	1:E:331:ILE:HB	2.23	0.65
1:C:688:ASP:OD1	1:C:688:ASP:N	2.30	0.65
1:D:568:LEU:C	1:D:568:LEU:HD23	2.22	0.65
1:B:112:SER:OG	1:B:689:ARG:NH2	2.30	0.64
1:A:564:ALA:O	1:A:567:LEU:HB3	1.96	0.64
2:J:1:FC0:CE2	2:J:2:ARG:HH21	2.10	0.64
1:D:93:SER:HB3	1:D:105:THR:HG22	1.79	0.64
1:C:470:ASP:C	1:C:472:LYS:H	2.06	0.64
1:C:213:ARG:HH22	1:C:236:ASP:HA	1.62	0.64
1:C:294:GLU:HG3	1:C:342:VAL:HG23	1.80	0.64
1:A:315:VAL:CG1	1:A:331:ILE:HB	2.27	0.63
1:F:478:MET:SD	1:F:560:GLU:HB2	2.38	0.63
1:E:307:LYS:HE2	1:E:308:ASP:OD1	1.99	0.63
1:C:61:GLU:HG2	1:C:675:LEU:CD2	2.08	0.63
1:F:209:ASP:OD2	1:F:215:ASN:ND2	2.31	0.63
1:A:100:ARG:HG2	1:A:100:ARG:NH1	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:712:LEU:HD12	1:F:712:LEU:H	1.63	0.63
2:J:1:FC0:HE2	2:J:2:ARG:HH21	1.62	0.63
1:A:61:GLU:CG	1:A:675:LEU:HD23	2.27	0.62
1:D:78:THR:O	1:D:82:GLU:HG3	2.00	0.62
1:A:262:THR:HA	1:A:289:VAL:O	1.98	0.62
1:D:104:TYR:CE1	1:D:117:CYS:HB2	2.34	0.62
1:F:279:LEU:H	1:F:279:LEU:CD2	2.11	0.62
1:F:330:LEU:HG	1:F:331:ILE:HG13	1.81	0.62
1:D:627:SER:HB3	1:D:630:ASP:HB2	1.81	0.62
1:A:5:ARG:HG2	1:A:6:GLY:H	1.64	0.61
1:B:209:ASP:HB2	1:B:215:ASN:CG	2.25	0.61
1:C:180:ARG:HB2	1:C:180:ARG:NH1	2.13	0.61
1:B:494:ASN:HD22	1:B:496:ARG:H	1.48	0.61
1:D:61:GLU:HG2	1:D:675:LEU:HD23	1.81	0.61
1:F:640:LEU:HD23	1:F:673:VAL:HG13	1.83	0.61
1:B:315:VAL:HG13	1:B:331:ILE:HB	1.81	0.61
1:B:614:PRO:HD3	1:B:623:MET:HE1	1.82	0.61
1:F:168:TYR:HE2	1:F:177:ARG:HH21	1.48	0.61
1:B:577:PRO:HG3	1:B:635:GLN:NE2	2.16	0.61
1:E:210:ALA:O	1:E:211:SER:HB2	2.00	0.61
1:C:488:CYS:HB3	1:C:517:GLU:HG3	1.83	0.61
1:E:639:HIS:CE1	1:E:671:ASN:HB3	2.36	0.61
1:F:168:TYR:CE2	1:F:177:ARG:NH2	2.67	0.60
1:B:543:ALA:O	1:B:547:ILE:HD12	2.00	0.60
1:C:536:PHE:CE1	1:C:568:LEU:HA	2.37	0.60
1:D:421:ASP:HB3	1:D:424:SER:OG	2.01	0.60
1:E:5:ARG:CG	1:E:6:GLY:H	2.15	0.60
1:A:219:ARG:NH2	1:A:276:HIS:O	2.35	0.60
1:C:712:LEU:HD12	1:C:712:LEU:H	1.67	0.60
1:F:395:GLN:OE1	1:F:405:ARG:HG2	2.01	0.60
1:B:681:SER:HB2	1:B:685:SER:HB2	1.83	0.60
1:E:79:ILE:HD11	1:E:499:PRO:HB3	1.84	0.60
1:A:216:LYS:HG3	1:A:234:THR:HG23	1.83	0.59
1:E:61:GLU:OE2	1:E:664:ARG:NH2	2.35	0.59
1:E:689:ARG:HH11	1:E:691:LYS:HG2	1.67	0.59
1:F:61:GLU:HG2	1:F:675:LEU:HD23	1.83	0.59
1:C:713:LEU:O	1:C:714:ARG:HD2	2.02	0.59
1:D:681:SER:HB2	1:D:685:SER:HB3	1.83	0.59
1:E:355:ARG:HG2	1:E:355:ARG:HH11	1.66	0.59
1:A:619:PHE:HB3	1:A:623:MET:HE2	1.85	0.59
1:E:547:ILE:CD1	1:E:554:PRO:HD3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:ILE:CG1	1:F:88:GLU:H	2.07	0.59
1:C:685:SER:C	1:C:687:SER:N	2.60	0.59
1:F:612:GLY:O	1:F:623:MET:HE1	2.01	0.59
1:A:623:MET:HA	1:A:626:TYR:CE2	2.37	0.59
1:F:261:GLU:HG2	1:F:609:GLU:OE1	2.02	0.59
1:F:644:ALA:HB3	1:F:677:MET:HE2	1.83	0.59
1:F:494:ASN:ND2	1:F:496:ARG:HD3	2.10	0.59
1:A:712:LEU:HD12	3:A:2109:HOH:O	2.02	0.59
1:E:325:ASP:O	1:E:326:TRP:HD1	1.86	0.59
1:F:476:PRO:HB2	1:F:505:MET:HG2	1.85	0.58
1:B:685:SER:HB3	1:B:687:SER:HA	1.85	0.58
1:A:110:GLY:C	1:A:111:LEU:HD23	2.29	0.58
1:A:404:LEU:HD21	1:A:406:LEU:HD21	1.85	0.58
1:B:478:MET:SD	1:B:560:GLU:HB2	2.43	0.58
1:C:552:THR:HG21	1:C:557:LEU:HB2	1.86	0.58
1:F:584:LEU:HD13	1:F:699:GLN:HG2	1.85	0.58
1:F:499:PRO:HB2	1:F:700:GLN:HE22	1.69	0.58
1:B:357:GLY:HA2	1:B:517:GLU:O	2.04	0.58
1:D:108:VAL:HB	1:D:111:LEU:HD12	1.86	0.58
1:E:689:ARG:HD3	1:E:691:LYS:H	1.69	0.58
1:D:650:ARG:NH2	1:D:684:PHE:CE2	2.71	0.58
1:E:685:SER:C	1:E:687:SER:N	2.62	0.58
1:F:5:ARG:HG2	1:F:6:GLY:H	1.69	0.58
1:F:641:MET:HE1	1:F:699:GLN:HA	1.86	0.58
1:A:691:LYS:HE2	1:A:694:ARG:HD3	1.86	0.58
1:F:687:SER:HB2	1:F:689:ARG:HG3	1.84	0.58
1:C:71:ASP:OD1	1:C:71:ASP:N	2.34	0.58
1:C:466:ASP:OD1	1:C:468:SER:OG	2.20	0.58
1:F:417:TRP:CE3	1:F:431:LYS:HD3	2.39	0.58
1:F:365:ARG:HH21	1:F:378:LYS:HB2	1.69	0.57
1:D:611:TRP:HB2	3:D:2037:HOH:O	2.02	0.57
1:B:96:TYR:CD2	1:B:395:GLN:HG2	2.39	0.57
1:B:115:LEU:HD23	1:B:133:ILE:HG21	1.87	0.57
1:B:639:HIS:ND1	1:B:671:ASN:HB3	2.19	0.57
1:B:691:LYS:HG3	3:B:2074:HOH:O	2.04	0.57
1:C:411:MET:HE1	1:C:462:SER:HB3	1.86	0.57
1:F:655:GLU:HB2	1:F:656:PRO:CD	2.34	0.57
1:A:163:ALA:HB2	1:A:178:PHE:CE2	2.40	0.57
1:A:357:GLY:HA2	1:A:517:GLU:O	2.04	0.57
1:C:552:THR:HG22	1:C:553:THR:O	2.04	0.57
1:E:113:TYR:HB3	1:E:137:GLU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASP:HB2	3:D:2022:HOH:O	2.04	0.57
1:B:15:GLU:O	1:B:15:GLU:HG3	2.02	0.57
1:E:582:VAL:HG22	1:E:583:ALA:N	2.19	0.57
1:F:696:ASN:O	1:F:700:GLN:HG3	2.05	0.57
1:A:418:TYR:CB	1:A:428:LYS:O	2.46	0.57
1:B:553:THR:OG1	1:B:556:GLN:NE2	2.26	0.57
1:D:304:LEU:CD2	1:D:341:ASP:HA	2.35	0.57
1:F:131:GLU:HG2	1:F:132:GLU:H	1.70	0.57
1:D:280:GLU:HB3	3:D:2018:HOH:O	2.03	0.57
1:E:653:TYR:O	1:E:656:PRO:HD2	2.05	0.57
1:F:552:THR:HG22	1:F:553:THR:H	1.68	0.57
1:A:213:ARG:HD3	3:A:2040:HOH:O	2.04	0.56
1:E:294:GLU:HG3	1:E:342:VAL:HG23	1.87	0.56
1:E:564:ALA:O	1:E:567:LEU:HB3	2.05	0.56
1:E:639:HIS:ND1	1:E:671:ASN:HB3	2.20	0.56
1:A:114:LYS:HG2	3:A:2023:HOH:O	2.04	0.56
1:C:180:ARG:HB2	1:C:180:ARG:HH11	1.70	0.56
1:C:614:PRO:N	1:C:623:MET:HE1	2.21	0.56
1:D:447:ARG:NH1	1:D:449:GLU:OE2	2.38	0.56
1:E:89:GLU:HB3	1:E:109:LYS:HA	1.86	0.56
1:F:162:VAL:O	1:F:179:VAL:HG23	2.06	0.56
1:F:685:SER:HB3	1:F:687:SER:HA	1.86	0.56
1:B:685:SER:C	1:B:687:SER:N	2.63	0.56
1:C:312:ASN:HD22	1:C:338:THR:HG1	1.49	0.56
1:E:235:ASP:OD2	1:E:285:ARG:NH2	2.39	0.56
1:A:173:VAL:CG1	1:A:189:GLY:HA2	2.35	0.56
1:B:358:LEU:HB2	1:B:360:ARG:HH11	1.70	0.56
1:B:477:THR:HB	1:B:557:LEU:CD1	2.35	0.56
1:D:87:ILE:O	1:D:88:GLU:HG2	2.05	0.56
1:D:639:HIS:ND1	1:D:671:ASN:HB3	2.20	0.56
1:F:221:ILE:O	1:F:224:GLN:HG3	2.04	0.56
1:F:626:TYR:O	1:F:627:SER:C	2.49	0.56
1:A:316:VAL:HG22	1:A:328:THR:O	2.06	0.56
1:B:292:THR:HG22	3:B:2032:HOH:O	2.05	0.56
1:C:204:PHE:CE1	1:C:219:ARG:HG3	2.40	0.56
1:D:688:ASP:C	1:D:689:ARG:HG3	2.29	0.56
1:F:79:ILE:HD11	1:F:499:PRO:HB3	1.88	0.56
1:F:539:PHE:CG	1:F:568:LEU:HD21	2.40	0.56
1:E:560:GLU:HG3	1:E:584:LEU:HB2	1.87	0.56
1:F:711:GLN:HA	1:F:711:GLN:NE2	2.20	0.56
1:D:611:TRP:CD1	3:D:2037:HOH:O	2.58	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:SER:CB	1:A:689:ARG:HG2	2.35	0.55
1:B:629:ILE:O	1:B:632:VAL:HG23	2.05	0.55
1:C:601:ILE:O	1:C:603:LEU:N	2.39	0.55
1:D:340:ASP:O	1:D:341:ASP:CB	2.47	0.55
1:E:461:ILE:HD11	1:E:542:CYS:HB3	1.88	0.55
1:B:482:TYR:HB3	1:B:483:GLY:HA2	1.89	0.55
1:D:88:GLU:HG3	1:D:91:ASP:HB2	1.88	0.55
1:D:667:LYS:HZ3	1:D:669:ASP:CG	2.15	0.55
1:F:25:ASP:O	1:F:599:PRO:HG3	2.05	0.55
1:B:332:PRO:HD2	3:B:2036:HOH:O	2.07	0.55
1:C:87:ILE:O	1:C:88:GLU:HG2	2.06	0.55
1:E:688:ASP:OD1	1:E:688:ASP:N	2.40	0.55
1:A:496:ARG:NH1	1:A:496:ARG:CG	2.61	0.55
1:C:81:GLN:OE1	1:C:81:GLN:HA	2.06	0.55
1:A:461:ILE:HG22	1:A:463:LEU:HD23	1.89	0.55
1:B:681:SER:HB2	1:B:685:SER:CB	2.37	0.55
1:C:61:GLU:CG	1:C:675:LEU:HD23	2.09	0.55
2:K:1:FC0:HA	2:K:2:ARG:HB2	1.88	0.55
1:E:586:GLY:O	1:E:587:VAL:C	2.49	0.54
1:E:646:LEU:HD22	1:E:679:LEU:HB3	1.87	0.54
1:D:247:SER:HB2	1:D:295:MET:HB2	1.89	0.54
1:E:367:GLY:C	1:E:369:ASP:H	2.14	0.54
1:F:85:SER:O	1:F:437:GLY:N	2.39	0.54
1:F:366:LEU:HD13	1:F:370:ASN:HA	1.89	0.54
1:A:304:LEU:HD22	1:A:341:ASP:HA	1.89	0.54
1:C:371:LEU:HD23	3:C:2017:HOH:O	2.06	0.54
1:F:79:ILE:CG1	1:F:499:PRO:HB3	2.38	0.54
1:A:221:ILE:HB	1:A:224:GLN:NE2	2.22	0.54
1:B:77:GLU:OE1	1:B:694:ARG:NH2	2.41	0.54
1:B:664:ARG:NH2	1:B:673:VAL:O	2.36	0.54
1:F:230:VAL:HG23	3:F:2020:HOH:O	2.07	0.54
1:E:523:TYR:OH	1:E:528:LYS:NZ	2.41	0.54
1:E:256:CYS:SG	1:E:258:MET:SD	2.99	0.54
1:D:482:TYR:O	1:D:565:GLY:HA2	2.08	0.54
1:A:641:MET:HE1	1:A:698:ILE:HG22	1.90	0.54
1:C:144:LYS:HE2	3:C:2007:HOH:O	2.08	0.54
1:C:650:ARG:CZ	1:C:684:PHE:HE2	2.20	0.54
1:F:82:GLU:O	1:F:86:HIS:ND1	2.41	0.54
1:E:568:LEU:O	1:E:572:VAL:HG23	2.08	0.53
1:A:455:ASP:OD1	1:A:457:THR:OG1	2.21	0.53
1:C:310:CYS:SG	1:C:314:LYS:HD3	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:HIS:O	1:F:60:LEU:HB2	2.08	0.53
1:A:474:PRO:HB2	1:A:556:GLN:HE22	1.73	0.53
1:C:482:TYR:O	1:C:565:GLY:HA2	2.08	0.53
1:A:568:LEU:C	1:A:568:LEU:HD23	2.33	0.53
1:C:563:SER:HA	1:C:587:VAL:O	2.09	0.53
1:E:482:TYR:HB3	1:E:483:GLY:CA	2.36	0.53
1:A:418:TYR:CZ	1:A:427:ARG:HD3	2.44	0.53
1:F:365:ARG:NH2	1:F:378:LYS:HB2	2.23	0.53
1:A:482:TYR:HB3	1:A:483:GLY:HA2	1.91	0.53
1:E:647:HIS:O	1:E:649:PRO:HD3	2.09	0.53
1:C:82:GLU:O	1:C:86:HIS:ND1	2.42	0.53
1:F:494:ASN:HD22	1:F:494:ASN:C	2.17	0.53
1:A:362:TRP:CD1	1:A:379:GLU:HA	2.45	0.52
1:B:568:LEU:C	1:B:568:LEU:HD23	2.34	0.52
1:C:711:GLN:HG3	1:C:712:LEU:O	2.09	0.52
1:D:113:TYR:HB3	1:D:137:GLU:HB2	1.92	0.52
1:A:633:ARG:NH2	1:B:621:ASP:OD2	2.41	0.52
1:D:354:ARG:NH2	1:D:490:GLU:OE2	2.42	0.52
1:D:396:MET:HE3	3:D:2025:HOH:O	2.10	0.52
1:A:340:ASP:O	1:A:341:ASP:HB3	2.09	0.52
1:A:393:CYS:HA	1:A:396:MET:HG3	1.92	0.52
1:A:577:PRO:HG2	3:A:2103:HOH:O	2.08	0.52
1:A:681:SER:CB	1:A:685:SER:HB2	2.28	0.52
1:D:466:ASP:O	1:D:469:ILE:HG12	2.09	0.52
1:E:482:TYR:CB	1:E:483:GLY:HA2	2.38	0.52
1:E:582:VAL:CG2	1:E:583:ALA:N	2.72	0.52
1:A:209:ASP:OD1	1:A:210:ALA:N	2.41	0.52
1:A:383:ASP:HA	3:A:2060:HOH:O	2.10	0.52
1:A:209:ASP:HB2	1:A:215:ASN:OD1	2.10	0.52
1:B:383:ASP:OD1	1:B:383:ASP:N	2.33	0.52
1:C:67:LYS:O	1:C:70:VAL:HG23	2.10	0.52
1:E:296:HIS:O	1:E:300:THR:HG23	2.09	0.52
1:E:521:THR:C	1:E:523:TYR:N	2.68	0.52
1:F:113:TYR:HB3	1:F:137:GLU:CB	2.40	0.52
1:A:355:ARG:O	1:A:360:ARG:NH1	2.43	0.52
1:B:112:SER:HB2	1:B:113:TYR:CD1	2.45	0.52
1:E:547:ILE:HD13	1:E:554:PRO:HD3	1.91	0.52
1:F:113:TYR:HB3	1:F:137:GLU:HB3	1.92	0.52
1:C:619:PHE:HB3	1:C:623:MET:CE	2.31	0.52
1:B:209:ASP:CG	1:B:210:ALA:N	2.65	0.52
1:A:57:HIS:HA	1:A:60:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HG2	1:A:674:LEU:HD21	1.91	0.52
1:A:209:ASP:OD2	1:A:215:ASN:ND2	2.43	0.52
1:C:32:ASP:HA	1:C:33:PRO:C	2.34	0.52
1:D:562:ARG:O	1:D:565:GLY:N	2.43	0.52
1:F:296:HIS:CD2	1:F:372:PHE:HE1	2.28	0.52
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.14	0.51
1:B:558:SER:HA	1:B:582:VAL:O	2.09	0.51
1:C:470:ASP:C	1:C:472:LYS:N	2.66	0.51
1:C:650:ARG:NH2	1:C:684:PHE:CE2	2.75	0.51
1:D:381:HIS:O	1:D:427:ARG:NH2	2.41	0.51
1:D:554:PRO:C	1:D:556:GLN:H	2.18	0.51
1:E:613:ASN:HB3	1:E:616:GLU:HG3	1.92	0.51
1:A:362:TRP:NE1	1:A:379:GLU:HG3	2.25	0.51
1:C:367:GLY:C	1:C:369:ASP:H	2.11	0.51
1:A:347:LYS:O	1:A:348:PHE:HB3	2.11	0.51
1:C:304:LEU:CD2	1:C:341:ASP:HA	2.40	0.51
1:E:306:ASN:HA	1:E:310:CYS:O	2.10	0.51
1:A:552:THR:HG21	1:A:557:LEU:HB2	1.93	0.51
1:E:499:PRO:O	1:E:503:ARG:HD2	2.10	0.51
1:E:558:SER:CB	1:E:582:VAL:HG13	2.40	0.51
1:F:131:GLU:HG2	1:F:132:GLU:N	2.25	0.51
1:A:312:ASN:HB3	1:A:338:THR:HA	1.93	0.51
1:D:489:ILE:HG22	1:D:509:ILE:HD13	1.92	0.51
1:E:113:TYR:HB3	1:E:137:GLU:CB	2.40	0.51
1:E:681:SER:CB	1:E:685:SER:HB2	2.39	0.51
1:A:483:GLY:CA	3:A:2074:HOH:O	2.56	0.51
1:F:134:VAL:O	1:F:179:VAL:HG11	2.11	0.51
1:B:686:ALA:HB1	1:B:695:GLU:HG3	1.93	0.51
1:C:114:LYS:C	1:C:115:LEU:HD12	2.36	0.51
1:C:213:ARG:NH2	1:C:236:ASP:HA	2.24	0.51
1:B:342:VAL:HG23	3:B:2032:HOH:O	2.10	0.50
1:F:644:ALA:HB3	1:F:677:MET:CE	2.41	0.50
1:A:331:ILE:HD13	1:A:351:LEU:HD21	1.93	0.50
1:C:291:TYR:HA	1:C:304:LEU:O	2.11	0.50
1:D:393:CYS:C	1:D:395:GLN:H	2.19	0.50
1:E:92:MET:O	1:E:431:LYS:NZ	2.45	0.50
1:F:482:TYR:HB3	1:F:483:GLY:CA	2.36	0.50
1:A:443:ASN:CG	1:A:714:ARG:HH12	2.20	0.50
1:D:80:TYR:O	1:D:84:ILE:HG12	2.10	0.50
1:D:455:ASP:CG	1:D:457:THR:HG1	2.16	0.50
1:E:640:LEU:HB3	1:E:673:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:GLU:OE1	1:F:442:LYS:HE2	2.12	0.50
1:A:424:SER:HB2	1:D:308:ASP:HB3	1.92	0.50
1:A:685:SER:C	1:A:687:SER:N	2.69	0.50
1:B:587:VAL:N	1:B:588:PRO:HD3	2.27	0.50
1:C:704:LEU:HD22	1:C:709:VAL:HG23	1.93	0.50
1:F:338:THR:HB	1:F:354:ARG:HB2	1.93	0.50
1:E:558:SER:HB3	1:E:582:VAL:HG13	1.94	0.50
1:F:460:PRO:HG3	1:F:518:MET:SD	2.52	0.50
1:F:499:PRO:HB2	1:F:700:GLN:NE2	2.26	0.50
1:C:489:ILE:HG22	1:C:509:ILE:HD13	1.93	0.50
1:E:337:VAL:HG22	1:E:355:ARG:HB2	1.93	0.50
1:B:411:MET:HE3	1:B:446:CYS:HB2	1.93	0.50
1:B:485:TYR:OH	2:H:4:OAR:HG2	2.12	0.50
1:C:318:THR:HB	1:C:325:ASP:O	2.11	0.50
1:E:325:ASP:C	1:E:326:TRP:HD1	2.18	0.50
1:E:497:PHE:CD1	1:E:497:PHE:C	2.90	0.50
1:F:349:ALA:HB3	1:F:364:VAL:HG12	1.92	0.50
1:F:496:ARG:HH11	1:F:496:ARG:HB2	1.77	0.49
1:A:79:ILE:HG22	1:A:697:ALA:HB1	1.94	0.49
1:C:173:VAL:HG13	1:C:189:GLY:HA2	1.94	0.49
1:D:552:THR:HG21	1:D:557:LEU:HB2	1.93	0.49
1:A:92:MET:HE1	1:A:126:GLY:HA2	1.92	0.49
1:B:418:TYR:CB	1:B:428:LYS:O	2.59	0.49
1:C:536:PHE:HE1	1:C:568:LEU:HA	1.75	0.49
1:C:539:PHE:CD2	1:C:572:VAL:HG21	2.48	0.49
1:D:213:ARG:HH22	1:D:236:ASP:HA	1.77	0.49
1:F:312:ASN:HB3	1:F:338:THR:HA	1.93	0.49
1:A:76:ALA:HB1	1:A:698:ILE:HD12	1.93	0.49
1:B:614:PRO:CD	1:B:623:MET:HE1	2.41	0.49
1:E:272:LYS:HB2	1:E:276:HIS:CD2	2.48	0.49
1:A:476:PRO:HA	1:A:556:GLN:HB3	1.94	0.49
1:B:338:THR:HG21	3:B:2037:HOH:O	2.13	0.49
1:C:398:THR:O	1:C:401:ALA:HB2	2.12	0.49
1:C:648:ASP:CG	1:C:683:HIS:HB2	2.37	0.49
1:D:439:PHE:HA	3:D:2027:HOH:O	2.12	0.49
1:D:445:VAL:HG12	3:D:2028:HOH:O	2.12	0.49
2:K:2:ARG:HG3	2:K:2:ARG:O	2.12	0.49
1:C:446:CYS:HA	1:C:463:LEU:O	2.12	0.49
1:D:567:LEU:HB2	1:D:589:PHE:O	2.12	0.49
1:E:83:HIS:HE1	1:E:499:PRO:HG2	1.76	0.49
1:F:501:VAL:C	1:F:503:ARG:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HG3	1:B:324:THR:HG22	1.95	0.49
1:E:366:LEU:HD12	1:E:366:LEU:N	2.19	0.49
1:E:695:GLU:O	1:E:698:ILE:HG22	2.13	0.49
1:F:220:HIS:ND1	1:F:229:ASP:OD1	2.39	0.49
1:B:225:PRO:O	1:B:228:GLU:HB2	2.12	0.49
1:D:404:LEU:HD22	1:D:422:VAL:HG22	1.93	0.49
1:E:264:GLU:HB2	1:E:285:ARG:HB3	1.95	0.49
1:F:357:GLY:HA2	1:F:517:GLU:O	2.13	0.49
1:F:521:THR:C	1:F:523:TYR:N	2.70	0.49
1:B:708:ASN:ND2	1:B:710:ARG:HH12	2.10	0.49
1:C:348:PHE:CD1	1:C:348:PHE:C	2.90	0.49
1:C:689:ARG:NH2	1:C:691:LYS:HG2	2.27	0.49
1:A:685:SER:O	1:A:686:ALA:HB3	2.13	0.49
1:D:354:ARG:NH2	1:D:490:GLU:CD	2.70	0.49
1:A:249:ASP:O	1:A:251:LYS:HD3	2.12	0.48
1:A:303:VAL:HB	1:A:316:VAL:HG12	1.95	0.48
1:B:68:ARG:HD2	3:B:2007:HOH:O	2.13	0.48
1:B:113:TYR:HB3	1:B:137:GLU:CB	2.43	0.48
1:C:485:TYR:CE2	2:I:3:VAL:HB	2.48	0.48
1:C:494:ASN:HD21	1:C:496:ARG:HB2	1.72	0.48
1:E:641:MET:HE1	1:E:698:ILE:HG23	1.95	0.48
1:F:418:TYR:CB	1:F:429:VAL:HA	2.42	0.48
1:C:500:TYR:CZ	1:C:700:GLN:HG2	2.48	0.48
1:C:635:GLN:HG2	1:C:637:TYR:CE1	2.48	0.48
1:D:411:MET:HE1	1:D:462:SER:HB3	1.95	0.48
1:E:211:SER:O	1:E:602:PRO:HA	2.13	0.48
1:F:552:THR:HG22	1:F:553:THR:N	2.28	0.48
1:B:646:LEU:HD22	1:B:679:LEU:HD22	1.94	0.48
1:C:338:THR:O	1:C:353:GLY:HA3	2.13	0.48
1:F:641:MET:CE	1:F:699:GLN:HA	2.43	0.48
1:B:51:ASP:OD2	1:B:54:VAL:HG23	2.13	0.48
1:F:382:PHE:HB3	1:F:408:TYR:HE2	1.79	0.48
1:F:383:ASP:OD1	1:F:383:ASP:N	2.46	0.48
1:F:482:TYR:CB	1:F:483:GLY:HA2	2.35	0.48
1:A:552:THR:HG22	1:A:553:THR:N	2.28	0.48
1:D:355:ARG:HB3	1:D:360:ARG:HD3	1.94	0.48
1:D:476:PRO:HB2	1:D:505:MET:HG2	1.94	0.48
1:D:554:PRO:O	1:D:556:GLN:N	2.47	0.48
1:F:544:GLU:HB2	3:F:2036:HOH:O	2.14	0.48
1:F:564:ALA:O	1:F:567:LEU:HB3	2.14	0.48
1:B:112:SER:CB	1:B:689:ARG:HH21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:CZ	1:B:148:VAL:HG23	2.48	0.48
1:C:407:ARG:HD2	1:C:417:TRP:CZ2	2.48	0.48
1:C:465:TYR:HB3	1:C:506:ILE:HG23	1.94	0.48
1:E:497:PHE:C	1:E:497:PHE:HD1	2.22	0.48
1:F:70:VAL:HA	1:F:73:LYS:HE2	1.96	0.48
1:F:279:LEU:N	1:F:279:LEU:CD2	2.72	0.48
1:A:707:LEU:HD12	1:A:707:LEU:HA	1.68	0.48
1:B:61:GLU:HG3	1:B:675:LEU:HB3	1.95	0.48
1:B:363:THR:HG22	3:B:2040:HOH:O	2.13	0.48
1:E:411:MET:HE3	1:E:446:CYS:HB2	1.96	0.48
1:C:177:ARG:HD3	1:C:186:LYS:CG	2.44	0.48
1:C:357:GLY:HA2	1:C:517:GLU:O	2.14	0.48
1:D:373:SER:HB3	1:D:376:THR:HG23	1.94	0.48
1:D:483:GLY:O	1:D:514:GLY:HA3	2.13	0.48
1:F:154:PRO:O	1:F:156:PRO:HD3	2.13	0.48
1:B:149:VAL:HG13	1:B:165:SER:O	2.14	0.48
1:C:183:VAL:HB	3:C:2010:HOH:O	2.13	0.48
1:E:654:TRP:O	1:E:658:LYS:HG3	2.14	0.48
1:F:164:TYR:OH	1:F:177:ARG:HD2	2.14	0.48
1:F:191:ASN:OD1	1:F:191:ASN:C	2.55	0.48
1:F:299:ASP:O	1:F:320:ARG:HB2	2.14	0.48
1:B:6:GLY:HA3	1:B:664:ARG:HD3	1.96	0.47
1:D:646:LEU:HD12	1:D:646:LEU:O	2.14	0.47
1:E:175:SER:OG	1:E:177:ARG:NH2	2.47	0.47
1:B:113:TYR:HB3	1:B:137:GLU:HB2	1.96	0.47
1:B:474:PRO:HA	1:B:551:LEU:O	2.13	0.47
1:B:476:PRO:HB2	1:B:505:MET:HG2	1.95	0.47
1:B:619:PHE:HB3	1:B:623:MET:CE	2.38	0.47
1:C:650:ARG:CZ	1:C:684:PHE:CE2	2.97	0.47
1:F:410:SER:O	1:F:493:PHE:HB2	2.14	0.47
1:A:45:ARG:HD2	1:A:654:TRP:CE2	2.48	0.47
1:A:392:VAL:O	1:A:396:MET:HG2	2.14	0.47
1:E:56:ALA:O	1:E:59:HIS:HB3	2.14	0.47
1:E:87:ILE:HD13	3:E:2025:HOH:O	2.13	0.47
1:E:210:ALA:C	1:E:212:LYS:H	2.21	0.47
1:E:396:MET:HE1	1:E:404:LEU:HA	1.95	0.47
1:B:570:GLY:O	1:B:571:ALA:C	2.56	0.47
1:C:413:THR:HG22	1:C:414:PRO:O	2.14	0.47
1:D:691:LYS:HD3	1:D:691:LYS:HA	1.69	0.47
1:F:498:LEU:HB2	1:F:499:PRO:HD3	1.97	0.47
1:F:650:ARG:NH2	1:F:684:PHE:HE2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:OD2	1:A:170:GLY:HA2	2.14	0.47
1:A:490:GLU:HA	1:A:490:GLU:OE1	2.15	0.47
1:D:83:HIS:HE1	1:D:496:ARG:HA	1.78	0.47
1:D:685:SER:C	1:D:687:SER:N	2.73	0.47
1:F:260:SER:HB3	1:F:609:GLU:HB3	1.97	0.47
1:B:362:TRP:CD1	1:B:379:GLU:HB2	2.49	0.47
1:B:487:ILE:CG2	1:B:488:CYS:N	2.78	0.47
1:A:233:TYR:HA	3:A:2044:HOH:O	2.14	0.47
1:C:528:LYS:O	1:C:529:TYR:C	2.58	0.47
1:F:494:ASN:ND2	1:F:494:ASN:C	2.73	0.47
1:A:534:ASN:O	1:A:535:THR:C	2.57	0.46
1:C:312:ASN:ND2	1:C:520:ARG:H	2.13	0.46
1:D:547:ILE:CD1	1:D:579:LEU:HD22	2.46	0.46
1:D:586:GLY:O	1:D:587:VAL:C	2.58	0.46
1:D:641:MET:HE2	1:D:699:GLN:CG	2.42	0.46
1:E:31:MET:HG3	1:E:615:ASN:O	2.15	0.46
1:E:210:ALA:O	1:E:211:SER:CB	2.62	0.46
1:F:93:SER:O	1:F:95:PRO:HD3	2.14	0.46
1:A:557:LEU:HD23	1:A:579:LEU:O	2.15	0.46
1:B:347:LYS:O	1:B:366:LEU:HG	2.15	0.46
1:B:440:GLU:O	1:B:443:ASN:HB2	2.15	0.46
1:B:616:GLU:O	1:B:617:TYR:C	2.58	0.46
1:D:162:VAL:HG13	1:D:179:VAL:HG21	1.97	0.46
1:D:355:ARG:O	1:D:360:ARG:NH1	2.47	0.46
1:E:50:ALA:O	1:E:51:ASP:C	2.59	0.46
1:E:312:ASN:HB3	1:E:338:THR:HA	1.96	0.46
1:C:100:ARG:O	1:C:100:ARG:HD3	2.16	0.46
1:C:598:ASP:HB3	1:C:601:ILE:CD1	2.41	0.46
1:C:638:PRO:HA	1:C:671:ASN:HD22	1.79	0.46
1:A:203:PHE:CD1	1:A:203:PHE:C	2.94	0.46
1:C:445:VAL:O	1:C:464:VAL:HA	2.16	0.46
1:E:607:GLU:HG2	1:E:611:TRP:HE1	1.80	0.46
1:B:68:ARG:HG2	1:B:674:LEU:HD21	1.97	0.46
1:B:577:PRO:HG3	1:B:635:GLN:HE21	1.81	0.46
1:C:190:THR:HA	1:C:206:ILE:O	2.16	0.46
1:B:294:GLU:HG2	3:B:2032:HOH:O	2.15	0.46
1:D:689:ARG:NH1	1:D:691:LYS:CG	2.77	0.46
1:A:167:ASP:OD2	1:A:170:GLY:CA	2.63	0.46
1:B:560:GLU:HG3	1:B:584:LEU:HD12	1.97	0.46
1:C:355:ARG:HB3	1:C:360:ARG:HH11	1.81	0.46
1:D:106:ARG:NH2	1:D:127:GLU:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ARG:HG2	1:D:186:LYS:HG2	1.98	0.46
1:D:308:ASP:OD2	1:D:314:LYS:NZ	2.48	0.46
1:E:191:ASN:C	1:E:191:ASN:OD1	2.59	0.46
1:F:639:HIS:ND1	1:F:671:ASN:HB3	2.31	0.46
1:D:349:ALA:HB3	1:D:364:VAL:HG12	1.96	0.46
1:A:552:THR:CG2	1:A:557:LEU:HB2	2.46	0.46
1:A:685:SER:HB3	1:A:687:SER:HA	1.98	0.46
1:C:213:ARG:NH2	1:C:235:ASP:O	2.49	0.46
1:D:498:LEU:O	1:D:499:PRO:C	2.58	0.46
1:E:39:ASP:OD2	1:E:658:LYS:NZ	2.48	0.46
1:F:553:THR:OG1	1:F:556:GLN:NE2	2.47	0.46
1:A:111:LEU:HD23	1:A:111:LEU:N	2.30	0.45
1:B:498:LEU:HB2	1:B:499:PRO:HD3	1.98	0.45
1:D:210:ALA:C	1:D:212:LYS:N	2.71	0.45
1:D:685:SER:O	1:D:686:ALA:HB3	2.16	0.45
1:E:49:ARG:HE	1:E:653:TYR:HE2	1.64	0.45
1:A:552:THR:CG2	1:A:553:THR:N	2.79	0.45
1:A:653:TYR:CD1	1:A:653:TYR:C	2.94	0.45
1:B:533:ARG:HD3	3:B:2057:HOH:O	2.17	0.45
1:C:685:SER:O	1:C:687:SER:N	2.49	0.45
1:D:266:HIS:CE1	1:D:281:MET:CE	2.99	0.45
1:D:676:LYS:HE3	1:D:695:GLU:HG2	1.98	0.45
1:F:9:ALA:HB3	1:F:41:LEU:HD22	1.98	0.45
1:F:291:TYR:HA	1:F:304:LEU:O	2.17	0.45
1:F:403:LEU:HD22	1:F:419:ASP:HB3	1.98	0.45
1:D:104:TYR:OH	1:D:131:GLU:HG3	2.17	0.45
1:F:588:PRO:HD2	1:F:656:PRO:HG3	1.98	0.45
1:F:710:ARG:HH11	1:F:710:ARG:HB2	1.80	0.45
1:B:626:TYR:O	1:B:627:SER:C	2.59	0.45
1:C:317:LEU:HD21	3:C:2017:HOH:O	2.16	0.45
1:C:689:ARG:CZ	1:C:691:LYS:HG2	2.47	0.45
1:D:103:TYR:CZ	1:D:118:ARG:HG3	2.52	0.45
1:E:406:LEU:O	1:E:417:TRP:HA	2.17	0.45
1:E:714:ARG:HB3	3:E:2037:HOH:O	2.16	0.45
1:F:418:TYR:HB3	1:F:429:VAL:HA	1.98	0.45
1:F:558:SER:HA	1:F:582:VAL:O	2.16	0.45
1:B:532:LYS:HE2	1:B:611:TRP:HZ3	1.81	0.45
1:C:689:ARG:NH1	1:C:691:LYS:HG2	2.31	0.45
1:D:151:CYS:O	1:D:164:TYR:HA	2.17	0.45
1:F:711:GLN:HE21	1:F:711:GLN:CA	2.23	0.45
1:C:588:PRO:HB2	1:C:590:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:THR:HB	1:D:325:ASP:O	2.17	0.45
1:F:499:PRO:O	1:F:503:ARG:HD2	2.16	0.45
1:F:601:ILE:HA	1:F:602:PRO:HD3	1.79	0.45
1:B:473:LYS:HB2	1:B:474:PRO:HD2	1.99	0.45
1:C:496:ARG:O	1:C:499:PRO:HD2	2.16	0.45
1:E:96:TYR:O	1:E:102:LEU:HA	2.17	0.45
1:E:337:VAL:CG2	1:E:355:ARG:HD3	2.47	0.45
1:F:463:LEU:HD12	1:F:506:ILE:HG21	1.98	0.45
1:C:563:SER:HB2	1:C:683:HIS:CE1	2.52	0.45
1:F:216:LYS:HD3	1:F:234:THR:OG1	2.17	0.45
1:C:113:TYR:HB3	1:C:137:GLU:CB	2.45	0.45
1:C:681:SER:CB	1:C:685:SER:HB2	2.45	0.45
1:F:386:VAL:HG22	1:F:386:VAL:O	2.17	0.45
1:A:173:VAL:HG13	1:A:189:GLY:HA2	1.97	0.45
1:B:354:ARG:NH2	1:B:490:GLU:OE2	2.50	0.45
1:C:158:GLU:O	1:C:159:HIS:HB2	2.16	0.45
1:F:19:GLY:O	1:F:26:ARG:HG3	2.17	0.45
1:A:101:PHE:CE1	1:A:118:ARG:HD3	2.52	0.44
1:C:78:THR:O	1:C:82:GLU:HG3	2.16	0.44
1:C:89:GLU:HB3	1:C:109:LYS:HA	1.98	0.44
1:D:528:LYS:HG3	1:D:529:TYR:N	2.31	0.44
1:E:101:PHE:HD1	1:E:120:PRO:HA	1.82	0.44
1:E:355:ARG:O	1:E:360:ARG:NH1	2.50	0.44
1:A:237:ASP:HA	1:A:238:PRO:HD2	1.61	0.44
1:B:342:VAL:HG12	1:B:351:LEU:HD12	1.99	0.44
1:B:552:THR:HG23	1:B:553:THR:H	1.81	0.44
1:E:484:SER:O	1:E:486:GLY:N	2.50	0.44
1:C:596:MET:HE1	1:C:604:THR:O	2.18	0.44
1:E:520:ARG:HG3	1:E:524:GLU:HG3	1.99	0.44
1:F:460:PRO:HG2	1:F:511:HIS:HB2	2.00	0.44
1:F:521:THR:C	1:F:523:TYR:H	2.25	0.44
1:B:112:SER:HB3	1:B:689:ARG:NE	2.31	0.44
1:C:162:VAL:O	1:C:179:VAL:HG23	2.17	0.44
1:E:88:GLU:O	1:E:88:GLU:HG3	2.17	0.44
1:E:172:GLU:HB2	1:E:649:PRO:HG3	1.99	0.44
1:F:46:ASP:OD2	1:F:50:ALA:N	2.44	0.44
1:F:642:ILE:CD1	1:F:660:ALA:HB2	2.47	0.44
1:F:712:LEU:HD12	1:F:712:LEU:N	2.29	0.44
1:B:263:SER:CB	1:B:291:TYR:H	2.30	0.44
1:E:69:ALA:O	1:E:71:ASP:N	2.51	0.44
1:E:707:LEU:HD12	1:E:707:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:SER:HB3	1:F:689:ARG:HA	1.99	0.44
1:A:18:PHE:CE2	1:A:597:CYS:HB3	2.52	0.44
1:A:175:SER:HA	1:A:187:VAL:O	2.17	0.44
1:C:88:GLU:C	1:C:90:THR:H	2.25	0.44
1:C:177:ARG:HD3	1:C:186:LYS:HG3	1.99	0.44
1:C:627:SER:HB3	1:C:630:ASP:HB2	1.98	0.44
1:A:96:TYR:CD1	1:A:395:GLN:HG2	2.52	0.44
1:A:119:VAL:HG13	1:A:123:LYS:HB2	1.99	0.44
1:A:261:GLU:HG2	1:A:609:GLU:OE1	2.18	0.44
1:A:521:THR:O	1:A:525:VAL:HG22	2.18	0.44
1:C:96:TYR:HE2	1:C:397:LYS:HG3	1.82	0.44
1:D:413:THR:O	1:D:493:PHE:HB2	2.18	0.44
1:D:666:LEU:HD23	1:D:666:LEU:HA	1.78	0.44
1:E:521:THR:C	1:E:523:TYR:H	2.26	0.44
1:A:488:CYS:HB3	1:A:517:GLU:HG3	1.98	0.44
1:B:261:GLU:HG2	1:B:609:GLU:OE1	2.18	0.44
1:C:497:PHE:CD1	1:C:497:PHE:C	2.96	0.44
1:E:342:VAL:HA	1:E:350:VAL:O	2.17	0.44
1:B:532:LYS:HE2	1:B:611:TRP:CZ3	2.53	0.44
1:D:88:GLU:O	1:D:88:GLU:CG	2.66	0.44
1:D:584:LEU:HD23	1:D:641:MET:HB3	2.00	0.44
1:E:679:LEU:HD12	1:E:679:LEU:H	1.83	0.44
1:A:482:TYR:HB3	3:A:2074:HOH:O	2.17	0.43
1:B:226:GLN:C	1:B:228:GLU:H	2.26	0.43
1:B:308:ASP:O	1:B:309:LYS:HB2	2.17	0.43
1:D:563:SER:HA	1:D:587:VAL:O	2.18	0.43
1:E:261:GLU:HA	1:E:290:ARG:HD2	2.00	0.43
1:E:307:LYS:HG2	1:E:308:ASP:OD1	2.18	0.43
1:F:573:LEU:HD23	1:F:573:LEU:HA	1.63	0.43
1:A:261:GLU:HA	1:A:290:ARG:HD2	2.00	0.43
1:C:534:ASN:O	1:C:535:THR:C	2.60	0.43
1:D:307:LYS:O	1:D:308:ASP:HB2	2.18	0.43
1:E:367:GLY:O	1:E:369:ASP:N	2.50	0.43
1:E:713:LEU:C	1:E:714:ARG:HE	2.26	0.43
1:F:219:ARG:HB2	1:F:232:LEU:HD11	2.00	0.43
1:A:299:ASP:OD1	1:A:299:ASP:N	2.50	0.43
1:A:479:LEU:HD11	1:A:510:ALA:HB2	2.00	0.43
1:B:627:SER:OG	1:B:630:ASP:OD2	2.27	0.43
1:C:413:THR:O	1:C:493:PHE:HB2	2.17	0.43
1:C:473:LYS:HA	1:C:474:PRO:HD2	1.88	0.43
1:A:236:ASP:O	1:A:238:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ARG:HG3	1:A:622:TYR:CZ	2.52	0.43
1:B:158:GLU:O	1:B:159:HIS:HB2	2.18	0.43
1:B:209:ASP:HB2	1:B:215:ASN:OD1	2.17	0.43
1:B:221:ILE:O	1:B:224:GLN:HG3	2.18	0.43
1:B:494:ASN:ND2	1:B:496:ARG:HB2	2.33	0.43
1:E:515:GLY:O	1:E:523:TYR:HB2	2.19	0.43
1:F:576:ARG:O	1:F:577:PRO:C	2.60	0.43
1:B:331:ILE:HA	1:B:332:PRO:HD3	1.85	0.43
1:C:504:GLY:HA3	1:C:713:LEU:HD12	2.01	0.43
1:D:446:CYS:O	1:D:446:CYS:SG	2.77	0.43
1:E:41:LEU:O	1:E:658:LYS:HE2	2.18	0.43
1:E:641:MET:HE1	1:E:698:ILE:CG2	2.48	0.43
1:E:650:ARG:NH2	1:E:684:PHE:HE2	2.16	0.43
1:F:74:ASP:O	1:F:77:GLU:HB3	2.18	0.43
1:A:179:VAL:O	1:A:181:ASP:N	2.52	0.43
1:A:230:VAL:HG11	1:A:277:ASN:ND2	2.34	0.43
1:D:162:VAL:HG13	1:D:179:VAL:CG2	2.49	0.43
1:D:393:CYS:C	1:D:395:GLN:N	2.77	0.43
1:E:482:TYR:O	1:E:565:GLY:HA2	2.19	0.43
1:F:100:ARG:O	1:F:121:ALA:HB2	2.18	0.43
1:F:449:GLU:HB2	1:F:461:ILE:HB	2.00	0.43
1:A:113:TYR:HB3	1:A:137:GLU:CB	2.43	0.43
1:A:247:SER:HB3	1:A:252:THR:HB	2.00	0.43
1:B:116:HIS:HB3	3:B:2012:HOH:O	2.18	0.43
1:D:283:ARG:HG3	1:D:324:THR:HG22	1.99	0.43
1:D:540:ILE:O	1:D:544:GLU:HG2	2.19	0.43
1:D:595:THR:HG23	1:D:601:ILE:HD13	2.00	0.43
1:D:712:LEU:HD12	1:D:712:LEU:H	1.83	0.43
1:E:613:ASN:O	1:E:619:PHE:HB2	2.18	0.43
1:A:61:GLU:HG2	1:A:675:LEU:CD2	2.36	0.43
1:A:204:PHE:CE1	1:A:219:ARG:HG3	2.53	0.43
1:F:61:GLU:HG2	1:F:675:LEU:HB3	2.01	0.43
1:F:153:ALA:HA	1:F:154:PRO:HD3	1.85	0.43
2:J:1:FC0:CD2	2:J:2:ARG:HH21	2.31	0.43
1:A:35:ARG:NH1	1:A:620:PHE:CD2	2.87	0.43
1:C:483:GLY:O	1:C:514:GLY:HA3	2.19	0.43
1:D:51:ASP:HA	1:D:52:PRO:HD3	1.91	0.43
1:E:209:ASP:OD1	1:E:210:ALA:N	2.51	0.43
1:F:115:LEU:HD23	1:F:133:ILE:HG12	2.00	0.43
1:F:689:ARG:HB2	1:F:691:LYS:H	1.84	0.43
1:A:294:GLU:HG3	1:A:342:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:O	1:B:156:PRO:HD3	2.19	0.43
1:B:685:SER:O	1:B:686:ALA:HB3	2.19	0.43
1:B:689:ARG:HD3	3:B:2074:HOH:O	2.18	0.43
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.92	0.43
1:C:104:TYR:CE2	1:C:117:CYS:HB2	2.53	0.43
1:C:479:LEU:O	1:C:559:CYS:HA	2.19	0.43
1:E:226:GLN:O	1:E:226:GLN:HG3	2.18	0.43
1:E:400:ASP:CB	3:E:2023:HOH:O	2.57	0.43
1:B:222:ILE:H	1:B:222:ILE:HG12	1.60	0.42
1:C:343:ALA:HB1	1:C:345:PHE:HE1	1.82	0.42
1:C:523:TYR:OH	1:C:528:LYS:NZ	2.48	0.42
1:D:496:ARG:HH11	1:D:496:ARG:CG	2.21	0.42
1:E:366:LEU:H	1:E:366:LEU:CD1	2.14	0.42
1:F:418:TYR:HB2	1:F:428:LYS:C	2.43	0.42
1:A:307:LYS:HG2	1:A:308:ASP:N	2.34	0.42
1:B:95:PRO:HA	1:B:103:TYR:O	2.19	0.42
1:C:179:VAL:O	1:C:180:ARG:C	2.62	0.42
1:E:108:VAL:HB	1:E:111:LEU:HD12	2.02	0.42
1:F:66:GLU:C	1:F:68:ARG:N	2.77	0.42
1:F:641:MET:HE2	1:F:699:GLN:HG3	2.01	0.42
1:B:244:VAL:HG23	1:B:255:ILE:HG12	2.01	0.42
1:C:542:CYS:O	1:C:546:LEU:HG	2.18	0.42
1:F:712:LEU:H	1:F:712:LEU:CD1	2.28	0.42
1:A:92:MET:HE3	1:A:92:MET:HB2	1.78	0.42
1:B:89:GLU:OE1	1:B:109:LYS:HE2	2.19	0.42
1:C:447:ARG:HG3	1:C:463:LEU:HD21	2.01	0.42
1:C:571:ALA:O	1:C:572:VAL:C	2.62	0.42
1:C:662:LYS:O	1:C:663:LEU:C	2.61	0.42
1:D:162:VAL:HG13	1:D:179:VAL:HB	2.00	0.42
1:D:563:SER:HB2	1:D:683:HIS:CE1	2.55	0.42
1:E:83:HIS:CE1	1:E:499:PRO:HG2	2.54	0.42
1:E:484:SER:C	1:E:486:GLY:H	2.27	0.42
1:E:689:ARG:HB2	1:E:690:TYR:H	1.59	0.42
1:A:689:ARG:HD3	1:A:691:LYS:HG2	1.99	0.42
1:B:641:MET:HE3	1:B:676:LYS:HB2	2.00	0.42
1:C:305:THR:OG1	1:C:307:LYS:HB2	2.20	0.42
1:C:533:ARG:HG3	1:C:622:TYR:CZ	2.54	0.42
1:D:220:HIS:HE1	1:D:224:GLN:O	2.01	0.42
1:E:325:ASP:C	1:E:326:TRP:CD1	2.97	0.42
1:E:446:CYS:HB3	1:E:464:VAL:HG23	2.02	0.42
1:F:179:VAL:C	1:F:181:ASP:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:592:VAL:O	1:F:596:MET:HB2	2.19	0.42
1:A:109:LYS:O	1:A:109:LYS:HG2	2.20	0.42
1:A:675:LEU:O	1:A:675:LEU:HG	2.18	0.42
1:B:449:GLU:HG3	1:B:463:LEU:HD21	2.00	0.42
1:C:381:HIS:O	1:C:427:ARG:NH2	2.42	0.42
1:D:89:GLU:OE1	1:D:109:LYS:HE3	2.20	0.42
1:D:96:TYR:CD1	1:D:395:GLN:HG2	2.55	0.42
1:B:424:SER:OG	1:B:426:GLU:HG2	2.20	0.42
1:C:162:VAL:HG12	3:C:2009:HOH:O	2.18	0.42
1:D:396:MET:HE1	1:D:403:LEU:O	2.20	0.42
1:D:592:VAL:HB	1:D:627:SER:OG	2.20	0.42
1:E:321:SER:O	1:E:323:PRO:HD3	2.19	0.42
1:E:400:ASP:OD1	1:E:400:ASP:O	2.37	0.42
1:E:653:TYR:CD1	1:E:653:TYR:C	2.98	0.42
1:F:79:ILE:CD1	1:F:499:PRO:HB3	2.48	0.42
1:A:363:THR:HG22	1:A:378:LYS:HB3	2.02	0.42
1:B:126:GLY:O	1:B:131:GLU:HB2	2.20	0.42
1:B:220:HIS:HE1	1:B:224:GLN:O	2.03	0.42
1:B:687:SER:HB2	1:B:689:ARG:HG3	2.01	0.42
1:C:637:TYR:N	1:C:669:ASP:OD2	2.40	0.42
1:D:61:GLU:CG	1:D:675:LEU:HB3	2.50	0.42
1:D:418:TYR:HB3	1:D:428:LYS:O	2.20	0.42
1:D:618:LYS:HD3	1:D:619:PHE:CE2	2.55	0.42
1:E:426:GLU:O	1:E:426:GLU:HG3	2.20	0.42
1:E:443:ASN:O	1:E:466:ASP:HA	2.19	0.42
1:E:659:TRP:CE2	1:E:663:LEU:HD11	2.55	0.42
1:F:199:ASN:HB2	1:F:201:GLU:HG3	2.02	0.42
1:F:393:CYS:HA	1:F:396:MET:HG3	2.02	0.42
1:A:268:LEU:HD13	1:A:279:LEU:HD13	2.02	0.42
1:D:382:PHE:HB3	1:D:408:TYR:CE1	2.55	0.42
1:C:373:SER:O	1:C:376:THR:OG1	2.36	0.42
1:C:539:PHE:HD2	1:C:572:VAL:HG21	1.83	0.42
1:C:614:PRO:CD	1:C:623:MET:HE1	2.50	0.42
1:D:421:ASP:HB3	1:D:424:SER:HG	1.83	0.42
1:D:639:HIS:CE1	1:D:671:ASN:HB3	2.55	0.42
1:E:713:LEU:O	1:E:714:ARG:NE	2.43	0.42
1:F:101:PHE:CD1	1:F:118:ARG:HD3	2.55	0.42
1:A:206:ILE:O	1:A:206:ILE:HG22	2.20	0.41
1:B:78:THR:O	1:B:82:GLU:HG3	2.19	0.41
1:C:249:ASP:OD1	1:C:249:ASP:C	2.63	0.41
1:C:418:TYR:HA	1:C:428:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:MET:HE3	1:F:446:CYS:HB2	2.01	0.41
1:A:31:MET:HG3	1:A:615:ASN:O	2.21	0.41
1:A:369:ASP:O	1:A:370:ASN:HB2	2.20	0.41
1:C:216:LYS:HG2	1:C:234:THR:HG23	2.02	0.41
1:D:554:PRO:C	1:D:556:GLN:N	2.77	0.41
1:F:304:LEU:HD12	1:F:314:LYS:O	2.19	0.41
1:F:498:LEU:HB2	1:F:499:PRO:CD	2.50	0.41
1:F:501:VAL:HG12	1:F:502:ASP:N	2.35	0.41
1:F:518:MET:HE3	1:F:518:MET:HB3	1.96	0.41
1:F:607:GLU:C	1:F:609:GLU:N	2.77	0.41
1:A:100:ARG:NH1	1:A:100:ARG:CG	2.77	0.41
1:A:595:THR:HA	1:A:601:ILE:HD12	2.00	0.41
1:B:439:PHE:CD1	1:B:439:PHE:C	2.99	0.41
1:D:134:VAL:HG12	1:D:162:VAL:HG11	2.02	0.41
1:D:210:ALA:C	1:D:212:LYS:H	2.26	0.41
1:E:476:PRO:HD3	1:E:556:GLN:OE1	2.20	0.41
1:E:648:ASP:OD1	1:E:683:HIS:HB2	2.21	0.41
1:E:703:VAL:HG12	1:E:707:LEU:HD22	2.02	0.41
1:F:69:ALA:O	1:F:70:VAL:C	2.63	0.41
1:F:713:LEU:C	1:F:714:ARG:HD2	2.45	0.41
1:B:648:ASP:OD1	1:B:683:HIS:HB2	2.21	0.41
1:C:331:ILE:HA	1:C:332:PRO:HD3	1.88	0.41
1:C:479:LEU:HD12	1:C:479:LEU:HA	1.87	0.41
1:E:260:SER:HB3	1:E:609:GLU:HB3	2.02	0.41
1:E:310:CYS:SG	1:E:314:LYS:HE2	2.60	0.41
1:F:315:VAL:HG13	1:F:331:ILE:HB	2.02	0.41
1:F:408:TYR:O	1:F:415:THR:HA	2.20	0.41
1:F:532:LYS:O	1:F:532:LYS:HG3	2.20	0.41
1:B:75:LEU:O	1:B:79:ILE:HD13	2.20	0.41
1:B:380:LEU:HD23	1:B:406:LEU:HD11	2.02	0.41
1:B:460:PRO:HB2	1:B:511:HIS:CD2	2.55	0.41
1:C:187:VAL:HA	1:C:226:GLN:OE1	2.20	0.41
1:C:500:TYR:OH	1:C:703:VAL:HG21	2.20	0.41
1:D:489:ILE:HD13	1:D:489:ILE:HA	1.88	0.41
1:D:655:GLU:HB2	1:D:656:PRO:CD	2.50	0.41
1:E:528:LYS:O	1:E:529:TYR:C	2.64	0.41
1:E:587:VAL:HG21	1:E:683:HIS:CE1	2.56	0.41
1:F:5:ARG:CG	1:F:6:GLY:H	2.31	0.41
1:F:418:TYR:HB2	1:F:429:VAL:HA	2.02	0.41
1:C:344:VAL:C	1:C:345:PHE:CD1	2.98	0.41
1:D:89:GLU:HB3	1:D:109:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:ALA:O	1:D:640:LEU:HA	2.21	0.41
1:D:593:MET:HE2	1:D:624:ASN:HB2	2.03	0.41
1:D:596:MET:HE1	1:D:604:THR:O	2.20	0.41
1:E:45:ARG:HD2	1:E:654:TRP:CZ2	2.56	0.41
1:E:482:TYR:CD2	1:E:483:GLY:HA2	2.55	0.41
1:E:632:VAL:CG1	1:E:666:LEU:HD12	2.36	0.41
1:A:582:VAL:HG22	1:A:583:ALA:N	2.36	0.41
1:C:681:SER:HB2	1:C:685:SER:HB3	1.98	0.41
1:D:573:LEU:HD23	1:D:573:LEU:HA	1.75	0.41
1:E:99:ASP:HB2	1:E:159:HIS:NE2	2.36	0.41
1:E:347:LYS:O	1:E:348:PHE:HB3	2.20	0.41
1:E:519:GLY:O	1:E:520:ARG:C	2.63	0.41
1:F:88:GLU:C	1:F:90:THR:N	2.79	0.41
1:A:165:SER:HA	1:A:175:SER:O	2.20	0.41
1:B:49:ARG:HH11	1:B:653:TYR:HD2	1.67	0.41
1:B:264:GLU:CD	1:B:285:ARG:HE	2.29	0.41
1:B:273:GLY:O	1:B:275:LYS:N	2.54	0.41
1:B:296:HIS:O	1:B:300:THR:HG23	2.21	0.41
1:B:629:ILE:HD11	1:B:659:TRP:N	2.36	0.41
1:B:707:LEU:HD12	1:B:707:LEU:HA	1.93	0.41
1:D:552:THR:HG22	1:D:553:THR:N	2.35	0.41
1:E:355:ARG:HB3	1:E:360:ARG:HD3	2.03	0.41
1:E:411:MET:HE3	1:E:446:CYS:CB	2.50	0.41
1:F:31:MET:SD	1:F:617:TYR:CD1	3.13	0.41
1:F:407:ARG:NE	3:F:2026:HOH:O	2.53	0.41
1:A:684:PHE:O	1:A:685:SER:O	2.39	0.41
1:A:707:LEU:O	1:A:708:ASN:CB	2.69	0.41
1:B:39:ASP:OD1	1:B:39:ASP:C	2.63	0.41
1:C:135:LEU:HD12	1:C:136:ASP:H	1.85	0.41
1:C:348:PHE:CD1	1:C:349:ALA:N	2.89	0.41
1:C:480:TYR:CD1	1:C:480:TYR:C	2.98	0.41
1:C:601:ILE:HA	1:C:602:PRO:HD3	1.91	0.41
1:C:691:LYS:HD3	1:C:691:LYS:HA	1.52	0.41
1:F:369:ASP:C	1:F:371:LEU:H	2.29	0.41
1:F:374:SER:C	1:F:376:THR:H	2.29	0.41
1:A:206:ILE:HA	1:A:216:LYS:O	2.20	0.41
1:A:554:PRO:HD2	3:A:2084:HOH:O	2.20	0.41
1:A:691:LYS:HD3	1:A:691:LYS:HA	1.86	0.41
1:D:191:ASN:OD1	1:D:191:ASN:C	2.63	0.41
1:D:220:HIS:CE1	1:D:224:GLN:O	2.73	0.41
1:D:619:PHE:CB	1:D:623:MET:CE	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ALA:C	1:E:212:LYS:N	2.79	0.41
1:E:367:GLY:C	1:E:369:ASP:N	2.79	0.41
1:E:476:PRO:HG2	1:E:709:VAL:HG11	2.02	0.41
1:F:21:VAL:O	1:F:22:GLU:C	2.63	0.41
1:F:382:PHE:HB3	1:F:408:TYR:CE2	2.55	0.41
1:A:596:MET:HA	1:A:604:THR:HG23	2.01	0.40
1:C:155:ALA:HA	1:C:156:PRO:HD2	1.95	0.40
1:C:704:LEU:CD2	1:C:709:VAL:HG23	2.50	0.40
1:D:688:ASP:OD1	1:D:688:ASP:N	2.54	0.40
1:E:295:MET:HE3	1:E:295:MET:HB3	2.01	0.40
1:E:552:THR:CG2	1:E:553:THR:N	2.84	0.40
1:E:704:LEU:HD22	1:E:709:VAL:HG23	2.02	0.40
1:A:51:ASP:HA	1:A:52:PRO:HD3	1.93	0.40
1:A:528:LYS:O	1:A:529:TYR:C	2.64	0.40
1:B:433:ARG:HG3	1:B:434:LYS:N	2.36	0.40
1:C:237:ASP:HA	1:C:238:PRO:HD2	1.92	0.40
1:E:450:LEU:HD23	1:E:460:PRO:HA	2.03	0.40
1:E:633:ARG:HH11	1:E:633:ARG:HD3	1.65	0.40
1:A:118:ARG:NH2	1:A:159:HIS:O	2.54	0.40
1:A:162:VAL:HG22	1:A:179:VAL:HG23	2.03	0.40
1:B:162:VAL:HG13	1:B:179:VAL:CG2	2.50	0.40
1:C:88:GLU:O	1:C:88:GLU:CG	2.70	0.40
1:C:614:PRO:HD3	1:C:623:MET:HE1	2.04	0.40
1:D:191:ASN:ND2	1:D:206:ILE:HB	2.36	0.40
1:E:277:ASN:O	1:E:279:LEU:HD13	2.22	0.40
1:F:687:SER:HB2	1:F:688:ASP:H	1.77	0.40
1:A:341:ASP:OD1	1:A:341:ASP:C	2.65	0.40
1:A:403:LEU:HD22	1:A:419:ASP:HB3	2.02	0.40
1:A:523:TYR:OH	1:A:528:LYS:NZ	2.44	0.40
1:A:598:ASP:OD1	1:A:598:ASP:C	2.64	0.40
1:A:654:TRP:O	1:A:658:LYS:HG3	2.21	0.40
1:B:106:ARG:NH2	1:B:131:GLU:OE1	2.47	0.40
1:B:139:LYS:HE3	3:B:2014:HOH:O	2.22	0.40
1:C:342:VAL:HA	1:C:350:VAL:O	2.22	0.40
1:C:463:LEU:N	1:C:463:LEU:CD2	2.84	0.40
1:D:445:VAL:HG23	1:D:465:TYR:CE1	2.56	0.40
1:D:494:ASN:OD1	1:D:496:ARG:HB2	2.22	0.40
1:E:62:LYS:HE2	1:E:62:LYS:HB3	1.69	0.40
1:E:417:TRP:CE3	1:E:431:LYS:HD3	2.56	0.40
1:E:558:SER:HA	1:E:582:VAL:O	2.21	0.40
1:F:253:LEU:HB3	1:F:268:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:GLU:HA	1:F:491:PRO:HD3	1.96	0.40
1:F:678:ASP:CG	1:F:680:GLU:H	2.30	0.40
1:B:115:LEU:HD23	1:B:133:ILE:HD13	2.02	0.40
1:B:215:ASN:OD1	1:B:216:LYS:HG2	2.22	0.40
1:F:646:LEU:HB3	1:F:679:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

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	708/715 (99%)	651 (92%)	48 (7%)	9 (1%)	9	21
1	B	708/715 (99%)	646 (91%)	51 (7%)	11 (2%)	7	17
1	C	708/715 (99%)	623 (88%)	69 (10%)	16 (2%)	5	11
1	D	708/715 (99%)	645 (91%)	49 (7%)	14 (2%)	6	13
1	E	708/715 (99%)	631 (89%)	63 (9%)	14 (2%)	6	13
1	F	708/715 (99%)	613 (87%)	82 (12%)	13 (2%)	6	15
2	G	1/4 (25%)	0	1 (100%)	0	100	100
2	H	1/4 (25%)	1 (100%)	0	0	100	100
2	I	1/4 (25%)	1 (100%)	0	0	100	100
2	J	1/4 (25%)	1 (100%)	0	0	100	100
2	K	1/4 (25%)	1 (100%)	0	0	100	100
2	L	1/4 (25%)	0	1 (100%)	0	100	100
All	All	4254/4314 (99%)	3813 (90%)	364 (9%)	77 (2%)	6	15

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	A	157	PRO
1	A	685	SER
1	B	157	PRO
1	B	274	VAL
1	B	401	ALA
1	C	156	PRO
1	C	157	PRO
1	D	156	PRO
1	D	157	PRO
1	E	70	VAL
1	E	121	ALA
1	E	156	PRO
1	E	157	PRO
1	F	142	GLU
1	F	157	PRO
1	A	180	ARG
1	B	93	SER
1	B	121	ALA
1	B	142	GLU
1	B	437	GLY
1	C	89	GLU
1	C	142	GLU
1	C	282	VAL
1	C	368	PRO
1	C	686	ALA
1	D	713	LEU
1	E	274	VAL
1	E	522	TRP
1	E	634	ALA
1	E	685	SER
1	F	159	HIS
1	A	142	GLU
1	B	620	PHE
1	C	341	ASP
1	C	471	LEU
1	C	474	PRO
1	D	180	ARG
1	D	555	ALA
1	D	563	SER
1	D	686	ALA
1	D	689	ARG
1	E	142	GLU

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Mol	Chain	Res	Type
1	E	368	PRO
1	F	156	PRO
1	F	578	ASP
1	A	467	THR
1	C	409	SER
1	C	602	PRO
1	E	88	GLU
1	E	282	VAL
1	E	686	ALA
1	F	84	ILE
1	F	370	ASN
1	F	620	PHE
1	A	208	LYS
1	A	411	MET
1	A	620	PHE
1	B	370	ASN
1	C	180	ARG
1	C	627	SER
1	C	628	PRO
1	D	63	ASP
1	D	142	GLU
1	D	308	ASP
1	E	429	VAL
1	F	437	GLY
1	F	502	ASP
1	C	181	ASP
1	D	341	ASP
1	B	156	PRO
1	F	282	VAL
1	F	94	ALA
1	B	628	PRO
1	D	13	PRO
1	D	527	GLY
1	F	628	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	614/619 (99%)	551 (90%)	63 (10%)	7	14
1	B	614/619 (99%)	535 (87%)	79 (13%)	4	7
1	C	614/619 (99%)	547 (89%)	67 (11%)	6	12
1	D	614/619 (99%)	533 (87%)	81 (13%)	4	7
1	E	614/619 (99%)	537 (88%)	77 (12%)	4	8
1	F	614/619 (99%)	533 (87%)	81 (13%)	4	7
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	L	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	3696/3726 (99%)	3244 (88%)	452 (12%)	5	9

All (452) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	37	ARG
1	A	49	ARG
1	A	62	LYS
1	A	66	GLU
1	A	78	THR
1	A	79	ILE
1	A	100	ARG
1	A	105	THR
1	A	114	LYS
1	A	119	VAL
1	A	140	LEU
1	A	144	LYS
1	A	156	PRO
1	A	162	VAL
1	A	175	SER
1	A	190	THR
1	A	199	ASN
1	A	201	GLU
1	A	226	GLN
1	A	251	LYS
1	A	258	MET

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Mol	Chain	Res	Type
1	A	262	THR
1	A	279	LEU
1	A	287	LYS
1	A	299	ASP
1	A	300	THR
1	A	316	VAL
1	A	317	LEU
1	A	320	ARG
1	A	328	THR
1	A	336	LYS
1	A	341	ASP
1	A	342	VAL
1	A	350	VAL
1	A	352	SER
1	A	361	VAL
1	A	391	VAL
1	A	396	MET
1	A	398	THR
1	A	404	LEU
1	A	412	THR
1	A	418	TYR
1	A	423	LEU
1	A	440	GLU
1	A	447	ARG
1	A	457	THR
1	A	463	LEU
1	A	473	LYS
1	A	496	ARG
1	A	497	PHE
1	A	562	ARG
1	A	592	VAL
1	A	628	PRO
1	A	675	LEU
1	A	679	LEU
1	A	685	SER
1	A	688	ASP
1	A	689	ARG
1	A	695	GLU
1	A	698	ILE
1	A	699	GLN
1	A	707	LEU
1	B	15	GLU

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Mol	Chain	Res	Type
1	B	16	VAL
1	B	37	ARG
1	B	53	GLU
1	B	67	LYS
1	B	70	VAL
1	B	84	ILE
1	B	93	SER
1	B	102	LEU
1	B	105	THR
1	B	109	LYS
1	B	119	VAL
1	B	124	THR
1	B	145	SER
1	B	151	CYS
1	B	156	PRO
1	B	157	PRO
1	B	161	LEU
1	B	190	THR
1	B	193	SER
1	B	199	ASN
1	B	216	LYS
1	B	227	SER
1	B	241	SER
1	B	251	LYS
1	B	260	SER
1	B	272	LYS
1	B	278	THR
1	B	279	LEU
1	B	285	ARG
1	B	287	LYS
1	B	292	THR
1	B	299	ASP
1	B	300	THR
1	B	302	ILE
1	B	315	VAL
1	B	316	VAL
1	B	319	LYS
1	B	320	ARG
1	B	321	SER
1	B	336	LYS
1	B	342	VAL
1	B	350	VAL

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Mol	Chain	Res	Type
1	B	361	VAL
1	B	363	THR
1	B	365	ARG
1	B	374	SER
1	B	376	THR
1	B	383	ASP
1	B	386	VAL
1	B	391	VAL
1	B	398	THR
1	B	402	SER
1	B	404	LEU
1	B	412	THR
1	B	418	TYR
1	B	424	SER
1	B	428	LYS
1	B	433	ARG
1	B	445	VAL
1	B	463	LEU
1	B	469	ILE
1	B	494	ASN
1	B	496	ARG
1	B	537	MET
1	B	562	ARG
1	B	575	MET
1	B	582	VAL
1	B	602	PRO
1	B	611	TRP
1	B	629	ILE
1	B	687	SER
1	B	688	ASP
1	B	689	ARG
1	B	691	LYS
1	B	695	GLU
1	B	698	ILE
1	B	707	LEU
1	B	711	GLN
1	C	5	ARG
1	C	8	ILE
1	C	15	GLU
1	C	36	ARG
1	C	38	VAL
1	C	60	LEU

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Mol	Chain	Res	Type
1	C	67	LYS
1	C	71	ASP
1	C	87	ILE
1	C	105	THR
1	C	106	ARG
1	C	114	LYS
1	C	119	VAL
1	C	129	GLU
1	C	158	GLU
1	C	162	VAL
1	C	180	ARG
1	C	186	LYS
1	C	207	THR
1	C	212	LYS
1	C	242	VAL
1	C	244	VAL
1	C	251	LYS
1	C	260	SER
1	C	265	SER
1	C	278	THR
1	C	279	LEU
1	C	285	ARG
1	C	287	LYS
1	C	299	ASP
1	C	308	ASP
1	C	311	VAL
1	C	315	VAL
1	C	316	VAL
1	C	317	LEU
1	C	320	ARG
1	C	337	VAL
1	C	350	VAL
1	C	360	ARG
1	C	361	VAL
1	C	363	THR
1	C	374	SER
1	C	377	LEU
1	C	386	VAL
1	C	388	THR
1	C	404	LEU
1	C	410	SER
1	C	423	LEU

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Mol	Chain	Res	Type
1	C	430	VAL
1	C	431	LYS
1	C	441	SER
1	C	445	VAL
1	C	463	LEU
1	C	473	LYS
1	C	488	CYS
1	C	496	ARG
1	C	497	PHE
1	C	525	VAL
1	C	611	TRP
1	C	616	GLU
1	C	628	PRO
1	C	629	ILE
1	C	688	ASP
1	C	691	LYS
1	C	694	ARG
1	C	698	ILE
1	C	714	ARG
1	D	24	GLU
1	D	36	ARG
1	D	37	ARG
1	D	38	VAL
1	D	46	ASP
1	D	67	LYS
1	D	68	ARG
1	D	87	ILE
1	D	100	ARG
1	D	105	THR
1	D	114	LYS
1	D	119	VAL
1	D	129	GLU
1	D	134	VAL
1	D	140	LEU
1	D	142	GLU
1	D	144	LYS
1	D	161	LEU
1	D	162	VAL
1	D	169	CYS
1	D	177	ARG
1	D	179	VAL
1	D	181	ASP

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Mol	Chain	Res	Type
1	D	185	ASP
1	D	216	LYS
1	D	251	LYS
1	D	252	THR
1	D	260	SER
1	D	265	SER
1	D	278	THR
1	D	279	LEU
1	D	285	ARG
1	D	287	LYS
1	D	289	VAL
1	D	299	ASP
1	D	302	ILE
1	D	311	VAL
1	D	314	LYS
1	D	315	VAL
1	D	316	VAL
1	D	318	THR
1	D	320	ARG
1	D	338	THR
1	D	341	ASP
1	D	342	VAL
1	D	350	VAL
1	D	356	ASP
1	D	358	LEU
1	D	361	VAL
1	D	363	THR
1	D	371	LEU
1	D	374	SER
1	D	383	ASP
1	D	386	VAL
1	D	396	MET
1	D	398	THR
1	D	404	LEU
1	D	410	SER
1	D	418	TYR
1	D	430	VAL
1	D	445	VAL
1	D	463	LEU
1	D	487	ILE
1	D	496	ARG
1	D	501	VAL

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Mol	Chain	Res	Type
1	D	525	VAL
1	D	528	LYS
1	D	537	MET
1	D	572	VAL
1	D	578	ASP
1	D	587	VAL
1	D	602	PRO
1	D	611	TRP
1	D	627	SER
1	D	628	PRO
1	D	629	ILE
1	D	687	SER
1	D	688	ASP
1	D	707	LEU
1	D	709	VAL
1	D	712	LEU
1	E	16	VAL
1	E	55	LEU
1	E	60	LEU
1	E	67	LYS
1	E	70	VAL
1	E	73	LYS
1	E	75	LEU
1	E	79	ILE
1	E	100	ARG
1	E	105	THR
1	E	114	LYS
1	E	117	CYS
1	E	119	VAL
1	E	156	PRO
1	E	162	VAL
1	E	185	ASP
1	E	190	THR
1	E	199	ASN
1	E	227	SER
1	E	241	SER
1	E	251	LYS
1	E	252	THR
1	E	255	ILE
1	E	265	SER
1	E	279	LEU
1	E	285	ARG

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Mol	Chain	Res	Type
1	E	292	THR
1	E	298	THR
1	E	300	THR
1	E	308	ASP
1	E	316	VAL
1	E	317	LEU
1	E	325	ASP
1	E	328	THR
1	E	336	LYS
1	E	350	VAL
1	E	352	SER
1	E	356	ASP
1	E	360	ARG
1	E	361	VAL
1	E	363	THR
1	E	366	LEU
1	E	374	SER
1	E	384	GLU
1	E	392	VAL
1	E	396	MET
1	E	398	THR
1	E	403	LEU
1	E	418	TYR
1	E	424	SER
1	E	434	LYS
1	E	443	ASN
1	E	445	VAL
1	E	447	ARG
1	E	463	LEU
1	E	464	VAL
1	E	471	LEU
1	E	472	LYS
1	E	473	LYS
1	E	487	ILE
1	E	497	PHE
1	E	528	LYS
1	E	552	THR
1	E	607	GLU
1	E	611	TRP
1	E	628	PRO
1	E	632	VAL
1	E	633	ARG

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Mol	Chain	Res	Type
1	E	662	LYS
1	E	679	LEU
1	E	685	SER
1	E	688	ASP
1	E	689	ARG
1	E	698	ILE
1	E	707	LEU
1	E	712	LEU
1	E	714	ARG
1	F	15	GLU
1	F	16	VAL
1	F	49	ARG
1	F	53	GLU
1	F	60	LEU
1	F	67	LYS
1	F	70	VAL
1	F	92	MET
1	F	97	VAL
1	F	105	THR
1	F	106	ARG
1	F	108	VAL
1	F	119	VAL
1	F	132	GLU
1	F	139	LYS
1	F	144	LYS
1	F	145	SER
1	F	162	VAL
1	F	169	CYS
1	F	177	ARG
1	F	179	VAL
1	F	180	ARG
1	F	224	GLN
1	F	241	SER
1	F	251	LYS
1	F	272	LYS
1	F	279	LEU
1	F	285	ARG
1	F	287	LYS
1	F	299	ASP
1	F	300	THR
1	F	311	VAL
1	F	315	VAL

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Mol	Chain	Res	Type
1	F	316	VAL
1	F	320	ARG
1	F	328	THR
1	F	336	LYS
1	F	342	VAL
1	F	352	SER
1	F	356	ASP
1	F	360	ARG
1	F	361	VAL
1	F	363	THR
1	F	364	VAL
1	F	374	SER
1	F	377	LEU
1	F	383	ASP
1	F	384	GLU
1	F	386	VAL
1	F	390	HIS
1	F	393	CYS
1	F	394	SER
1	F	396	MET
1	F	402	SER
1	F	418	TYR
1	F	447	ARG
1	F	472	LYS
1	F	494	ASN
1	F	496	ARG
1	F	497	PHE
1	F	499	PRO
1	F	501	VAL
1	F	518	MET
1	F	525	VAL
1	F	537	MET
1	F	548	SER
1	F	552	THR
1	F	562	ARG
1	F	582	VAL
1	F	587	VAL
1	F	602	PRO
1	F	629	ILE
1	F	633	ARG
1	F	677	MET
1	F	688	ASP

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Mol	Chain	Res	Type
1	F	694	ARG
1	F	695	GLU
1	F	698	ILE
1	F	699	GLN
1	F	711	GLN
1	F	712	LEU
2	H	2	ARG
2	I	2	ARG
2	K	2	ARG
2	L	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	14	HIS
1	A	57	HIS
1	A	224	GLN
1	A	266	HIS
1	A	381	HIS
1	A	390	HIS
1	A	556	GLN
1	A	671	ASN
1	A	699	GLN
1	A	708	ASN
1	B	14	HIS
1	B	59	HIS
1	B	395	GLN
1	B	494	ASN
1	B	556	GLN
1	B	708	ASN
1	C	224	GLN
1	C	266	HIS
1	C	276	HIS
1	C	312	ASN
1	C	494	ASN
1	C	556	GLN
1	C	581	HIS
1	C	671	ASN
1	C	708	ASN
1	D	83	HIS
1	D	266	HIS

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Mol	Chain	Res	Type
1	D	581	HIS
1	D	699	GLN
1	E	14	HIS
1	E	59	HIS
1	E	83	HIS
1	E	683	HIS
1	E	706	HIS
1	F	29	ASN
1	F	83	HIS
1	F	475	ASN
1	F	494	ASN
1	F	545	HIS
1	F	556	GLN
1	F	700	GLN
1	F	708	ASN
1	F	711	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FC0	J	1	2	14,14,15	1.39	1 (7%)	16,17,19	1.42	2 (12%)
2	OAR	H	4	2	10,10,10	1.51	1 (10%)	9,11,11	1.21	1 (11%)
2	OAR	I	4	2	10,10,10	1.60	2 (20%)	9,11,11	1.08	0
2	FC0	G	1	2	14,14,15	1.08	0	16,17,19	1.26	3 (18%)
2	OAR	J	4	2	10,10,10	1.61	1 (10%)	9,11,11	1.41	3 (33%)
2	FC0	L	1	2	14,14,15	1.08	0	16,17,19	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OAR	L	4	2	10,10,10	1.53	1 (10%)	9,11,11	0.49	0
2	FC0	I	1	2	14,14,15	0.87	0	16,17,19	1.15	2 (12%)
2	FC0	H	1	2	14,14,15	1.04	0	16,17,19	1.46	2 (12%)
2	FC0	K	1	2	14,14,15	1.07	0	16,17,19	1.29	1 (6%)
2	OAR	G	4	2	10,10,10	1.63	1 (10%)	9,11,11	1.12	1 (11%)
2	OAR	K	4	2	10,10,10	1.49	2 (20%)	9,11,11	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FC0	J	1	2	-	8/11/11/12	0/1/1/1
2	OAR	H	4	2	1/1/2/3	5/9/9/9	-
2	OAR	J	4	2	1/1/2/3	1/9/9/9	-
2	OAR	I	4	2	1/1/2/3	4/9/9/9	-
2	FC0	G	1	2	-	5/11/11/12	0/1/1/1
2	FC0	L	1	2	-	1/11/11/12	0/1/1/1
2	OAR	L	4	2	1/1/2/3	5/9/9/9	-
2	FC0	I	1	2	-	5/11/11/12	0/1/1/1
2	FC0	H	1	2	-	7/11/11/12	0/1/1/1
2	FC0	K	1	2	-	7/11/11/12	0/1/1/1
2	OAR	G	4	2	1/1/2/3	3/9/9/9	-
2	OAR	K	4	2	1/1/2/3	2/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	OAR	O-C	-4.61	1.23	1.42
2	I	4	OAR	O-C	-4.40	1.23	1.42
2	L	4	OAR	O-C	-4.37	1.24	1.42
2	H	4	OAR	O-C	-4.16	1.25	1.42
2	J	4	OAR	O-C	-4.11	1.25	1.42
2	K	4	OAR	O-C	-4.09	1.25	1.42
2	J	1	FC0	CA-N	2.74	1.49	1.45
2	I	4	OAR	CZ-NH1	-2.05	1.26	1.34
2	K	4	OAR	CZ-NH1	-2.04	1.26	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FC0	CA-N-C1	-3.90	116.82	122.82
2	G	1	FC0	O1-C1-N	-3.08	117.37	125.32
2	K	1	FC0	O1-C1-N	-3.01	117.54	125.32
2	H	4	OAR	CB-CA-C	2.99	116.35	112.25
2	J	1	FC0	CG-CB-CA	2.63	120.35	113.36
2	I	1	FC0	O1-C1-N	-2.62	118.54	125.32
2	J	4	OAR	CG-CB-CA	-2.48	103.28	116.12
2	G	4	OAR	CB-CA-C	-2.43	108.93	112.25
2	H	1	FC0	CB-CA-C	2.30	115.92	110.45
2	J	1	FC0	OXT-C-O	-2.24	119.00	124.08
2	J	4	OAR	CG-CD-NE	-2.21	105.99	112.20
2	L	1	FC0	CA-N-C1	-2.21	119.43	122.82
2	I	1	FC0	OXT-C-CA	2.14	120.76	113.51
2	J	4	OAR	O-C-CA	2.09	119.57	111.52
2	G	1	FC0	OXT-C-CA	2.09	120.57	113.51
2	G	1	FC0	C-CA-N	2.01	115.21	110.56

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	4	OAR	CA
2	H	4	OAR	CA
2	I	4	OAR	CA
2	J	4	OAR	CA
2	K	4	OAR	CA
2	L	4	OAR	CA

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	FC0	C-CA-CB-CG
2	G	1	FC0	O1-C1-N-CA
2	G	4	OAR	C-CA-CB-CG
2	H	1	FC0	O1-C1-N-CA
2	H	4	OAR	NH1-CZ-NE-CD
2	H	4	OAR	O-C-CA-N
2	H	4	OAR	O-C-CA-CB
2	I	1	FC0	C-CA-N-C1
2	I	1	FC0	O1-C1-N-CA
2	I	4	OAR	C-CA-CB-CG
2	J	1	FC0	O1-C1-N-CA

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Mol	Chain	Res	Type	Atoms
2	J	4	OAR	O-C-CA-CB
2	K	1	FC0	C-CA-CB-CG
2	K	1	FC0	O1-C1-N-CA
2	K	4	OAR	O-C-CA-CB
2	L	1	FC0	O1-C1-N-CA
2	L	4	OAR	NH1-CZ-NE-CD
2	L	4	OAR	NH2-CZ-NE-CD
2	L	4	OAR	O-C-CA-N
2	L	4	OAR	O-C-CA-CB
2	K	1	FC0	N-CA-CB-CG
2	H	1	FC0	C-CA-CB-CG
2	G	4	OAR	NE-CD-CG-CB
2	G	1	FC0	N-CA-CB-CG
2	I	4	OAR	NE-CD-CG-CB
2	H	1	FC0	N-CA-CB-CG
2	I	1	FC0	C-CA-CB-CG
2	J	1	FC0	C-CA-CB-CG
2	I	1	FC0	N-CA-CB-CG
2	H	1	FC0	CA-CB-CG-CD2
2	H	1	FC0	CA-CB-CG-CD1
2	J	1	FC0	CA-CB-CG-CD1
2	J	1	FC0	CA-CB-CG-CD2
2	G	1	FC0	CA-CB-CG-CD2
2	G	1	FC0	CA-CB-CG-CD1
2	J	1	FC0	CB-CA-N-C1
2	K	1	FC0	OXT-C-CA-CB
2	K	1	FC0	O-C-CA-CB
2	H	4	OAR	NH2-CZ-NE-CD
2	H	4	OAR	CG-CD-NE-CZ
2	I	4	OAR	O-C-CA-CB
2	L	4	OAR	CG-CD-NE-CZ
2	J	1	FC0	N-CA-CB-CG
2	H	1	FC0	OXT-C-CA-CB
2	K	4	OAR	O-C-CA-N
2	H	1	FC0	O-C-CA-CB
2	I	1	FC0	CB-CA-N-C1
2	K	1	FC0	CA-CB-CG-CD2
2	J	1	FC0	OXT-C-CA-CB
2	J	1	FC0	O-C-CA-CB
2	K	1	FC0	CA-CB-CG-CD1
2	G	4	OAR	O-C-CA-CB
2	I	4	OAR	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	FC0	4	0
2	H	4	OAR	1	0
2	G	1	FC0	1	0
2	K	1	FC0	1	0

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

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	710/715 (99%)	-0.03	5 (0%) 84 80	33, 45, 64, 79	0
1	B	710/715 (99%)	0.03	5 (0%) 84 80	34, 49, 78, 108	0
1	C	710/715 (99%)	0.26	8 (1%) 78 73	44, 62, 94, 109	0
1	D	710/715 (99%)	0.11	3 (0%) 88 87	38, 54, 79, 93	0
1	E	710/715 (99%)	0.25	8 (1%) 78 73	37, 63, 106, 130	0
1	F	710/715 (99%)	0.33	20 (2%) 55 46	38, 66, 115, 144	0
2	G	2/4 (50%)	0.33	0 100 100	29, 29, 29, 58	0
2	H	2/4 (50%)	0.63	0 100 100	29, 29, 29, 55	0
2	I	2/4 (50%)	1.04	0 100 100	42, 42, 42, 66	0
2	J	2/4 (50%)	0.92	0 100 100	38, 38, 38, 60	0
2	K	2/4 (50%)	1.28	1 (50%) 0 0	33, 33, 33, 65	0
2	L	2/4 (50%)	0.59	0 100 100	39, 39, 39, 62	0
All	All	4272/4314 (99%)	0.16	50 (1%) 76 71	29, 55, 97, 144	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	686	ALA	4.9
1	F	686	ALA	4.7
1	D	686	ALA	4.1
1	C	686	ALA	4.0
1	F	423	LEU	3.7
1	F	368	PRO	3.6
1	B	686	ALA	3.4
1	A	687	SER	3.3
1	C	687	SER	3.3
1	F	209	ASP	3.3
1	F	418	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	ASP	3.1
1	C	684	PHE	2.9
1	A	689	ARG	2.8
1	E	87	ILE	2.8
1	C	209	ASP	2.8
1	B	423	LEU	2.7
1	A	400	ASP	2.7
1	F	97	VAL	2.7
1	A	686	ALA	2.6
1	A	209	ASP	2.6
1	E	423	LEU	2.5
1	F	690	TYR	2.4
1	C	381	HIS	2.4
1	F	385	PRO	2.4
1	F	687	SER	2.4
1	E	5	ARG	2.4
1	F	6	GLY	2.3
2	K	2	ARG	2.3
1	B	367	GLY	2.3
1	E	121	ALA	2.3
1	F	139	LYS	2.3
1	F	711	GLN	2.2
1	E	128	GLY	2.2
1	E	340	ASP	2.2
1	F	5	ARG	2.2
1	F	122	GLY	2.2
1	F	375	ALA	2.2
1	F	100	ARG	2.1
1	B	368	PRO	2.1
1	D	401	ALA	2.1
1	C	688	ASP	2.1
1	C	438	GLY	2.1
1	D	209	ASP	2.1
1	C	210	ALA	2.1
1	F	129	GLU	2.1
1	F	381	HIS	2.0
1	E	400	ASP	2.0
1	F	87	ILE	2.0
1	F	362	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FC0	H	1	14/15	0.67	0.24	68,81,87,88	0
2	FC0	K	1	14/15	0.70	0.22	72,83,84,84	0
2	FC0	L	1	14/15	0.72	0.27	74,88,91,91	0
2	FC0	I	1	14/15	0.73	0.20	70,84,87,88	0
2	FC0	G	1	14/15	0.75	0.21	69,77,79,80	0
2	FC0	J	1	14/15	0.75	0.21	65,83,86,86	0
2	OAR	H	4	11/11	0.94	0.10	23,27,32,33	0
2	OAR	I	4	11/11	0.95	0.09	19,25,35,37	0
2	OAR	G	4	11/11	0.96	0.09	16,18,27,28	0
2	OAR	K	4	11/11	0.96	0.08	19,25,30,30	0
2	OAR	J	4	11/11	0.96	0.07	20,23,27,31	0
2	OAR	L	4	11/11	0.96	0.09	24,26,35,38	0

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.