



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:00 PM UTC

PDB ID : 3HVD / pdb_00003hvd
Title : The Protective Antigen Component of Anthrax Toxin Forms Functional Octameric Complexes
Authors : Kintzer, A.F.; Dong, K.C.; Berger, J.M.; Krantz, B.A.
Deposited on : 2009-06-15
Resolution : 3.21 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

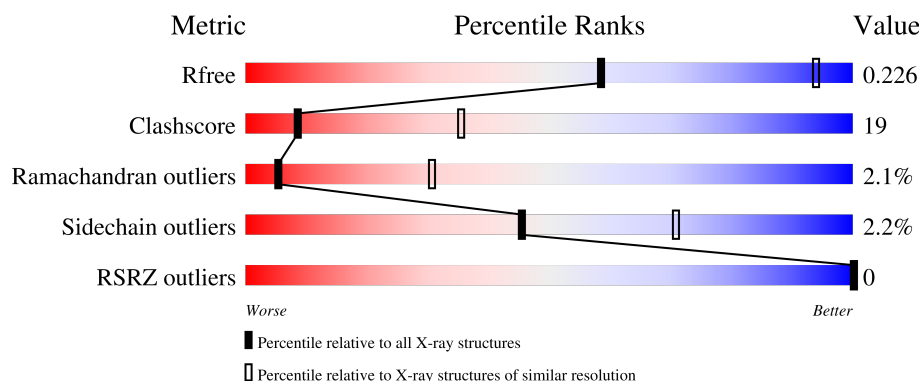
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	548	56% 36% • 5%
1	B	548	58% 34% • 5%
1	C	548	57% 36% • 6%
1	D	548	59% 34% • 5%
1	E	548	55% 37% • 5%

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Mol	Chain	Length	Quality of chain
1	F	548	 58% 34% • 5%
1	G	548	 54% 38% • 5%
1	H	548	 57% 35% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32701 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 Protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4067	2555	698	808	6			
1	B	523	Total	C	N	O	S	0	0	0
			4075	2555	704	810	6			
1	C	517	Total	C	N	O	S	0	0	0
			4078	2562	701	809	6			
1	D	518	Total	C	N	O	S	0	0	0
			4066	2554	698	808	6			
1	E	519	Total	C	N	O	S	0	0	0
			4091	2568	703	814	6			
1	F	519	Total	C	N	O	S	0	0	0
			4098	2572	706	814	6			
1	G	518	Total	C	N	O	S	0	0	0
			4094	2570	703	815	6			
1	H	518	Total	C	N	O	S	0	0	0
			4108	2578	704	820	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	PRO	VAL	engineered mutation	UNP Q08G54
A	324	GLY	HIS	engineered mutation	UNP Q08G54
A	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
B	303	PRO	VAL	engineered mutation	UNP Q08G54
B	304	GLY	HIS	engineered mutation	UNP Q08G54
B	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
C	323	PRO	VAL	engineered mutation	UNP Q08G54
C	324	GLY	HIS	engineered mutation	UNP Q08G54
C	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
D	323	PRO	VAL	engineered mutation	UNP Q08G54
D	324	GLY	HIS	engineered mutation	UNP Q08G54
D	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
E	303	PRO	VAL	engineered mutation	UNP Q08G54

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Chain	Residue	Modelled	Actual	Comment	Reference
E	324	GLY	HIS	engineered mutation	UNP Q08G54
E	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
F	323	PRO	VAL	engineered mutation	UNP Q08G54
F	324	GLY	HIS	engineered mutation	UNP Q08G54
F	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
G	323	PRO	VAL	engineered mutation	UNP Q08G54
G	324	GLY	HIS	engineered mutation	UNP Q08G54
G	669	ARG	GLN	SEE REMARK 999	UNP Q08G54
H	323	PRO	VAL	engineered mutation	UNP Q08G54
H	324	GLY	HIS	engineered mutation	UNP Q08G54
H	669	ARG	GLN	SEE REMARK 999	UNP Q08G54

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0
2	G	2	Total Ca 2 2	0	0
2	H	2	Total Ca 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

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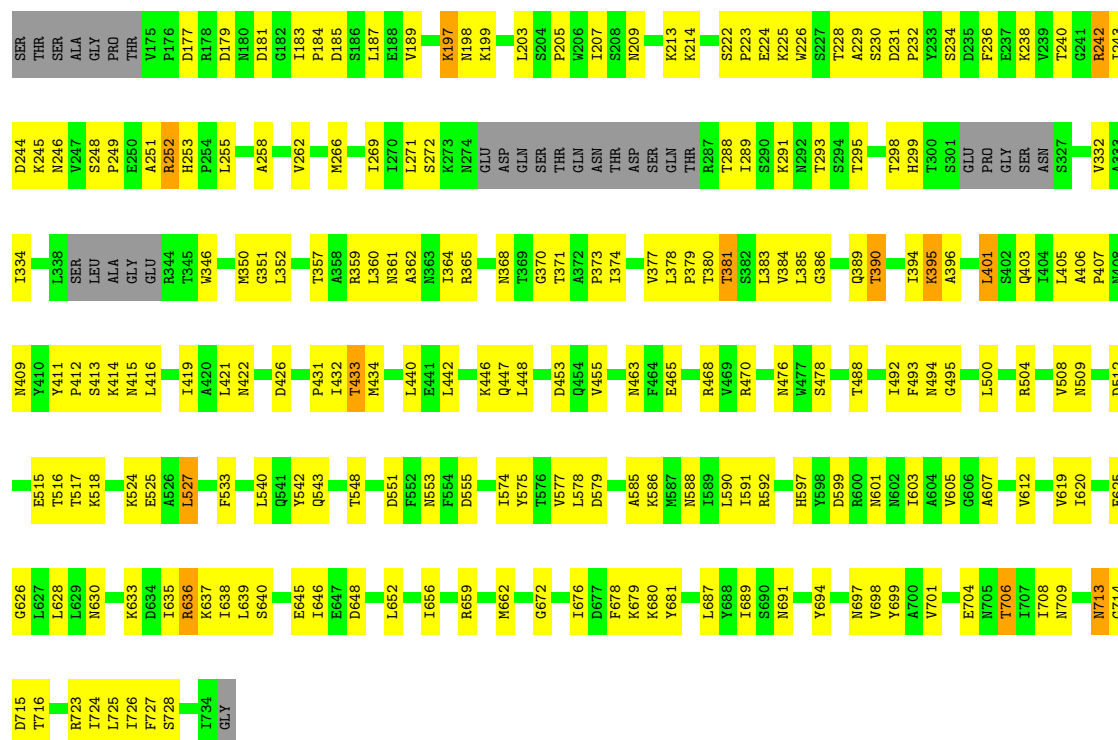
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

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.

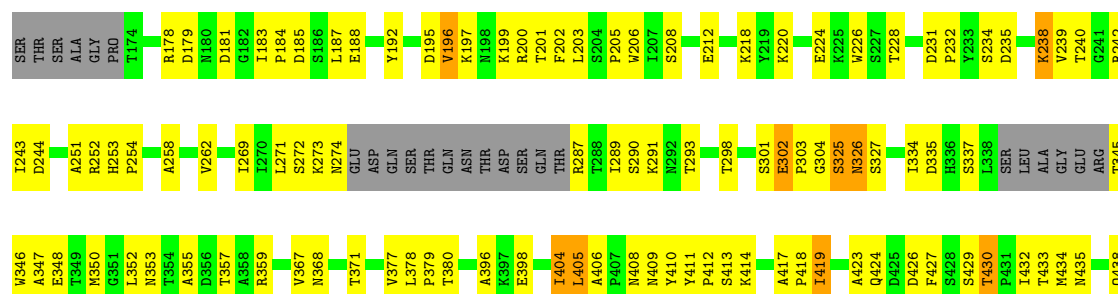
• Molecule 1: Protective antigen

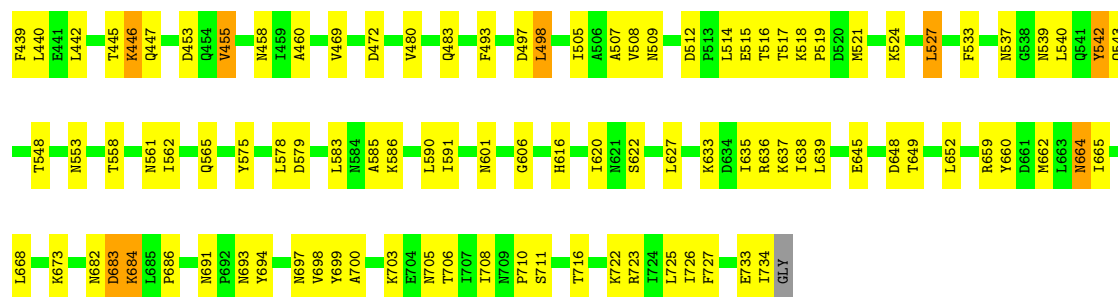
Chain A: 



• Molecule 1: Protective antigen

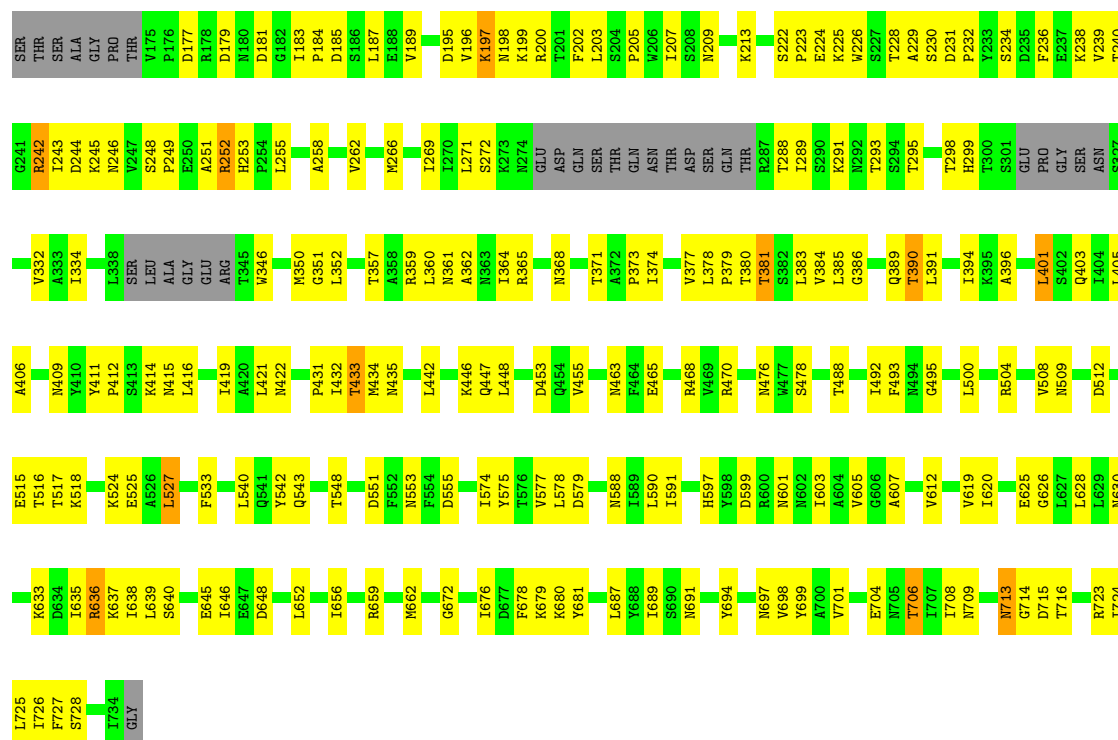
Chain B: 





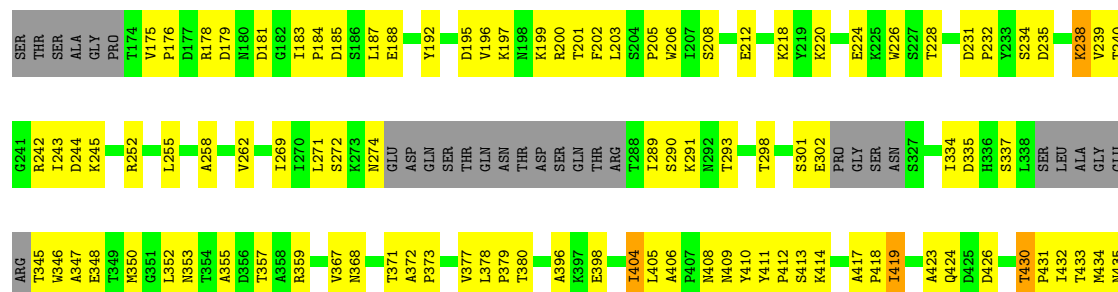
• Molecule 1: Protective antigen

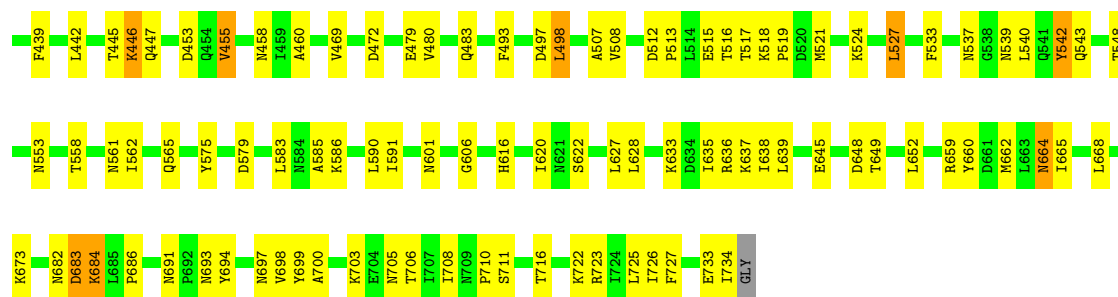
Chain C: 57% 36% 6%



• Molecule 1: Protective antigen

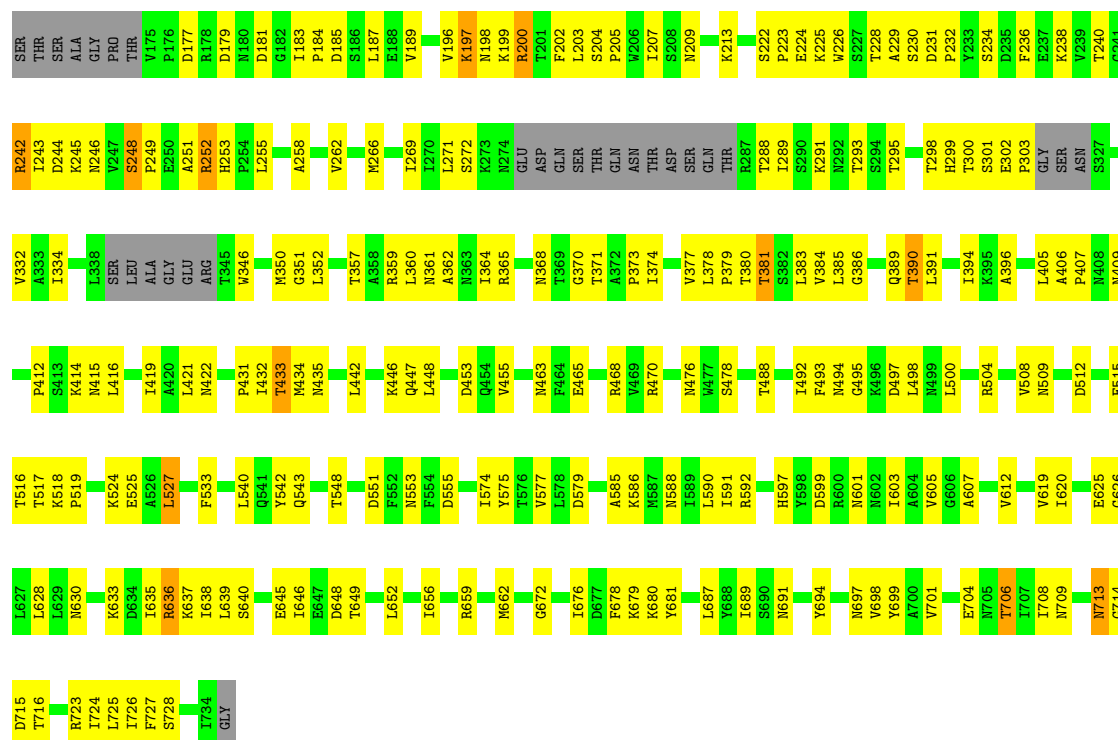
Chain D: 59% 34% 5%





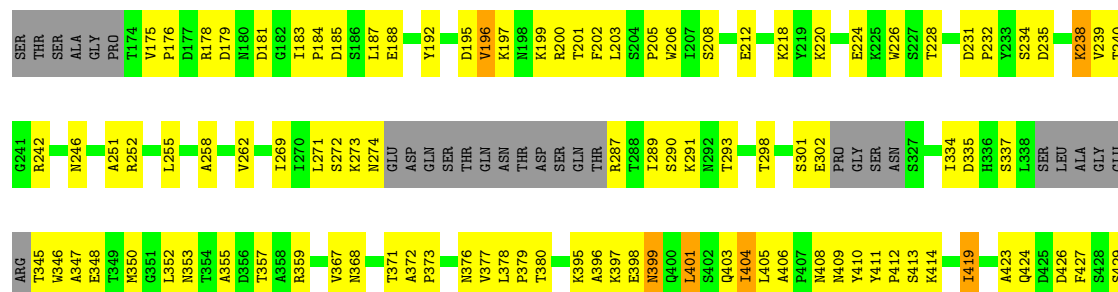
• Molecule 1: Protective antigen

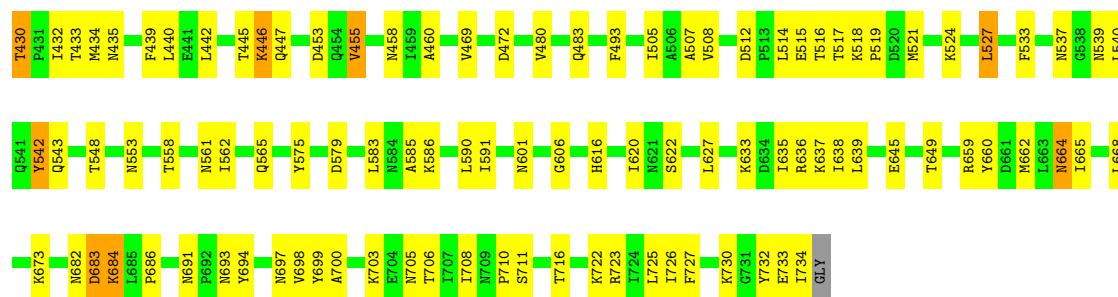
Chain E: 55% 37% 5%



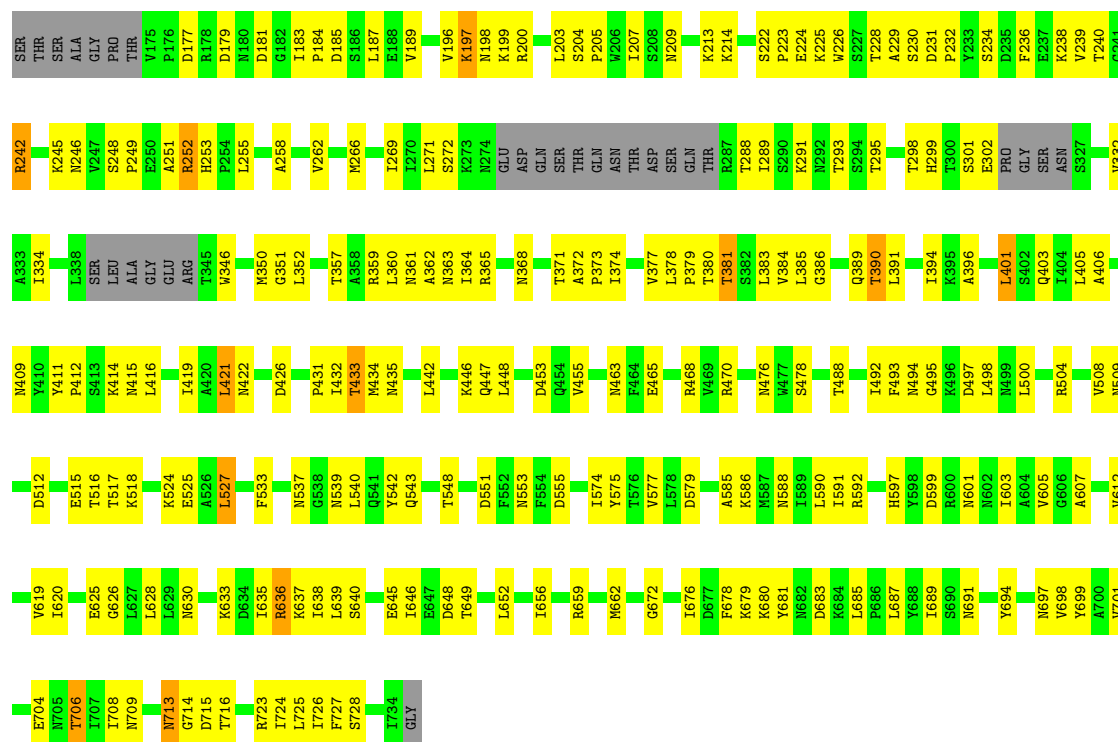
• Molecule 1: Protective antigen

Chain F: 58% 34% 5%

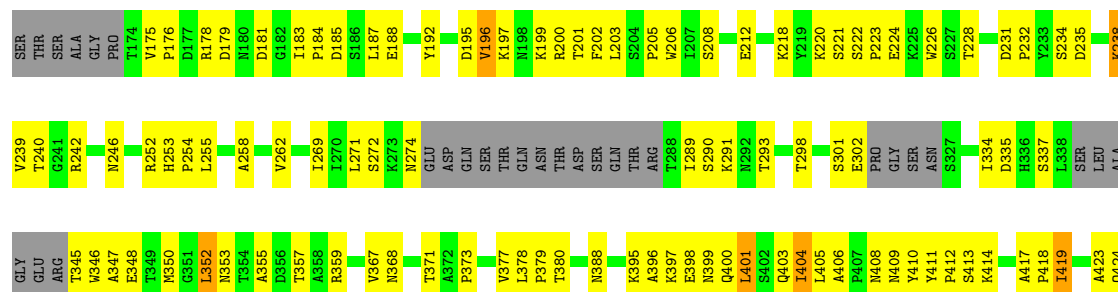




- Molecule 1: Protective antigen



- Molecule 1: Protective antigen



D425	D426		T430	P431	I432	T433	M434	M435		F439		L442		T445	K446	Q447		D453	Q454	V455		N458	I459	A460		V469		D472		V480		Q483		F493		D497	L498		I505	A506	A507	V508		D512	P513	L514	E515	T516	T517	K518	P519	D520	M521		K524		L527		F533
	N537	G538	N539	L540	Q541	Y542	Q543		T548		N553		T558		N561	I562		Q565		Y575		D579		L583	N584	A585	K586		L590	I591		N601		G606		H616		I620	N621	S622		L627	L628		K633	D634	I635	R636	K637	I638	L639		E645		D648	T649		L652	
R659	Y660	D661	M662	L663	N664	I665		L668		K673		N682	D683	K684	L685	P686		N691	P692	N693	Y694		N697	V698	Y699	A700		K703	E704	N705	T706	I707	I708	N709	P710	S711		T716		K722	R723	I724	L725	I726	F727		E733	I734	GLY										

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	125.60Å 125.67Å 125.82Å 106.64° 110.82° 110.98°	Depositor
Resolution (Å)	47.27 – 3.21 47.27 – 3.21	Depositor EDS
% Data completeness (in resolution range)	90.3 (47.27-3.21) 90.2 (47.27-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2009_02_15_2320_3)	Depositor
R, R_{free}	0.210 , 0.249 0.190 , 0.226	Depositor DCC
R_{free} test set	1840 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.438 for -l,-h,h+k+l 0.438 for -k,h+k+l,-h 0.032 for k,h,-h-k-l 0.458 for -h-k-l,l,k 0.033 for h+k+l,-k,-l 0.033 for l,-h-k-l,h 0.032 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32701	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.31	0/4136	0.75	2/5617 (0.0%)
1	B	0.31	0/4144	0.78	8/5632 (0.1%)
1	C	0.31	0/4147	0.75	2/5629 (0.0%)
1	D	0.30	0/4134	0.76	4/5614 (0.1%)
1	E	0.31	0/4161	0.75	4/5650 (0.1%)
1	F	0.30	0/4167	0.76	4/5655 (0.1%)
1	G	0.31	0/4163	0.75	2/5650 (0.0%)
1	H	0.30	0/4177	0.76	4/5667 (0.1%)
All	All	0.31	0/33229	0.76	30/45114 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	GLU	CA-C-N	6.62	128.12	119.84
1	B	302	GLU	C-N-CA	6.62	128.12	119.84
1	H	426	ASP	N-CA-C	-5.94	106.65	114.31
1	B	426	ASP	N-CA-C	-5.93	106.66	114.31
1	D	426	ASP	N-CA-C	-5.93	106.66	114.31
1	F	426	ASP	N-CA-C	-5.54	107.16	114.31
1	E	509	ASN	CA-C-N	5.42	126.62	119.84
1	E	509	ASN	C-N-CA	5.42	126.62	119.84
1	A	509	ASN	CA-C-N	5.41	126.60	119.84
1	A	509	ASN	C-N-CA	5.41	126.60	119.84
1	H	665	ILE	N-CA-C	5.41	117.40	112.43
1	C	509	ASN	CA-C-N	5.39	126.58	119.84
1	C	509	ASN	C-N-CA	5.39	126.58	119.84
1	G	509	ASN	CA-C-N	5.39	126.57	119.84
1	G	509	ASN	C-N-CA	5.39	126.57	119.84
1	B	430	THR	CA-C-N	5.38	125.37	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	430	THR	C-N-CA	5.38	125.37	120.21
1	B	665	ILE	N-CA-C	5.34	117.34	112.43
1	H	430	THR	CA-C-N	5.31	125.31	120.21
1	H	430	THR	C-N-CA	5.31	125.31	120.21
1	E	248	SER	CA-C-N	5.29	124.47	118.97
1	E	248	SER	C-N-CA	5.29	124.47	118.97
1	F	430	THR	CA-C-N	5.29	125.29	120.21
1	F	430	THR	C-N-CA	5.29	125.29	120.21
1	D	430	THR	CA-C-N	5.20	125.20	120.21
1	D	430	THR	C-N-CA	5.20	125.20	120.21
1	D	665	ILE	N-CA-C	5.15	117.17	112.43
1	F	665	ILE	N-CA-C	5.14	117.16	112.43
1	B	509	ASN	CA-C-N	5.06	126.17	119.84
1	B	509	ASN	C-N-CA	5.06	126.17	119.84

There are no chirality outliers.

There are no planarity outliers.

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	4067	0	4005	167	0
1	B	4075	0	3995	149	0
1	C	4078	0	4036	166	0
1	D	4066	0	4005	147	0
1	E	4091	0	4035	166	0
1	F	4098	0	4057	153	0
1	G	4094	0	4050	175	0
1	H	4108	0	4078	158	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	32701	0	32261	1229	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 19.

All (1229) 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:H:648:ASP:HB3	1:H:652:LEU:HB3	1.40	1.03
1:D:648:ASP:HB3	1:D:652:LEU:HB3	1.48	0.94
1:B:274:ASN:HD21	1:B:359:ARG:HB3	1.32	0.92
1:B:187:LEU:HD21	1:B:205:PRO:HG3	1.53	0.90
1:B:231:ASP:HB2	1:B:232:PRO:HD2	1.55	0.89
1:F:187:LEU:HD21	1:F:205:PRO:HG3	1.52	0.89
1:H:187:LEU:HD21	1:H:205:PRO:HG3	1.54	0.89
1:H:231:ASP:HB2	1:H:232:PRO:HD2	1.54	0.89
1:D:187:LEU:HD21	1:D:205:PRO:HG3	1.54	0.89
1:D:231:ASP:HB2	1:D:232:PRO:HD2	1.54	0.88
1:F:231:ASP:HB2	1:F:232:PRO:HD2	1.54	0.88
1:F:345:THR:HB	1:F:348:GLU:HG2	1.58	0.85
1:F:399:ASN:HD22	1:F:399:ASN:H	1.23	0.85
1:B:274:ASN:ND2	1:B:359:ARG:HB3	1.92	0.85
1:F:524:LYS:HD3	1:F:579:ASP:HB3	1.59	0.84
1:D:345:THR:HB	1:D:348:GLU:HG2	1.59	0.84
1:D:524:LYS:HD3	1:D:579:ASP:HB3	1.60	0.84
1:H:345:THR:HB	1:H:348:GLU:HG2	1.59	0.83
1:B:345:THR:HB	1:B:348:GLU:HG2	1.59	0.83
1:H:524:LYS:HD3	1:H:579:ASP:HB3	1.59	0.83
1:B:524:LYS:HD3	1:B:579:ASP:HB3	1.59	0.82
1:H:401:LEU:HG	1:H:401:LEU:O	1.79	0.80
1:G:242:ARG:HH11	1:G:242:ARG:HG3	1.47	0.79
1:E:236:PHE:O	1:E:240:THR:HG22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:ARG:HG3	1:E:242:ARG:HH11	1.47	0.78
1:C:242:ARG:HG3	1:C:242:ARG:HH11	1.48	0.78
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.47	0.78
1:G:249:PRO:O	1:G:252:ARG:HB2	1.85	0.76
1:A:236:PHE:O	1:A:240:THR:HG22	1.85	0.76
1:A:378:LEU:HD13	1:A:401:LEU:HD12	1.67	0.75
1:E:249:PRO:O	1:E:252:ARG:HB2	1.86	0.75
1:G:236:PHE:O	1:G:240:THR:HG22	1.86	0.75
1:C:249:PRO:O	1:C:252:ARG:HB2	1.85	0.75
1:H:240:THR:HG23	1:H:242:ARG:H	1.52	0.75
1:A:249:PRO:O	1:A:252:ARG:HB2	1.86	0.75
1:C:365:ARG:HH11	1:C:414:LYS:HD2	1.52	0.74
1:C:378:LEU:HD13	1:C:401:LEU:HD12	1.68	0.74
1:C:236:PHE:O	1:C:240:THR:HG22	1.86	0.74
1:A:365:ARG:HH11	1:A:414:LYS:HD2	1.53	0.74
1:C:245:LYS:H	1:D:483:GLN:HE22	1.36	0.74
1:D:433:THR:HG22	1:D:434:MET:H	1.53	0.74
1:F:240:THR:HG23	1:F:242:ARG:H	1.53	0.74
1:H:433:THR:HG22	1:H:434:MET:H	1.53	0.74
1:F:399:ASN:HD22	1:F:399:ASN:N	1.84	0.73
1:G:245:LYS:H	1:H:483:GLN:HE22	1.36	0.73
1:G:365:ARG:HH11	1:G:414:LYS:HD2	1.54	0.73
1:D:240:THR:HG23	1:D:242:ARG:H	1.53	0.73
1:E:648:ASP:HB2	1:E:652:LEU:HB2	1.71	0.73
1:B:433:THR:HG22	1:B:434:MET:H	1.52	0.73
1:C:524:LYS:HD3	1:C:579:ASP:HB3	1.71	0.73
1:F:433:THR:HG22	1:F:434:MET:H	1.53	0.73
1:G:648:ASP:HB2	1:G:652:LEU:HB2	1.71	0.73
1:E:365:ARG:HH11	1:E:414:LYS:HD2	1.53	0.72
1:F:184:PRO:HD2	1:F:187:LEU:HD12	1.71	0.72
1:A:231:ASP:HB2	1:A:232:PRO:HD3	1.72	0.72
1:G:524:LYS:HD3	1:G:579:ASP:HB3	1.71	0.72
1:C:648:ASP:HB2	1:C:652:LEU:HB2	1.71	0.71
1:E:524:LYS:HD3	1:E:579:ASP:HB3	1.71	0.71
1:A:648:ASP:HB2	1:A:652:LEU:HB2	1.71	0.71
1:B:240:THR:HG23	1:B:242:ARG:H	1.54	0.71
1:B:184:PRO:HD2	1:B:187:LEU:HD12	1.72	0.71
1:A:524:LYS:HD3	1:A:579:ASP:HB3	1.71	0.71
1:G:187:LEU:HD21	1:G:205:PRO:HG3	1.71	0.71
1:A:648:ASP:HB3	1:A:652:LEU:H	1.56	0.71
1:C:231:ASP:HB2	1:C:232:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:ASP:HB2	1:E:232:PRO:HD3	1.72	0.71
1:G:262:VAL:HG11	1:G:379:PRO:HG2	1.72	0.71
1:D:184:PRO:HD2	1:D:187:LEU:HD12	1.73	0.71
1:C:187:LEU:HD21	1:C:205:PRO:HG3	1.72	0.71
1:A:228:THR:HG23	1:A:518:LYS:HG2	1.73	0.70
1:A:262:VAL:HG11	1:A:379:PRO:HG2	1.74	0.70
1:G:231:ASP:HB2	1:G:232:PRO:HD3	1.71	0.70
1:G:648:ASP:HB3	1:G:652:LEU:H	1.56	0.70
1:C:262:VAL:HG11	1:C:379:PRO:HG2	1.73	0.70
1:E:187:LEU:HD21	1:E:205:PRO:HG3	1.73	0.70
1:B:298:THR:HB	1:B:601:ASN:HB3	1.74	0.70
1:H:184:PRO:HD2	1:H:187:LEU:HD12	1.73	0.69
1:H:298:THR:HB	1:H:601:ASN:HB3	1.74	0.69
1:E:648:ASP:HB3	1:E:652:LEU:H	1.56	0.69
1:G:242:ARG:HH11	1:G:242:ARG:CG	2.05	0.69
1:E:262:VAL:HG11	1:E:379:PRO:HG2	1.73	0.69
1:A:533:PHE:HB3	1:A:540:LEU:HD11	1.75	0.69
1:E:533:PHE:HB3	1:E:540:LEU:HD11	1.75	0.69
1:C:228:THR:HG23	1:C:518:LYS:HG2	1.74	0.69
1:H:274:ASN:HD21	1:H:359:ARG:HB3	1.55	0.69
1:A:187:LEU:HD21	1:A:205:PRO:HG3	1.72	0.69
1:D:298:THR:HB	1:D:601:ASN:HB3	1.74	0.69
1:F:298:THR:HB	1:F:601:ASN:HB3	1.74	0.69
1:C:533:PHE:HB3	1:C:540:LEU:HD11	1.75	0.68
1:E:228:THR:HG23	1:E:518:LYS:HG2	1.74	0.68
1:G:228:THR:HG23	1:G:518:LYS:HG2	1.74	0.68
1:C:231:ASP:HB2	1:C:232:PRO:CD	2.24	0.68
1:E:242:ARG:HH11	1:E:242:ARG:CG	2.06	0.68
1:E:231:ASP:HB2	1:E:232:PRO:CD	2.24	0.68
1:D:291:LYS:HB3	1:D:335:ASP:HB3	1.76	0.68
1:E:245:LYS:H	1:F:483:GLN:HE22	1.39	0.67
1:A:242:ARG:HH11	1:A:242:ARG:CG	2.06	0.67
1:C:242:ARG:HH11	1:C:242:ARG:CG	2.06	0.67
1:H:291:LYS:HB3	1:H:335:ASP:HB3	1.76	0.67
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.24	0.67
1:C:648:ASP:HB3	1:C:652:LEU:H	1.56	0.67
1:G:231:ASP:HB2	1:G:232:PRO:CD	2.24	0.67
1:F:291:LYS:HB3	1:F:335:ASP:HB3	1.77	0.67
1:A:245:LYS:H	1:B:483:GLN:HE22	1.41	0.67
1:B:648:ASP:CB	1:B:652:LEU:HB3	2.25	0.67
1:G:533:PHE:HB3	1:G:540:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LYS:O	1:B:706:THR:HG22	1.95	0.66
1:A:659:ARG:HA	1:A:716:THR:O	1.96	0.66
1:H:703:LYS:O	1:H:706:THR:HG22	1.95	0.66
1:D:703:LYS:O	1:D:706:THR:HG22	1.96	0.66
1:F:703:LYS:O	1:F:706:THR:HG22	1.96	0.66
1:A:713:ASN:HD21	1:A:715:ASP:HB2	1.61	0.65
1:B:291:LYS:HB3	1:B:335:ASP:HB3	1.77	0.65
1:C:713:ASN:HD21	1:C:715:ASP:HB2	1.61	0.65
1:B:410:TYR:CE1	1:B:414:LYS:HE2	2.31	0.65
1:C:701:VAL:HG12	1:C:706:THR:HG22	1.79	0.65
1:G:713:ASN:HD21	1:G:715:ASP:HB2	1.61	0.65
1:H:410:TYR:CE1	1:H:414:LYS:HE2	2.32	0.65
1:A:662:MET:HE3	1:A:681:TYR:HD1	1.62	0.65
1:F:410:TYR:CE1	1:F:414:LYS:HE2	2.32	0.65
1:C:659:ARG:HA	1:C:716:THR:O	1.96	0.65
1:E:659:ARG:HA	1:E:716:THR:O	1.97	0.65
1:G:298:THR:HG22	1:G:603:ILE:HD11	1.79	0.65
1:E:713:ASN:HD21	1:E:715:ASP:HB2	1.61	0.65
1:F:423:ALA:HB1	1:F:430:THR:O	1.97	0.65
1:G:636:ARG:HA	1:G:639:LEU:HD13	1.78	0.65
1:E:701:VAL:HG12	1:E:706:THR:HG22	1.79	0.64
1:F:700:ALA:HB2	1:F:726:ILE:HD11	1.79	0.64
1:H:700:ALA:HB2	1:H:726:ILE:CD1	2.27	0.64
1:A:298:THR:HG22	1:A:603:ILE:HD11	1.79	0.64
1:B:423:ALA:HB1	1:B:430:THR:O	1.98	0.64
1:D:700:ALA:HB2	1:D:726:ILE:CD1	2.28	0.64
1:A:603:ILE:O	1:A:605:VAL:HG23	1.97	0.64
1:B:700:ALA:HB2	1:B:726:ILE:CD1	2.27	0.64
1:E:298:THR:HG22	1:E:603:ILE:HD11	1.78	0.64
1:E:662:MET:HE3	1:E:681:TYR:HD1	1.62	0.64
1:C:298:THR:HG22	1:C:603:ILE:HD11	1.79	0.64
1:F:700:ALA:HB2	1:F:726:ILE:CD1	2.27	0.64
1:G:659:ARG:HA	1:G:716:THR:O	1.97	0.64
1:A:488:THR:OG1	1:A:504:ARG:HD3	1.98	0.64
1:D:423:ALA:HB1	1:D:430:THR:O	1.98	0.64
1:G:197:LYS:HG3	1:G:198:ASN:N	2.13	0.64
1:H:648:ASP:CB	1:H:652:LEU:HB3	2.23	0.64
1:C:636:ARG:HA	1:C:639:LEU:HD13	1.79	0.64
1:H:700:ALA:HB2	1:H:726:ILE:HD11	1.79	0.64
1:A:701:VAL:HG12	1:A:706:THR:HG22	1.79	0.63
1:D:699:TYR:HD1	1:D:725:LEU:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:636:ARG:HA	1:E:639:LEU:HD13	1.79	0.63
1:C:662:MET:HE3	1:C:681:TYR:HD1	1.62	0.63
1:H:423:ALA:HB1	1:H:430:THR:O	1.98	0.63
1:A:636:ARG:HA	1:A:639:LEU:HD13	1.79	0.63
1:B:700:ALA:HB2	1:B:726:ILE:HD11	1.79	0.63
1:C:524:LYS:HG3	1:C:540:LEU:HD22	1.80	0.63
1:E:603:ILE:O	1:E:605:VAL:HG23	1.98	0.63
1:G:240:THR:HG23	1:G:242:ARG:H	1.64	0.63
1:G:701:VAL:HG12	1:G:706:THR:HG22	1.79	0.63
1:B:699:TYR:HD1	1:B:725:LEU:HA	1.63	0.63
1:D:410:TYR:CE1	1:D:414:LYS:HE2	2.33	0.63
1:D:648:ASP:CB	1:D:652:LEU:HB3	2.24	0.63
1:G:603:ILE:O	1:G:605:VAL:HG23	1.97	0.63
1:A:181:ASP:O	1:A:236:PHE:HB2	1.99	0.63
1:A:512:ASP:HB3	1:A:515:GLU:HB2	1.81	0.63
1:A:553:ASN:HB2	1:A:590:LEU:HB3	1.80	0.63
1:B:710:PRO:HG3	1:B:716:THR:HG22	1.81	0.63
1:E:553:ASN:HB2	1:E:590:LEU:HB3	1.80	0.63
1:G:662:MET:HE3	1:G:681:TYR:HD1	1.63	0.63
1:C:488:THR:OG1	1:C:504:ARG:HD3	1.99	0.63
1:D:622:SER:HB3	1:D:734:ILE:CG1	2.29	0.63
1:G:488:THR:OG1	1:G:504:ARG:HD3	1.98	0.63
1:C:603:ILE:O	1:C:605:VAL:HG23	1.97	0.63
1:H:699:TYR:HD1	1:H:725:LEU:HA	1.63	0.63
1:E:659:ARG:HB2	1:E:662:MET:SD	2.39	0.63
1:D:700:ALA:HB2	1:D:726:ILE:HD11	1.80	0.62
1:E:512:ASP:HB3	1:E:515:GLU:HB2	1.81	0.62
1:F:622:SER:HB3	1:F:734:ILE:CG1	2.29	0.62
1:G:197:LYS:HG3	1:G:198:ASN:H	1.63	0.62
1:H:710:PRO:HG3	1:H:716:THR:HG22	1.81	0.62
1:B:691:ASN:HB3	1:B:694:TYR:CE1	2.34	0.62
1:F:691:ASN:HB3	1:F:694:TYR:CE1	2.35	0.62
1:G:181:ASP:O	1:G:236:PHE:HB2	1.99	0.62
1:C:181:ASP:O	1:C:236:PHE:HB2	1.99	0.62
1:C:508:VAL:HG13	1:C:516:THR:HA	1.80	0.62
1:F:733:GLU:C	1:F:734:ILE:HD12	2.24	0.62
1:C:226:TRP:CZ2	1:C:234:SER:HB3	2.35	0.62
1:H:691:ASN:HB3	1:H:694:TYR:CE1	2.35	0.62
1:D:710:PRO:HG3	1:D:716:THR:HG22	1.82	0.62
1:D:733:GLU:C	1:D:734:ILE:HD12	2.24	0.62
1:H:622:SER:HB3	1:H:734:ILE:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG23	1:A:242:ARG:H	1.64	0.62
1:B:622:SER:HB3	1:B:734:ILE:CG1	2.29	0.62
1:E:488:THR:OG1	1:E:504:ARG:HD3	1.99	0.62
1:E:508:VAL:HG13	1:E:516:THR:HA	1.81	0.62
1:A:659:ARG:HB2	1:A:662:MET:SD	2.39	0.62
1:C:240:THR:HG23	1:C:242:ARG:H	1.65	0.62
1:C:553:ASN:HB2	1:C:590:LEU:HB3	1.82	0.62
1:B:508:VAL:HG13	1:B:516:THR:HA	1.82	0.62
1:E:442:LEU:HD13	1:E:448:LEU:HD21	1.82	0.62
1:G:508:VAL:HG13	1:G:516:THR:HA	1.81	0.62
1:G:524:LYS:HG3	1:G:540:LEU:HD22	1.81	0.62
1:A:226:TRP:CZ2	1:A:234:SER:HB3	2.35	0.61
1:F:710:PRO:HG3	1:F:716:THR:HG22	1.80	0.61
1:G:226:TRP:CZ2	1:G:234:SER:HB3	2.35	0.61
1:H:508:VAL:HG13	1:H:516:THR:HA	1.82	0.61
1:E:181:ASP:O	1:E:236:PHE:HB2	2.00	0.61
1:C:197:LYS:HD3	1:C:202:PHE:HD2	1.64	0.61
1:F:699:TYR:HD1	1:F:725:LEU:HA	1.63	0.61
1:G:512:ASP:HB3	1:G:515:GLU:HB2	1.82	0.61
1:A:508:VAL:HG13	1:A:516:THR:HA	1.81	0.61
1:E:240:THR:HG23	1:E:242:ARG:H	1.65	0.61
1:G:659:ARG:HB2	1:G:662:MET:SD	2.39	0.61
1:C:512:ASP:HB3	1:C:515:GLU:HB2	1.82	0.61
1:C:659:ARG:HB2	1:C:662:MET:SD	2.40	0.61
1:G:553:ASN:HB2	1:G:590:LEU:HB3	1.81	0.61
1:G:555:ASP:OD2	1:G:588:ASN:HB2	2.00	0.61
1:H:733:GLU:C	1:H:734:ILE:HD12	2.24	0.61
1:A:524:LYS:HG3	1:A:540:LEU:HD22	1.81	0.61
1:C:269:ILE:HG22	1:C:362:ALA:HB2	1.83	0.61
1:E:555:ASP:OD2	1:E:588:ASN:HB2	2.00	0.61
1:D:691:ASN:HB3	1:D:694:TYR:CE1	2.35	0.61
1:E:524:LYS:HG3	1:E:540:LEU:HD22	1.82	0.61
1:A:442:LEU:HD13	1:A:448:LEU:HD21	1.83	0.61
1:F:508:VAL:HG13	1:F:516:THR:HA	1.82	0.61
1:B:733:GLU:C	1:B:734:ILE:HD12	2.25	0.60
1:E:385:LEU:O	1:E:389:GLN:HB2	2.02	0.60
1:F:410:TYR:CD1	1:F:414:LYS:HE2	2.36	0.60
1:D:293:THR:HG22	1:D:334:ILE:HA	1.83	0.60
1:G:442:LEU:HD13	1:G:448:LEU:HD21	1.82	0.60
1:A:555:ASP:OD2	1:A:588:ASN:HB2	2.01	0.60
1:E:226:TRP:CZ2	1:E:234:SER:HB3	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ALA:HB1	1:C:258:ALA:HB2	1.83	0.60
1:C:442:LEU:HD13	1:C:448:LEU:HD21	1.82	0.60
1:D:508:VAL:HG13	1:D:516:THR:HA	1.82	0.60
1:A:640:SER:HB3	1:A:706:THR:HG21	1.83	0.60
1:B:206:TRP:CG	1:B:218:LYS:HD2	2.36	0.60
1:C:640:SER:HB3	1:C:706:THR:HG21	1.84	0.60
1:G:377:VAL:HG12	1:G:378:LEU:N	2.17	0.60
1:B:410:TYR:CD1	1:B:414:LYS:HE2	2.36	0.60
1:E:251:ALA:HB1	1:E:258:ALA:HB2	1.82	0.60
1:G:251:ALA:HB1	1:G:258:ALA:HB2	1.84	0.60
1:A:385:LEU:O	1:A:389:GLN:HB2	2.01	0.60
1:A:453:ASP:HB2	1:H:403:GLN:OE1	2.02	0.60
1:C:385:LEU:O	1:C:389:GLN:HB2	2.02	0.60
1:D:224:GLU:HB2	1:D:517:THR:HG21	1.84	0.60
1:A:251:ALA:HB1	1:A:258:ALA:HB2	1.83	0.59
1:F:206:TRP:CG	1:F:218:LYS:HD2	2.37	0.59
1:E:199:LYS:O	1:F:517:THR:HG23	2.02	0.59
1:H:206:TRP:CG	1:H:218:LYS:HD2	2.37	0.59
1:G:385:LEU:O	1:G:389:GLN:HB2	2.02	0.59
1:D:410:TYR:CD1	1:D:414:LYS:HE2	2.38	0.59
1:F:293:THR:HG22	1:F:334:ILE:HA	1.84	0.59
1:E:377:VAL:HG12	1:E:378:LEU:N	2.17	0.59
1:H:293:THR:HG22	1:H:334:ILE:HA	1.84	0.59
1:H:410:TYR:CD1	1:H:414:LYS:HE2	2.37	0.59
1:C:269:ILE:HG22	1:C:362:ALA:CB	2.32	0.59
1:D:699:TYR:HB3	1:D:723:ARG:HB2	1.84	0.59
1:A:269:ILE:HG22	1:A:362:ALA:HB2	1.85	0.59
1:C:468:ARG:HD2	1:C:470:ARG:HH21	1.68	0.59
1:C:555:ASP:OD2	1:C:588:ASN:HB2	2.03	0.59
1:D:206:TRP:CG	1:D:218:LYS:HD2	2.37	0.59
1:G:269:ILE:HG22	1:G:362:ALA:HB2	1.84	0.59
1:F:699:TYR:HB3	1:F:723:ARG:HB2	1.85	0.59
1:G:468:ARG:HD2	1:G:470:ARG:HH21	1.68	0.59
1:H:699:TYR:HB3	1:H:723:ARG:HB2	1.85	0.59
1:C:377:VAL:HG12	1:C:378:LEU:N	2.18	0.58
1:G:640:SER:HB3	1:G:706:THR:HG21	1.84	0.58
1:H:224:GLU:HB2	1:H:517:THR:HG21	1.84	0.58
1:A:289:ILE:HD13	1:A:346:TRP:CD1	2.38	0.58
1:G:378:LEU:HD13	1:G:401:LEU:CD2	2.33	0.58
1:E:640:SER:HB3	1:E:706:THR:HG21	1.85	0.58
1:F:199:LYS:HB2	1:G:189:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:401:LEU:HD12	1:G:403:GLN:H	1.66	0.58
1:B:224:GLU:HB2	1:B:517:THR:HG21	1.85	0.58
1:E:289:ILE:HD13	1:E:346:TRP:CD1	2.39	0.58
1:E:468:ARG:HD2	1:E:470:ARG:HH21	1.69	0.58
1:B:699:TYR:HB3	1:B:723:ARG:HB2	1.84	0.58
1:H:627:LEU:HD11	1:H:727:PHE:CD2	2.39	0.58
1:B:627:LEU:HD11	1:B:727:PHE:CD2	2.39	0.58
1:A:377:VAL:HG12	1:A:378:LEU:N	2.17	0.58
1:E:229:ALA:O	1:E:230:SER:HB2	2.04	0.58
1:F:627:LEU:HD11	1:F:727:PHE:CD2	2.39	0.58
1:C:289:ILE:HD13	1:C:346:TRP:CD1	2.39	0.58
1:E:269:ILE:HG22	1:E:362:ALA:HB2	1.85	0.57
1:G:289:ILE:HD13	1:G:346:TRP:CD1	2.39	0.57
1:F:224:GLU:HB2	1:F:517:THR:HG21	1.86	0.57
1:A:229:ALA:O	1:A:230:SER:HB2	2.04	0.57
1:A:468:ARG:HD2	1:A:470:ARG:HH21	1.69	0.57
1:B:293:THR:HG22	1:B:334:ILE:HA	1.84	0.57
1:G:269:ILE:HG22	1:G:362:ALA:CB	2.33	0.57
1:H:274:ASN:ND2	1:H:359:ARG:HB3	2.18	0.57
1:A:269:ILE:HG22	1:A:362:ALA:CB	2.34	0.57
1:E:269:ILE:HG22	1:E:362:ALA:CB	2.34	0.57
1:E:295:THR:OG1	1:E:332:VAL:HG12	2.05	0.57
1:G:527:LEU:HB3	1:G:533:PHE:CD1	2.40	0.57
1:H:347:ALA:HA	1:H:352:LEU:HD22	1.85	0.57
1:A:493:PHE:CZ	1:A:495:GLY:HA3	2.40	0.57
1:E:493:PHE:CZ	1:E:495:GLY:HA3	2.40	0.57
1:D:262:VAL:HG11	1:D:379:PRO:HG2	1.87	0.57
1:F:691:ASN:HB3	1:F:694:TYR:CZ	2.40	0.57
1:G:229:ALA:O	1:G:230:SER:HB2	2.05	0.57
1:B:691:ASN:HB3	1:B:694:TYR:CZ	2.40	0.57
1:B:262:VAL:HG11	1:B:379:PRO:HG2	1.87	0.56
1:B:458:ASN:HB3	1:B:472:ASP:O	2.05	0.56
1:E:527:LEU:HB3	1:E:533:PHE:CD1	2.40	0.56
1:D:691:ASN:HB3	1:D:694:TYR:CZ	2.40	0.56
1:H:262:VAL:HG11	1:H:379:PRO:HG2	1.87	0.56
1:H:397:LYS:HD3	1:H:400:GLN:OE1	2.04	0.56
1:A:527:LEU:HB3	1:A:533:PHE:CD1	2.41	0.56
1:C:295:THR:OG1	1:C:332:VAL:HG12	2.06	0.56
1:D:627:LEU:HD11	1:D:727:PHE:CD2	2.39	0.56
1:H:691:ASN:HB3	1:H:694:TYR:CZ	2.40	0.56
1:B:199:LYS:HB2	1:C:189:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:493:PHE:CZ	1:G:495:GLY:HA3	2.40	0.56
1:C:229:ALA:O	1:C:230:SER:HB2	2.05	0.56
1:C:493:PHE:CZ	1:C:495:GLY:HA3	2.40	0.56
1:E:713:ASN:CG	1:E:714:GLY:H	2.13	0.56
1:F:395:LYS:NZ	1:F:397:LYS:HG2	2.20	0.56
1:F:698:VAL:O	1:F:726:ILE:HB	2.06	0.56
1:G:295:THR:OG1	1:G:332:VAL:HG12	2.05	0.56
1:C:527:LEU:HB3	1:C:533:PHE:CD1	2.40	0.56
1:F:401:LEU:HD22	1:F:401:LEU:O	2.05	0.56
1:A:359:ARG:HH21	1:A:431:PRO:CG	2.19	0.56
1:E:699:TYR:HB3	1:E:723:ARG:HB2	1.88	0.56
1:C:633:LYS:HE3	1:C:672:GLY:O	2.06	0.56
1:E:359:ARG:HH21	1:E:431:PRO:CG	2.19	0.56
1:G:699:TYR:HB3	1:G:723:ARG:HB2	1.88	0.56
1:A:648:ASP:CB	1:A:652:LEU:HB2	2.36	0.55
1:F:423:ALA:HA	1:F:432:ILE:HG13	1.88	0.55
1:H:698:VAL:O	1:H:726:ILE:HB	2.06	0.55
1:A:295:THR:OG1	1:A:332:VAL:HG12	2.06	0.55
1:C:648:ASP:CB	1:C:652:LEU:HB2	2.36	0.55
1:G:245:LYS:HE3	1:H:512:ASP:OD1	2.06	0.55
1:A:633:LYS:HE3	1:A:672:GLY:O	2.06	0.55
1:B:698:VAL:O	1:B:726:ILE:HB	2.06	0.55
1:C:200:ARG:HB3	1:D:178:ARG:NH1	2.22	0.55
1:H:458:ASN:HB3	1:H:472:ASP:O	2.06	0.55
1:C:359:ARG:HH21	1:C:431:PRO:CG	2.19	0.55
1:D:458:ASN:HB3	1:D:472:ASP:O	2.06	0.55
1:E:689:ILE:HG22	1:E:691:ASN:H	1.71	0.55
1:G:648:ASP:CB	1:G:652:LEU:HB2	2.37	0.55
1:G:713:ASN:CG	1:G:714:GLY:H	2.14	0.55
1:D:698:VAL:O	1:D:726:ILE:HB	2.06	0.55
1:F:458:ASN:HB3	1:F:472:ASP:O	2.06	0.55
1:F:262:VAL:HG11	1:F:379:PRO:HG2	1.88	0.55
1:A:659:ARG:HD3	1:A:662:MET:SD	2.47	0.55
1:B:380:THR:OG1	1:B:396:ALA:HB2	2.07	0.55
1:B:460:ALA:HB1	1:B:469:VAL:HG12	1.88	0.55
1:G:359:ARG:HH21	1:G:431:PRO:CG	2.19	0.55
1:G:633:LYS:HE3	1:G:672:GLY:O	2.06	0.55
1:D:346:TRP:CZ2	1:D:446:LYS:HE3	2.42	0.55
1:D:460:ALA:HB1	1:D:469:VAL:HG12	1.89	0.55
1:E:633:LYS:HE3	1:E:672:GLY:O	2.06	0.55
1:H:346:TRP:CZ2	1:H:446:LYS:HE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:THR:OG1	1:H:396:ALA:HB2	2.07	0.55
1:B:304:GLY:O	1:B:326:ASN:N	2.40	0.54
1:B:423:ALA:HA	1:B:432:ILE:HG13	1.88	0.54
1:C:199:LYS:O	1:D:517:THR:HG23	2.07	0.54
1:D:228:THR:HG23	1:D:518:LYS:HG2	1.90	0.54
1:G:659:ARG:HD3	1:G:662:MET:SD	2.47	0.54
1:H:423:ALA:HA	1:H:432:ILE:HG13	1.88	0.54
1:H:460:ALA:HB1	1:H:469:VAL:HG12	1.89	0.54
1:A:395:LYS:HB3	1:A:426:ASP:CB	2.38	0.54
1:A:699:TYR:HB3	1:A:723:ARG:HB2	1.88	0.54
1:C:699:TYR:HB3	1:C:723:ARG:HB2	1.89	0.54
1:F:346:TRP:CZ2	1:F:446:LYS:HE3	2.42	0.54
1:G:364:ILE:HG12	1:G:421:LEU:HD22	1.89	0.54
1:H:397:LYS:HD3	1:H:400:GLN:CD	2.32	0.54
1:F:460:ALA:HB1	1:F:469:VAL:HG12	1.88	0.54
1:D:423:ALA:HA	1:D:432:ILE:HG13	1.88	0.54
1:A:189:VAL:HG13	1:H:199:LYS:HB2	1.88	0.54
1:E:242:ARG:CG	1:E:242:ARG:NH1	2.70	0.54
1:E:360:LEU:HD12	1:E:361:ASN:H	1.72	0.54
1:G:689:ILE:HG22	1:G:691:ASN:H	1.72	0.54
1:A:368:ASN:HB2	1:A:405:LEU:HG	1.89	0.54
1:C:689:ILE:HG22	1:C:691:ASN:H	1.72	0.54
1:E:300:THR:C	1:E:302:GLU:H	2.15	0.54
1:E:659:ARG:HD3	1:E:662:MET:SD	2.48	0.54
1:C:368:ASN:HB2	1:C:405:LEU:HG	1.89	0.54
1:G:200:ARG:HB3	1:H:178:ARG:NH1	2.23	0.54
1:A:242:ARG:CG	1:A:242:ARG:NH1	2.70	0.54
1:A:689:ILE:HG22	1:A:691:ASN:H	1.72	0.54
1:A:199:LYS:O	1:B:517:THR:HG23	2.07	0.54
1:C:238:LYS:HB3	1:C:252:ARG:O	2.08	0.54
1:E:648:ASP:CB	1:E:652:LEU:HB2	2.36	0.54
1:H:337:SER:HB3	1:H:664:ASN:HB2	1.91	0.54
1:A:360:LEU:HD12	1:A:361:ASN:H	1.73	0.53
1:C:246:ASN:HB3	1:C:373:PRO:HG3	1.90	0.53
1:D:380:THR:OG1	1:D:396:ALA:HB2	2.07	0.53
1:B:337:SER:HB3	1:B:664:ASN:HB2	1.91	0.53
1:B:346:TRP:CZ2	1:B:446:LYS:HE3	2.43	0.53
1:F:337:SER:HB3	1:F:664:ASN:HB2	1.90	0.53
1:D:337:SER:HB3	1:D:664:ASN:HB2	1.90	0.53
1:A:365:ARG:HH12	1:A:414:LYS:HA	1.74	0.53
1:C:659:ARG:HD3	1:C:662:MET:SD	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:ASN:HB2	1:G:405:LEU:HG	1.89	0.53
1:G:635:ILE:C	1:G:637:LYS:H	2.16	0.53
1:C:245:LYS:HE3	1:D:512:ASP:OD1	2.07	0.53
1:E:248:SER:HB2	1:E:371:THR:HB	1.91	0.53
1:A:635:ILE:C	1:A:637:LYS:H	2.17	0.53
1:E:246:ASN:HB3	1:E:373:PRO:HG3	1.90	0.53
1:F:622:SER:HB3	1:F:734:ILE:HG13	1.91	0.53
1:B:446:LYS:HB2	1:B:708:ILE:HD12	1.91	0.53
1:D:446:LYS:HB2	1:D:708:ILE:HD12	1.91	0.53
1:F:380:THR:OG1	1:F:396:ALA:HB2	2.08	0.53
1:G:238:LYS:HB3	1:G:252:ARG:O	2.09	0.53
1:H:228:THR:HG23	1:H:518:LYS:HG2	1.89	0.53
1:A:656:ILE:HD13	1:A:656:ILE:N	2.24	0.53
1:C:645:GLU:HG2	1:C:697:ASN:HB2	1.91	0.53
1:G:360:LEU:HD12	1:G:361:ASN:H	1.74	0.53
1:D:524:LYS:CD	1:D:579:ASP:HB3	2.37	0.52
1:F:376:ASN:O	1:F:401:LEU:HD13	2.08	0.52
1:H:397:LYS:HG2	1:H:400:GLN:CB	2.39	0.52
1:A:645:GLU:HG2	1:A:697:ASN:HB2	1.91	0.52
1:C:635:ILE:C	1:C:637:LYS:H	2.16	0.52
1:C:662:MET:HE3	1:C:681:TYR:CD1	2.43	0.52
1:E:365:ARG:HH12	1:E:414:LYS:HA	1.75	0.52
1:E:635:ILE:C	1:E:637:LYS:H	2.16	0.52
1:E:645:GLU:HG2	1:E:697:ASN:HB2	1.91	0.52
1:C:385:LEU:HD12	1:C:386:GLY:H	1.75	0.52
1:D:231:ASP:HB2	1:D:232:PRO:CD	2.35	0.52
1:E:368:ASN:HB2	1:E:405:LEU:HG	1.89	0.52
1:F:524:LYS:CD	1:F:579:ASP:HB3	2.36	0.52
1:G:199:LYS:O	1:H:517:THR:HG23	2.09	0.52
1:H:231:ASP:HB2	1:H:232:PRO:CD	2.35	0.52
1:C:551:ASP:O	1:C:591:ILE:HA	2.10	0.52
1:F:445:THR:O	1:F:447:GLN:N	2.43	0.52
1:A:248:SER:HB2	1:A:371:THR:HB	1.92	0.52
1:B:226:TRP:CZ2	1:B:234:SER:HB3	2.45	0.52
1:B:445:THR:O	1:B:447:GLN:N	2.42	0.52
1:C:360:LEU:HD12	1:C:361:ASN:H	1.74	0.52
1:F:197:LYS:HB2	1:F:202:PHE:HE2	1.74	0.52
1:A:246:ASN:HB3	1:A:373:PRO:HG3	1.90	0.52
1:A:640:SER:CB	1:A:706:THR:HG21	2.39	0.52
1:G:662:MET:HE3	1:G:681:TYR:CD1	2.44	0.52
1:H:446:LYS:HB2	1:H:708:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:SER:CB	1:C:706:THR:HG21	2.40	0.52
1:E:238:LYS:HB3	1:E:252:ARG:O	2.10	0.52
1:G:246:ASN:HB3	1:G:373:PRO:HG3	1.90	0.52
1:G:645:GLU:HG2	1:G:697:ASN:HB2	1.91	0.52
1:D:542:TYR:CE2	1:D:543:GLN:HG3	2.45	0.52
1:E:662:MET:HE3	1:E:681:TYR:CD1	2.44	0.52
1:H:445:THR:O	1:H:447:GLN:N	2.42	0.52
1:B:197:LYS:HB2	1:B:202:PHE:HE2	1.75	0.52
1:F:638:ILE:O	1:F:703:LYS:HG3	2.10	0.52
1:A:551:ASP:O	1:A:591:ILE:HA	2.10	0.51
1:B:638:ILE:O	1:B:703:LYS:HG3	2.11	0.51
1:E:724:ILE:O	1:E:726:ILE:HD13	2.10	0.51
1:C:365:ARG:HH12	1:C:414:LYS:HA	1.75	0.51
1:H:524:LYS:CD	1:H:579:ASP:HB3	2.36	0.51
1:B:542:TYR:CE2	1:B:543:GLN:HG3	2.45	0.51
1:E:476:ASN:OD1	1:E:478:SER:HB2	2.11	0.51
1:E:640:SER:CB	1:E:706:THR:HG21	2.40	0.51
1:F:542:TYR:CE2	1:F:543:GLN:HG3	2.45	0.51
1:G:683:ASP:O	1:G:685:LEU:HG	2.10	0.51
1:A:238:LYS:HB3	1:A:252:ARG:O	2.10	0.51
1:A:620:ILE:HB	1:A:628:LEU:O	2.11	0.51
1:B:228:THR:HG23	1:B:518:LYS:HG2	1.92	0.51
1:D:445:THR:O	1:D:447:GLN:N	2.43	0.51
1:E:713:ASN:N	1:E:713:ASN:OD1	2.43	0.51
1:G:248:SER:HB2	1:G:371:THR:HB	1.92	0.51
1:H:537:ASN:C	1:H:539:ASN:H	2.19	0.51
1:A:476:ASN:OD1	1:A:478:SER:HB2	2.10	0.51
1:E:253:HIS:HE1	1:E:255:LEU:HG	1.76	0.51
1:F:226:TRP:CZ2	1:F:234:SER:HB3	2.45	0.51
1:G:713:ASN:ND2	1:G:715:ASP:HB2	2.25	0.51
1:C:656:ILE:HD13	1:C:656:ILE:N	2.26	0.51
1:C:724:ILE:O	1:C:726:ILE:HD13	2.11	0.51
1:D:638:ILE:O	1:D:703:LYS:HG3	2.11	0.51
1:F:446:LYS:HB2	1:F:708:ILE:HD12	1.92	0.51
1:G:476:ASN:OD1	1:G:478:SER:HB2	2.10	0.51
1:H:645:GLU:HG2	1:H:697:ASN:HB2	1.93	0.51
1:A:713:ASN:OD1	1:A:713:ASN:N	2.43	0.51
1:G:385:LEU:HD12	1:G:386:GLY:H	1.75	0.51
1:D:498:LEU:HD23	1:D:637:LYS:HD3	1.93	0.51
1:D:622:SER:HB3	1:D:734:ILE:HG13	1.92	0.51
1:E:551:ASP:O	1:E:591:ILE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LYS:HB2	1:H:202:PHE:HE2	1.75	0.51
1:H:622:SER:HB3	1:H:734:ILE:HG13	1.92	0.51
1:D:699:TYR:CD1	1:D:725:LEU:HA	2.46	0.51
1:E:385:LEU:HD12	1:E:386:GLY:H	1.76	0.51
1:F:537:ASN:C	1:F:539:ASN:H	2.19	0.51
1:G:365:ARG:HH12	1:G:414:LYS:HA	1.76	0.51
1:H:226:TRP:CZ2	1:H:234:SER:HB3	2.46	0.51
1:A:385:LEU:HD12	1:A:386:GLY:H	1.76	0.51
1:A:646:ILE:HD11	1:A:687:LEU:HD21	1.92	0.51
1:C:476:ASN:OD1	1:C:478:SER:HB2	2.11	0.51
1:D:274:ASN:OD1	1:D:359:ARG:HB3	2.11	0.51
1:D:226:TRP:CZ2	1:D:234:SER:HB3	2.46	0.50
1:D:537:ASN:C	1:D:539:ASN:H	2.19	0.50
1:E:620:ILE:HB	1:E:628:LEU:O	2.11	0.50
1:G:551:ASP:O	1:G:591:ILE:HA	2.10	0.50
1:G:713:ASN:N	1:G:713:ASN:OD1	2.44	0.50
1:B:524:LYS:CD	1:B:579:ASP:HB3	2.36	0.50
1:B:542:TYR:CD2	1:B:543:GLN:HG3	2.47	0.50
1:D:622:SER:HB3	1:D:734:ILE:HG12	1.94	0.50
1:F:542:TYR:HE2	1:F:543:GLN:HE21	1.60	0.50
1:H:498:LEU:HD23	1:H:637:LYS:HD3	1.93	0.50
1:B:515:GLU:HA	1:B:518:LYS:HD3	1.93	0.50
1:B:537:ASN:C	1:B:539:ASN:H	2.19	0.50
1:C:620:ILE:HB	1:C:628:LEU:O	2.12	0.50
1:C:625:GLU:HG2	1:C:679:LYS:HD3	1.93	0.50
1:G:365:ARG:NH1	1:G:414:LYS:HD2	2.26	0.50
1:G:724:ILE:O	1:G:726:ILE:HD13	2.10	0.50
1:A:245:LYS:HB2	1:B:483:GLN:NE2	2.26	0.50
1:B:262:VAL:HA	1:B:367:VAL:O	2.11	0.50
1:B:622:SER:HB3	1:B:734:ILE:HG13	1.92	0.50
1:C:713:ASN:OD1	1:C:713:ASN:N	2.43	0.50
1:F:635:ILE:O	1:F:638:ILE:HG12	2.12	0.50
1:H:622:SER:HB3	1:H:734:ILE:HG12	1.94	0.50
1:H:638:ILE:O	1:H:703:LYS:HG3	2.11	0.50
1:A:724:ILE:O	1:A:726:ILE:HD13	2.11	0.50
1:B:635:ILE:O	1:B:638:ILE:HG12	2.12	0.50
1:B:645:GLU:HG2	1:B:697:ASN:HB2	1.93	0.50
1:B:699:TYR:CD1	1:B:725:LEU:HA	2.45	0.50
1:F:395:LYS:HZ3	1:F:397:LYS:HG2	1.76	0.50
1:F:660:TYR:CZ	1:F:710:PRO:HD3	2.47	0.50
1:G:640:SER:CB	1:G:706:THR:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:620:ILE:HG13	1:H:673:LYS:HD3	1.94	0.50
1:A:625:GLU:HG2	1:A:679:LYS:HD3	1.94	0.50
1:B:620:ILE:HG13	1:B:673:LYS:HD3	1.94	0.50
1:D:199:LYS:HB2	1:E:189:VAL:HG13	1.93	0.50
1:F:262:VAL:HA	1:F:367:VAL:O	2.12	0.50
1:F:622:SER:HB3	1:F:734:ILE:HG12	1.94	0.50
1:D:515:GLU:HA	1:D:518:LYS:HD3	1.93	0.50
1:D:645:GLU:HG2	1:D:697:ASN:HB2	1.93	0.50
1:E:200:ARG:HB2	1:F:178:ARG:NH1	2.27	0.50
1:E:713:ASN:ND2	1:E:715:ASP:HB2	2.26	0.50
1:A:662:MET:HE3	1:A:681:TYR:CD1	2.44	0.50
1:B:542:TYR:HE2	1:B:543:GLN:HE21	1.60	0.50
1:C:248:SER:HB2	1:C:371:THR:HB	1.93	0.50
1:C:253:HIS:HE1	1:C:255:LEU:HG	1.77	0.50
1:C:381:THR:HG23	1:C:394:ILE:HB	1.94	0.50
1:F:228:THR:HG23	1:F:518:LYS:HG2	1.93	0.50
1:F:645:GLU:HG2	1:F:697:ASN:HB2	1.93	0.50
1:G:207:ILE:HG22	1:G:209:ASN:OD1	2.12	0.50
1:G:298:THR:HG21	1:G:601:ASN:HD22	1.77	0.50
1:H:635:ILE:O	1:H:638:ILE:HG12	2.12	0.50
1:B:325:SER:O	1:B:327:SER:N	2.45	0.50
1:F:542:TYR:CD2	1:F:543:GLN:HG3	2.47	0.50
1:F:699:TYR:CD1	1:F:725:LEU:HA	2.46	0.50
1:G:620:ILE:HB	1:G:628:LEU:O	2.11	0.50
1:H:515:GLU:HA	1:H:518:LYS:HD3	1.94	0.50
1:D:258:ALA:HA	1:D:371:THR:OG1	2.12	0.49
1:E:625:GLU:HG2	1:E:679:LYS:HD3	1.94	0.49
1:A:381:THR:HG23	1:A:394:ILE:HB	1.95	0.49
1:A:413:SER:HB3	1:B:304:GLY:HA2	1.94	0.49
1:D:240:THR:CG2	1:D:242:ARG:H	2.24	0.49
1:D:542:TYR:CD2	1:D:543:GLN:HG3	2.47	0.49
1:D:620:ILE:HG13	1:D:673:LYS:HD3	1.93	0.49
1:G:374:ILE:HD11	1:G:405:LEU:HD23	1.94	0.49
1:A:298:THR:HG21	1:A:601:ASN:HD22	1.78	0.49
1:C:646:ILE:HD11	1:C:687:LEU:HD21	1.94	0.49
1:E:207:ILE:HG22	1:E:209:ASN:OD1	2.12	0.49
1:G:656:ILE:N	1:G:656:ILE:HD13	2.26	0.49
1:H:542:TYR:CE2	1:H:543:GLN:HG3	2.46	0.49
1:H:542:TYR:CD2	1:H:543:GLN:HG3	2.47	0.49
1:A:713:ASN:ND2	1:A:715:ASP:HB2	2.26	0.49
1:C:207:ILE:HG22	1:C:209:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:LYS:NZ	1:H:397:LYS:HE2	2.28	0.49
1:A:207:ILE:HG22	1:A:209:ASN:OD1	2.13	0.49
1:A:253:HIS:HE1	1:A:255:LEU:HG	1.76	0.49
1:B:498:LEU:HD23	1:B:637:LYS:HD3	1.93	0.49
1:F:620:ILE:HG13	1:F:673:LYS:HD3	1.93	0.49
1:C:196:VAL:HG21	1:D:516:THR:HG21	1.95	0.49
1:D:197:LYS:HB2	1:D:202:PHE:HE2	1.76	0.49
1:F:493:PHE:HD1	1:F:591:ILE:HB	1.78	0.49
1:G:253:HIS:HE1	1:G:255:LEU:HG	1.77	0.49
1:B:493:PHE:HD1	1:B:591:ILE:HB	1.78	0.49
1:F:682:ASN:O	1:F:683:ASP:C	2.56	0.49
1:G:646:ILE:HD11	1:G:687:LEU:HD21	1.95	0.49
1:B:660:TYR:CZ	1:B:710:PRO:HD3	2.47	0.49
1:D:493:PHE:HD1	1:D:591:ILE:HB	1.77	0.49
1:G:401:LEU:HD13	1:G:411:TYR:CZ	2.46	0.49
1:H:493:PHE:HD1	1:H:591:ILE:HB	1.77	0.49
1:B:258:ALA:HA	1:B:371:THR:OG1	2.12	0.49
1:F:515:GLU:HA	1:F:518:LYS:HD3	1.94	0.49
1:H:258:ALA:HA	1:H:371:THR:OG1	2.12	0.49
1:H:682:ASN:O	1:H:683:ASP:C	2.56	0.49
1:G:271:LEU:HD21	1:G:360:LEU:HD13	1.94	0.48
1:G:381:THR:HG23	1:G:394:ILE:HB	1.93	0.48
1:H:636:ARG:CZ	1:H:668:LEU:HD22	2.43	0.48
1:A:183:ILE:HG12	1:A:203:LEU:HD21	1.95	0.48
1:A:271:LEU:HD21	1:A:360:LEU:HD13	1.95	0.48
1:B:636:ARG:CZ	1:B:668:LEU:HD22	2.43	0.48
1:G:359:ARG:HH21	1:G:431:PRO:HG2	1.78	0.48
1:H:262:VAL:HA	1:H:367:VAL:O	2.12	0.48
1:A:374:ILE:HD11	1:A:405:LEU:HD23	1.95	0.48
1:A:725:LEU:O	1:A:726:ILE:HD12	2.13	0.48
1:B:357:THR:HG22	1:B:435:ASN:HA	1.96	0.48
1:C:713:ASN:ND2	1:C:715:ASP:HB2	2.26	0.48
1:D:272:SER:CA	1:D:350:MET:HE3	2.44	0.48
1:D:357:THR:HG22	1:D:435:ASN:HA	1.96	0.48
1:E:271:LEU:HD21	1:E:360:LEU:HD13	1.95	0.48
1:E:374:ILE:HD11	1:E:405:LEU:HD23	1.94	0.48
1:E:656:ILE:N	1:E:656:ILE:HD13	2.27	0.48
1:G:183:ILE:HG12	1:G:203:LEU:HD21	1.95	0.48
1:G:625:GLU:HG2	1:G:679:LYS:HD3	1.93	0.48
1:H:660:TYR:CZ	1:H:710:PRO:HD3	2.48	0.48
1:A:680:LYS:HG2	1:A:681:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:THR:CB	1:B:601:ASN:HB3	2.43	0.48
1:B:682:ASN:O	1:B:683:ASP:C	2.56	0.48
1:C:271:LEU:HD21	1:C:360:LEU:HD13	1.94	0.48
1:D:635:ILE:O	1:D:638:ILE:HG12	2.12	0.48
1:F:636:ARG:CZ	1:F:668:LEU:HD22	2.43	0.48
1:G:242:ARG:CG	1:G:242:ARG:NH1	2.69	0.48
1:B:622:SER:HB3	1:B:734:ILE:HG12	1.94	0.48
1:C:289:ILE:HD13	1:C:346:TRP:CG	2.49	0.48
1:D:298:THR:CB	1:D:601:ASN:HB3	2.43	0.48
1:D:660:TYR:CZ	1:D:710:PRO:HD3	2.48	0.48
1:E:357:THR:HB	1:E:433:THR:HG22	1.96	0.48
1:H:240:THR:CG2	1:H:242:ARG:H	2.23	0.48
1:H:397:LYS:HG2	1:H:400:GLN:HB2	1.95	0.48
1:B:558:THR:O	1:B:562:ILE:HG12	2.14	0.48
1:C:713:ASN:CG	1:C:714:GLY:H	2.21	0.48
1:F:258:ALA:HA	1:F:371:THR:OG1	2.13	0.48
1:H:699:TYR:CD1	1:H:725:LEU:HA	2.45	0.48
1:A:245:LYS:HE3	1:B:512:ASP:OD1	2.13	0.48
1:D:682:ASN:O	1:D:683:ASP:C	2.56	0.48
1:E:381:THR:HG23	1:E:394:ILE:HB	1.94	0.48
1:F:200:ARG:HH11	1:G:185:ASP:HB3	1.78	0.48
1:G:725:LEU:O	1:G:726:ILE:HD12	2.14	0.48
1:H:272:SER:CA	1:H:350:MET:HE3	2.43	0.48
1:A:222:SER:HB3	1:A:225:LYS:HB2	1.96	0.48
1:C:266:MET:HB3	1:C:332:VAL:HG11	1.96	0.48
1:D:262:VAL:HA	1:D:367:VAL:O	2.13	0.48
1:D:636:ARG:CZ	1:D:668:LEU:HD22	2.43	0.48
1:E:289:ILE:HD13	1:E:346:TRP:CG	2.49	0.48
1:E:646:ILE:HD11	1:E:687:LEU:HD21	1.94	0.48
1:A:289:ILE:HD13	1:A:346:TRP:CG	2.49	0.48
1:C:298:THR:HG21	1:C:601:ASN:HD22	1.78	0.48
1:C:378:LEU:HD13	1:C:401:LEU:CD1	2.41	0.48
1:G:253:HIS:CE1	1:G:255:LEU:HB2	2.48	0.48
1:G:289:ILE:HD13	1:G:346:TRP:CG	2.49	0.48
1:H:368:ASN:HB2	1:H:405:LEU:HG	1.96	0.48
1:B:206:TRP:CD1	1:B:218:LYS:HD2	2.49	0.48
1:C:183:ILE:HG12	1:C:203:LEU:HD21	1.96	0.48
1:C:680:LYS:HG2	1:C:681:TYR:CD2	2.49	0.48
1:D:199:LYS:O	1:E:517:THR:HG23	2.14	0.48
1:E:183:ILE:HG12	1:E:203:LEU:HD21	1.95	0.48
1:C:253:HIS:CE1	1:C:255:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:NH1	1:C:414:LYS:HD2	2.25	0.47
1:D:206:TRP:CD1	1:D:218:LYS:HD2	2.49	0.47
1:D:558:THR:O	1:D:562:ILE:HG12	2.14	0.47
1:E:680:LYS:HG2	1:E:681:TYR:CD2	2.48	0.47
1:E:725:LEU:O	1:E:726:ILE:HD12	2.13	0.47
1:F:197:LYS:HD2	1:F:202:PHE:CE2	2.49	0.47
1:F:272:SER:CA	1:F:350:MET:HE3	2.44	0.47
1:H:633:LYS:O	1:H:637:LYS:HG3	2.14	0.47
1:A:713:ASN:CG	1:A:714:GLY:H	2.20	0.47
1:F:558:THR:O	1:F:562:ILE:HG12	2.13	0.47
1:H:357:THR:HG22	1:H:435:ASN:HA	1.96	0.47
1:A:253:HIS:CE1	1:A:255:LEU:HB2	2.49	0.47
1:C:374:ILE:HD11	1:C:405:LEU:HD23	1.95	0.47
1:C:626:GLY:HA3	1:C:676:ILE:O	2.14	0.47
1:D:542:TYR:HE2	1:D:543:GLN:HE21	1.60	0.47
1:F:231:ASP:HB2	1:F:232:PRO:CD	2.35	0.47
1:G:377:VAL:CG1	1:G:378:LEU:N	2.77	0.47
1:G:626:GLY:HA3	1:G:676:ILE:O	2.14	0.47
1:H:208:SER:O	1:H:212:GLU:HB2	2.14	0.47
1:A:378:LEU:HD13	1:A:401:LEU:CD1	2.40	0.47
1:E:377:VAL:CG1	1:E:378:LEU:N	2.76	0.47
1:F:199:LYS:O	1:G:517:THR:HG23	2.13	0.47
1:F:208:SER:O	1:F:212:GLU:HB2	2.14	0.47
1:E:245:LYS:HB2	1:F:483:GLN:NE2	2.29	0.47
1:E:359:ARG:HH21	1:E:431:PRO:HG2	1.79	0.47
1:F:298:THR:CB	1:F:601:ASN:HB3	2.43	0.47
1:F:357:THR:HG22	1:F:435:ASN:HA	1.96	0.47
1:G:222:SER:HB3	1:G:225:LYS:HB2	1.95	0.47
1:B:199:LYS:O	1:C:517:THR:HG23	2.14	0.47
1:B:272:SER:CA	1:B:350:MET:HE3	2.44	0.47
1:C:359:ARG:HH21	1:C:431:PRO:HG2	1.78	0.47
1:D:347:ALA:HA	1:D:352:LEU:HD12	1.97	0.47
1:D:455:VAL:HG13	1:D:455:VAL:O	2.14	0.47
1:E:302:GLU:HA	1:E:303:PRO:HD2	1.64	0.47
1:G:680:LYS:HG2	1:G:681:TYR:CD2	2.49	0.47
1:A:377:VAL:CG1	1:A:378:LEU:N	2.77	0.47
1:B:633:LYS:O	1:B:637:LYS:HG3	2.14	0.47
1:E:298:THR:HG21	1:E:601:ASN:HD22	1.79	0.47
1:F:368:ASN:HB2	1:F:405:LEU:HG	1.96	0.47
1:F:412:PRO:HD3	1:F:419:ILE:HG13	1.96	0.47
1:G:357:THR:HB	1:G:433:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LYS:HD2	1:H:202:PHE:CE2	2.49	0.47
1:H:206:TRP:CD1	1:H:218:LYS:HD2	2.49	0.47
1:H:412:PRO:HD3	1:H:419:ILE:HG13	1.97	0.47
1:B:208:SER:O	1:B:212:GLU:HB2	2.14	0.47
1:D:197:LYS:HD2	1:D:202:PHE:CE2	2.50	0.47
1:H:455:VAL:O	1:H:455:VAL:HG13	2.15	0.47
1:H:542:TYR:HE2	1:H:543:GLN:HE21	1.61	0.47
1:H:558:THR:O	1:H:562:ILE:HG12	2.14	0.47
1:A:245:LYS:NZ	1:B:514:LEU:HD23	2.29	0.47
1:A:365:ARG:NH1	1:A:414:LYS:HD2	2.25	0.47
1:B:197:LYS:HD2	1:B:202:PHE:CE2	2.49	0.47
1:D:606:GLY:C	1:D:638:ILE:HD12	2.40	0.47
1:E:245:LYS:HE3	1:F:512:ASP:OD1	2.15	0.47
1:E:380:THR:OG1	1:E:396:ALA:HB2	2.15	0.47
1:C:648:ASP:HA	1:C:694:TYR:CE2	2.50	0.47
1:D:200:ARG:HH11	1:E:185:ASP:HB3	1.80	0.47
1:E:626:GLY:HA3	1:E:676:ILE:O	2.15	0.47
1:F:206:TRP:CD1	1:F:218:LYS:HD2	2.49	0.47
1:F:455:VAL:HG13	1:F:455:VAL:O	2.14	0.47
1:F:633:LYS:O	1:F:637:LYS:HG3	2.14	0.47
1:G:446:LYS:NZ	1:G:709:ASN:HD21	2.13	0.47
1:H:350:MET:HE2	1:H:352:LEU:HD21	1.97	0.47
1:A:266:MET:HB3	1:A:332:VAL:HG11	1.96	0.46
1:B:455:VAL:HG13	1:B:455:VAL:O	2.14	0.46
1:C:332:VAL:O	1:C:447:GLN:HB2	2.16	0.46
1:C:357:THR:HB	1:C:433:THR:HG22	1.96	0.46
1:C:377:VAL:CG1	1:C:378:LEU:N	2.77	0.46
1:C:380:THR:OG1	1:C:396:ALA:HB2	2.16	0.46
1:D:368:ASN:HB2	1:D:405:LEU:HG	1.96	0.46
1:H:378:LEU:HB2	1:H:401:LEU:HD22	1.97	0.46
1:A:492:ILE:HB	1:A:590:LEU:HD12	1.97	0.46
1:A:648:ASP:HA	1:A:694:TYR:CE2	2.51	0.46
1:B:412:PRO:HD3	1:B:419:ILE:HG13	1.96	0.46
1:C:196:VAL:HG21	1:D:516:THR:CG2	2.44	0.46
1:D:208:SER:O	1:D:212:GLU:HB2	2.14	0.46
1:D:412:PRO:HD3	1:D:419:ILE:HG13	1.96	0.46
1:E:253:HIS:CE1	1:E:255:LEU:HB2	2.50	0.46
1:E:446:LYS:NZ	1:E:709:ASN:HD21	2.14	0.46
1:A:245:LYS:HB2	1:B:483:GLN:HE22	1.79	0.46
1:A:626:GLY:HA3	1:A:676:ILE:O	2.15	0.46
1:D:633:LYS:O	1:D:637:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:MET:HB3	1:E:332:VAL:HG11	1.96	0.46
1:H:298:THR:CB	1:H:601:ASN:HB3	2.42	0.46
1:H:606:GLY:C	1:H:638:ILE:HD12	2.40	0.46
1:A:359:ARG:HH21	1:A:431:PRO:HG2	1.78	0.46
1:G:648:ASP:HA	1:G:694:TYR:CE2	2.51	0.46
1:B:200:ARG:HH11	1:C:185:ASP:HB3	1.80	0.46
1:B:347:ALA:HA	1:B:352:LEU:HD12	1.97	0.46
1:D:507:ALA:HB1	1:D:583:LEU:O	2.16	0.46
1:E:209:ASN:O	1:E:213:LYS:HE3	2.15	0.46
1:E:648:ASP:HA	1:E:694:TYR:CE2	2.50	0.46
1:F:178:ARG:HG3	1:F:185:ASP:OD2	2.16	0.46
1:G:266:MET:HB3	1:G:332:VAL:HG11	1.95	0.46
1:G:380:THR:OG1	1:G:396:ALA:HB2	2.15	0.46
1:A:357:THR:HB	1:A:433:THR:HG22	1.96	0.46
1:B:427:PHE:HD2	1:B:429:SER:HG	1.62	0.46
1:E:222:SER:HB3	1:E:225:LYS:HB2	1.97	0.46
1:A:380:THR:OG1	1:A:396:ALA:HB2	2.15	0.46
1:A:646:ILE:CD1	1:A:687:LEU:HD21	2.46	0.46
1:B:195:ASP:O	1:B:202:PHE:N	2.47	0.46
1:D:533:PHE:HB3	1:D:540:LEU:HD11	1.98	0.46
1:F:274:ASN:OD1	1:F:359:ARG:HB3	2.16	0.46
1:D:548:THR:HA	1:D:575:TYR:CE1	2.51	0.46
1:C:242:ARG:CG	1:C:242:ARG:NH1	2.70	0.46
1:D:232:PRO:HD3	1:D:480:VAL:HG11	1.98	0.46
1:G:209:ASN:O	1:G:213:LYS:HE3	2.16	0.46
1:H:682:ASN:O	1:H:684:LYS:N	2.49	0.46
1:A:612:VAL:HG12	1:A:726:ILE:HD11	1.99	0.45
1:B:289:ILE:HG12	1:B:290:SER:N	2.31	0.45
1:E:360:LEU:HD12	1:E:361:ASN:N	2.31	0.45
1:G:197:LYS:CG	1:G:198:ASN:H	2.24	0.45
1:G:492:ILE:HB	1:G:590:LEU:HD12	1.97	0.45
1:H:507:ALA:HB1	1:H:583:LEU:O	2.16	0.45
1:B:178:ARG:HG3	1:B:185:ASP:OD2	2.15	0.45
1:B:606:GLY:C	1:B:638:ILE:HD12	2.41	0.45
1:C:184:PRO:HD2	1:C:187:LEU:HD12	1.98	0.45
1:C:222:SER:HB3	1:C:225:LYS:HB2	1.98	0.45
1:E:605:VAL:HG12	1:E:704:GLU:N	2.31	0.45
1:F:606:GLY:C	1:F:638:ILE:HD12	2.42	0.45
1:G:301:SER:O	1:G:302:GLU:C	2.60	0.45
1:A:209:ASN:O	1:A:213:LYS:HE3	2.17	0.45
1:C:446:LYS:NZ	1:C:709:ASN:HD21	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ILE:HG12	1:D:290:SER:N	2.31	0.45
1:E:332:VAL:O	1:E:447:GLN:HB2	2.16	0.45
1:F:682:ASN:O	1:F:684:LYS:N	2.49	0.45
1:G:332:VAL:O	1:G:447:GLN:HB2	2.15	0.45
1:H:183:ILE:HD13	1:H:192:TYR:CZ	2.52	0.45
1:H:368:ASN:O	1:H:408:ASN:N	2.50	0.45
1:A:332:VAL:O	1:A:447:GLN:HB2	2.15	0.45
1:A:542:TYR:O	1:A:543:GLN:C	2.60	0.45
1:F:273:LYS:HB3	1:F:352:LEU:CD2	2.47	0.45
1:B:199:LYS:HD2	1:B:199:LYS:HA	1.74	0.45
1:B:633:LYS:HA	1:B:636:ARG:HG2	1.98	0.45
1:C:492:ILE:HB	1:C:590:LEU:HD12	1.98	0.45
1:F:527:LEU:HB3	1:F:533:PHE:CD1	2.52	0.45
1:G:378:LEU:HD13	1:G:401:LEU:HD22	1.97	0.45
1:H:220:LYS:O	1:H:519:PRO:HG2	2.17	0.45
1:C:365:ARG:NH2	1:C:416:LEU:O	2.47	0.45
1:C:411:TYR:HA	1:C:412:PRO:HA	1.83	0.45
1:F:289:ILE:HG12	1:F:290:SER:N	2.31	0.45
1:F:548:THR:HA	1:F:575:TYR:CE1	2.52	0.45
1:A:446:LYS:NZ	1:A:709:ASN:HD21	2.14	0.45
1:A:605:VAL:HG12	1:A:704:GLU:N	2.32	0.45
1:B:273:LYS:HB3	1:B:352:LEU:CD2	2.47	0.45
1:C:725:LEU:O	1:C:726:ILE:HD12	2.16	0.45
1:D:195:ASP:O	1:D:202:PHE:N	2.48	0.45
1:F:730:LYS:HD3	1:F:732:TYR:HE1	1.82	0.45
1:A:453:ASP:OD2	1:A:455:VAL:HG12	2.17	0.45
1:B:368:ASN:O	1:B:408:ASN:N	2.49	0.45
1:E:492:ILE:HB	1:E:590:LEU:HD12	1.98	0.45
1:F:347:ALA:HA	1:F:352:LEU:HD12	1.97	0.45
1:G:360:LEU:HD12	1:G:361:ASN:N	2.32	0.45
1:G:612:VAL:HG12	1:G:726:ILE:HD11	1.99	0.45
1:H:271:LEU:HB2	1:H:289:ILE:CG2	2.47	0.45
1:A:515:GLU:OE1	1:A:518:LYS:NZ	2.50	0.45
1:B:659:ARG:HB2	1:B:662:MET:HB2	1.99	0.45
1:D:633:LYS:HA	1:D:636:ARG:HG2	1.99	0.45
1:G:196:VAL:HG21	1:H:516:THR:HG21	1.99	0.45
1:G:384:VAL:HG22	1:G:390:THR:HB	1.99	0.45
1:G:605:VAL:HG12	1:G:704:GLU:N	2.32	0.45
1:H:533:PHE:HB3	1:H:540:LEU:HD11	1.98	0.45
1:C:406:ALA:O	1:C:409:ASN:HB2	2.17	0.45
1:C:453:ASP:OD2	1:C:455:VAL:HG12	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:ILE:CD1	1:C:687:LEU:HD21	2.47	0.45
1:E:542:TYR:O	1:E:543:GLN:C	2.60	0.45
1:G:378:LEU:HD12	1:G:378:LEU:HA	1.85	0.45
1:B:302:GLU:HA	1:B:303:PRO:HD3	1.70	0.44
1:B:406:ALA:O	1:B:409:ASN:HB2	2.17	0.44
1:D:183:ILE:HD13	1:D:192:TYR:CZ	2.52	0.44
1:D:433:THR:HG22	1:D:434:MET:N	2.27	0.44
1:E:200:ARG:HG3	1:E:202:PHE:CE2	2.52	0.44
1:E:293:THR:HG22	1:E:334:ILE:HA	1.99	0.44
1:F:334:ILE:CD1	1:F:442:LEU:HD11	2.47	0.44
1:H:289:ILE:HG12	1:H:290:SER:N	2.32	0.44
1:H:378:LEU:HD12	1:H:379:PRO:HD3	2.00	0.44
1:A:626:GLY:HA2	1:A:678:PHE:CE2	2.53	0.44
1:B:548:THR:HA	1:B:575:TYR:CE1	2.52	0.44
1:C:605:VAL:HG12	1:C:704:GLU:N	2.32	0.44
1:D:271:LEU:HB2	1:D:289:ILE:CG2	2.47	0.44
1:F:271:LEU:HB2	1:F:289:ILE:CG2	2.47	0.44
1:F:633:LYS:HA	1:F:636:ARG:HG2	1.99	0.44
1:G:184:PRO:HD2	1:G:187:LEU:HD12	2.00	0.44
1:G:266:MET:HA	1:G:364:ILE:HG22	1.99	0.44
1:A:360:LEU:HD12	1:A:361:ASN:N	2.31	0.44
1:B:533:PHE:HB3	1:B:540:LEU:HD11	1.99	0.44
1:B:553:ASN:HB2	1:B:590:LEU:HB3	2.00	0.44
1:E:378:LEU:HD12	1:E:378:LEU:HA	1.85	0.44
1:E:626:GLY:HA2	1:E:678:PHE:CE2	2.52	0.44
1:F:232:PRO:HD3	1:F:480:VAL:HG11	2.00	0.44
1:H:232:PRO:HD3	1:H:480:VAL:HG11	1.99	0.44
1:H:334:ILE:CD1	1:H:442:LEU:HD11	2.48	0.44
1:B:240:THR:CG2	1:B:242:ARG:H	2.25	0.44
1:B:682:ASN:O	1:B:684:LYS:N	2.50	0.44
1:C:209:ASN:O	1:C:213:LYS:HE3	2.17	0.44
1:E:245:LYS:HZ1	1:F:514:LEU:HD23	1.82	0.44
1:E:463:ASN:OD1	1:E:465:GLU:HG2	2.18	0.44
1:E:646:ILE:CD1	1:E:687:LEU:HD21	2.47	0.44
1:F:507:ALA:HB1	1:F:583:LEU:O	2.17	0.44
1:G:542:TYR:O	1:G:543:GLN:C	2.60	0.44
1:G:646:ILE:CD1	1:G:687:LEU:HD21	2.48	0.44
1:H:187:LEU:HD23	1:H:187:LEU:HA	1.75	0.44
1:H:633:LYS:HA	1:H:636:ARG:HG2	1.99	0.44
1:C:612:VAL:HG12	1:C:726:ILE:HD11	1.99	0.44
1:E:612:VAL:HG12	1:E:726:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:THR:CG2	1:F:242:ARG:H	2.25	0.44
1:F:406:ALA:O	1:F:409:ASN:HB2	2.17	0.44
1:G:406:ALA:O	1:G:409:ASN:HB2	2.18	0.44
1:H:406:ALA:O	1:H:409:ASN:HB2	2.17	0.44
1:H:548:THR:HA	1:H:575:TYR:CE1	2.52	0.44
1:B:183:ILE:HG12	1:B:203:LEU:HD21	1.99	0.44
1:B:527:LEU:HB3	1:B:533:PHE:CD1	2.53	0.44
1:C:266:MET:HA	1:C:364:ILE:HG22	1.99	0.44
1:D:183:ILE:HG12	1:D:203:LEU:HD21	2.00	0.44
1:D:220:LYS:O	1:D:519:PRO:HG2	2.17	0.44
1:E:272:SER:HB3	1:E:288:THR:HG22	2.00	0.44
1:E:637:LYS:HB3	1:E:637:LYS:HE2	1.59	0.44
1:F:183:ILE:HD13	1:F:192:TYR:CZ	2.53	0.44
1:F:200:ARG:NH1	1:G:185:ASP:HB3	2.33	0.44
1:F:533:PHE:HB3	1:F:540:LEU:HD11	1.99	0.44
1:B:226:TRP:CE2	1:B:234:SER:HB3	2.53	0.44
1:B:440:LEU:HD23	1:B:440:LEU:HA	1.85	0.44
1:E:266:MET:HA	1:E:364:ILE:HG22	2.00	0.44
1:G:599:ASP:HB3	1:G:605:VAL:HG21	2.00	0.44
1:A:517:THR:HG23	1:H:199:LYS:O	2.18	0.44
1:B:220:LYS:O	1:B:519:PRO:HG2	2.18	0.44
1:C:378:LEU:HD12	1:C:378:LEU:HA	1.85	0.44
1:D:406:ALA:O	1:D:409:ASN:HB2	2.17	0.44
1:D:616:HIS:CD2	1:D:726:ILE:HD13	2.53	0.44
1:F:235:ASP:O	1:F:239:VAL:HG22	2.18	0.44
1:F:561:ASN:O	1:F:565:GLN:HG3	2.18	0.44
1:F:659:ARG:HB2	1:F:662:MET:HB2	2.00	0.44
1:H:199:LYS:HA	1:H:199:LYS:HD2	1.74	0.44
1:H:659:ARG:HB2	1:H:662:MET:HB2	2.00	0.44
1:A:293:THR:HG22	1:A:334:ILE:HA	1.98	0.44
1:A:384:VAL:HG22	1:A:390:THR:HB	2.00	0.44
1:B:183:ILE:HD13	1:B:192:TYR:CZ	2.52	0.44
1:B:196:VAL:HG12	1:B:201:THR:HG22	2.00	0.44
1:B:271:LEU:HB2	1:B:289:ILE:CG2	2.47	0.44
1:B:334:ILE:CD1	1:B:442:LEU:HD11	2.48	0.44
1:C:578:LEU:HD12	1:C:578:LEU:HA	1.89	0.44
1:D:178:ARG:HG3	1:D:185:ASP:OD2	2.17	0.44
1:D:334:ILE:CD1	1:D:442:LEU:HD11	2.48	0.44
1:D:553:ASN:HB2	1:D:590:LEU:HB3	2.00	0.44
1:D:682:ASN:O	1:D:684:LYS:N	2.50	0.44
1:E:185:ASP:O	1:E:189:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:VAL:HG21	1:H:516:THR:CG2	2.48	0.44
1:G:378:LEU:HA	1:G:379:PRO:HD3	1.86	0.44
1:H:616:HIS:CD2	1:H:726:ILE:HD13	2.53	0.44
1:C:197:LYS:HB2	1:C:202:PHE:CE2	2.53	0.43
1:C:542:TYR:O	1:C:543:GLN:C	2.60	0.43
1:C:637:LYS:HB3	1:C:637:LYS:HE2	1.60	0.43
1:E:262:VAL:CG1	1:E:379:PRO:HG2	2.46	0.43
1:E:599:ASP:HB3	1:E:605:VAL:HG21	2.00	0.43
1:H:301:SER:O	1:H:302:GLU:HG3	2.18	0.43
1:A:222:SER:HA	1:A:223:PRO:HD2	1.81	0.43
1:A:406:ALA:O	1:A:409:ASN:HB2	2.18	0.43
1:C:599:ASP:HB3	1:C:605:VAL:HG21	2.00	0.43
1:H:433:THR:HG22	1:H:434:MET:N	2.27	0.43
1:B:200:ARG:NH1	1:C:185:ASP:HB3	2.33	0.43
1:B:232:PRO:HD3	1:B:480:VAL:HG11	2.00	0.43
1:B:353:ASN:C	1:B:355:ALA:H	2.26	0.43
1:B:616:HIS:CD2	1:B:726:ILE:HD13	2.52	0.43
1:C:195:ASP:HB3	1:C:197:LYS:NZ	2.33	0.43
1:D:659:ARG:HB2	1:D:662:MET:HB2	1.99	0.43
1:F:195:ASP:O	1:F:202:PHE:N	2.48	0.43
1:F:353:ASN:C	1:F:355:ALA:H	2.26	0.43
1:F:616:HIS:CD2	1:F:726:ILE:HD13	2.53	0.43
1:G:453:ASP:OD2	1:G:455:VAL:HG12	2.18	0.43
1:G:626:GLY:HA2	1:G:678:PHE:CE2	2.53	0.43
1:H:377:VAL:HG12	1:H:378:LEU:N	2.34	0.43
1:H:553:ASN:HB2	1:H:590:LEU:HB3	2.00	0.43
1:A:599:ASP:HB3	1:A:605:VAL:HG21	2.01	0.43
1:C:197:LYS:O	1:C:198:ASN:C	2.61	0.43
1:C:463:ASN:OD1	1:C:465:GLU:HG2	2.18	0.43
1:D:301:SER:O	1:D:302:GLU:HG3	2.18	0.43
1:D:345:THR:HG22	1:D:347:ALA:H	1.84	0.43
1:E:289:ILE:HG21	1:E:346:TRP:NE1	2.33	0.43
1:G:463:ASN:OD1	1:G:465:GLU:HG2	2.18	0.43
1:H:178:ARG:HG3	1:H:185:ASP:OD2	2.18	0.43
1:A:266:MET:HA	1:A:364:ILE:HG22	2.00	0.43
1:A:289:ILE:HG21	1:A:346:TRP:NE1	2.34	0.43
1:B:578:LEU:HD12	1:B:578:LEU:HA	1.83	0.43
1:C:179:ASP:HB3	1:C:224:GLU:C	2.44	0.43
1:C:384:VAL:HG22	1:C:390:THR:HB	1.99	0.43
1:D:353:ASN:C	1:D:355:ALA:H	2.26	0.43
1:D:561:ASN:O	1:D:565:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:SER:HA	1:E:223:PRO:HD2	1.81	0.43
1:E:406:ALA:O	1:E:409:ASN:HB2	2.18	0.43
1:F:220:LYS:O	1:F:519:PRO:HG2	2.18	0.43
1:G:204:SER:HA	1:G:205:PRO:HD3	1.89	0.43
1:H:585:ALA:O	1:H:586:LYS:HB2	2.19	0.43
1:A:179:ASP:HB3	1:A:224:GLU:C	2.44	0.43
1:B:231:ASP:HB2	1:B:232:PRO:CD	2.35	0.43
1:D:368:ASN:O	1:D:408:ASN:N	2.50	0.43
1:E:453:ASP:OD2	1:E:455:VAL:HG12	2.19	0.43
1:E:698:VAL:HB	1:E:727:PHE:HB3	2.01	0.43
1:F:368:ASN:O	1:F:408:ASN:N	2.49	0.43
1:F:585:ALA:O	1:F:586:LYS:HB2	2.18	0.43
1:A:197:LYS:O	1:A:198:ASN:C	2.61	0.43
1:A:350:MET:O	1:A:352:LEU:N	2.51	0.43
1:A:463:ASN:OD1	1:A:465:GLU:HG2	2.19	0.43
1:B:188:GLU:HA	1:B:192:TYR:CE2	2.54	0.43
1:B:235:ASP:O	1:B:239:VAL:HG22	2.18	0.43
1:B:411:TYR:CD1	1:B:412:PRO:HA	2.54	0.43
1:B:497:ASP:O	1:B:498:LEU:HB2	2.18	0.43
1:B:585:ALA:O	1:B:586:LYS:HB2	2.18	0.43
1:D:245:LYS:HA	1:D:245:LYS:HD3	1.88	0.43
1:E:179:ASP:HB3	1:E:224:GLU:C	2.44	0.43
1:F:269:ILE:HG13	1:F:293:THR:HG21	2.01	0.43
1:G:272:SER:HB3	1:G:288:THR:HG22	2.00	0.43
1:G:293:THR:HG22	1:G:334:ILE:HA	1.99	0.43
1:A:184:PRO:HD2	1:A:187:LEU:HD12	2.01	0.43
1:B:507:ALA:HB1	1:B:583:LEU:O	2.18	0.43
1:C:470:ARG:HG3	1:D:479:GLU:CD	2.44	0.43
1:E:223:PRO:HD2	1:E:517:THR:HG22	2.00	0.43
1:E:245:LYS:HB2	1:F:483:GLN:HE22	1.83	0.43
1:F:183:ILE:HG12	1:F:203:LEU:HD21	1.99	0.43
1:G:597:HIS:HD2	1:G:607:ALA:CA	2.32	0.43
1:H:397:LYS:HG2	1:H:400:GLN:HB3	2.00	0.43
1:H:417:ALA:HA	1:H:418:PRO:HD3	1.93	0.43
1:A:243:ILE:HG12	1:A:244:ASP:N	2.34	0.43
1:A:272:SER:HB3	1:A:288:THR:HG22	2.00	0.43
1:B:238:LYS:HD3	1:B:251:ALA:O	2.19	0.43
1:B:378:LEU:HA	1:B:379:PRO:HD3	1.87	0.43
1:C:197:LYS:HD3	1:C:202:PHE:CD2	2.48	0.43
1:C:597:HIS:HD2	1:C:607:ALA:CA	2.32	0.43
1:D:372:ALA:HA	1:D:373:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:MET:O	1:E:352:LEU:N	2.52	0.43
1:E:384:VAL:HG22	1:E:390:THR:HB	2.00	0.43
1:E:525:GLU:OE1	1:E:525:GLU:HA	2.19	0.43
1:F:378:LEU:HD12	1:F:379:PRO:HD3	2.01	0.43
1:F:399:ASN:N	1:F:399:ASN:ND2	2.56	0.43
1:F:705:ASN:CG	1:F:722:LYS:HB3	2.44	0.43
1:G:365:ARG:NH2	1:G:416:LEU:O	2.47	0.43
1:H:253:HIS:HA	1:H:254:PRO:HD3	1.90	0.43
1:H:353:ASN:C	1:H:355:ALA:H	2.26	0.43
1:A:185:ASP:O	1:A:189:VAL:HG23	2.18	0.43
1:A:223:PRO:HD2	1:A:517:THR:HG22	2.01	0.43
1:A:378:LEU:HA	1:A:379:PRO:HD3	1.85	0.43
1:A:585:ALA:O	1:A:586:LYS:HB2	2.19	0.43
1:A:638:ILE:HG13	1:A:639:LEU:HD12	2.01	0.43
1:B:453:ASP:OD2	1:B:455:VAL:HG12	2.19	0.43
1:C:365:ARG:NH1	1:C:414:LYS:HA	2.34	0.43
1:D:196:VAL:HG11	1:E:516:THR:HB	2.00	0.43
1:E:196:VAL:HG21	1:F:516:THR:CG2	2.49	0.43
1:E:494:ASN:OD1	1:E:592:ARG:HA	2.18	0.43
1:E:638:ILE:HG13	1:E:639:LEU:HD12	2.01	0.43
1:F:226:TRP:CE2	1:F:234:SER:HB3	2.53	0.43
1:H:373:PRO:HB3	1:H:404:ILE:HD11	2.01	0.43
1:H:453:ASP:OD2	1:H:455:VAL:HG12	2.19	0.43
1:C:185:ASP:O	1:C:189:VAL:HG23	2.19	0.42
1:C:350:MET:O	1:C:352:LEU:N	2.52	0.42
1:C:455:VAL:O	1:C:455:VAL:HG13	2.19	0.42
1:D:196:VAL:HG12	1:D:201:THR:HG22	2.00	0.42
1:D:235:ASP:O	1:D:239:VAL:HG22	2.19	0.42
1:D:238:LYS:HB3	1:D:252:ARG:O	2.19	0.42
1:E:204:SER:HA	1:E:205:PRO:HD3	1.88	0.42
1:F:188:GLU:HA	1:F:192:TYR:CE2	2.54	0.42
1:F:553:ASN:HB2	1:F:590:LEU:HB3	2.00	0.42
1:G:350:MET:O	1:G:352:LEU:N	2.52	0.42
1:H:235:ASP:O	1:H:239:VAL:HG22	2.19	0.42
1:H:345:THR:HG22	1:H:347:ALA:H	1.84	0.42
1:A:185:ASP:HB3	1:H:200:ARG:HH11	1.84	0.42
1:A:525:GLU:OE1	1:A:525:GLU:HA	2.19	0.42
1:B:345:THR:HG22	1:B:347:ALA:H	1.83	0.42
1:B:561:ASN:O	1:B:565:GLN:HG3	2.18	0.42
1:C:293:THR:HG22	1:C:334:ILE:HA	2.00	0.42
1:C:446:LYS:HD2	1:C:708:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:GLY:HA2	1:C:678:PHE:CE2	2.54	0.42
1:D:269:ILE:HG13	1:D:293:THR:HG21	2.01	0.42
1:E:548:THR:HA	1:E:575:TYR:CE1	2.54	0.42
1:F:453:ASP:OD2	1:F:455:VAL:HG12	2.18	0.42
1:H:183:ILE:HG12	1:H:203:LEU:HD21	2.01	0.42
1:H:411:TYR:CD1	1:H:412:PRO:HA	2.54	0.42
1:A:412:PRO:HD3	1:A:419:ILE:HG13	2.02	0.42
1:A:597:HIS:HD2	1:A:607:ALA:CA	2.33	0.42
1:C:360:LEU:HD12	1:C:361:ASN:N	2.32	0.42
1:D:527:LEU:HB3	1:D:533:PHE:CD1	2.54	0.42
1:E:197:LYS:O	1:E:198:ASN:C	2.61	0.42
1:E:243:ILE:HG12	1:E:244:ASP:N	2.34	0.42
1:E:597:HIS:HD2	1:E:607:ALA:CA	2.32	0.42
1:F:377:VAL:HG12	1:F:378:LEU:N	2.33	0.42
1:H:188:GLU:HA	1:H:192:TYR:CE2	2.55	0.42
1:H:196:VAL:HG12	1:H:201:THR:HG22	2.01	0.42
1:H:222:SER:HA	1:H:223:PRO:HD2	1.87	0.42
1:H:561:ASN:O	1:H:565:GLN:HG3	2.19	0.42
1:H:684:LYS:HA	1:H:684:LYS:HD2	1.61	0.42
1:A:370:GLY:O	1:A:407:PRO:HB3	2.19	0.42
1:A:401:LEU:HD22	1:A:403:GLN:O	2.19	0.42
1:A:578:LEU:HD12	1:A:578:LEU:HA	1.88	0.42
1:C:272:SER:HB3	1:C:288:THR:HG22	2.00	0.42
1:E:291:LYS:HD3	1:E:291:LYS:HA	1.78	0.42
1:E:370:GLY:O	1:E:407:PRO:HB3	2.19	0.42
1:E:383:LEU:HD22	1:E:391:LEU:HD12	2.02	0.42
1:F:403:GLN:OE1	1:G:453:ASP:HB2	2.20	0.42
1:F:433:THR:HG22	1:F:434:MET:N	2.27	0.42
1:G:289:ILE:HG21	1:G:346:TRP:NE1	2.34	0.42
1:A:365:ARG:NH2	1:A:416:LEU:O	2.47	0.42
1:A:648:ASP:HB3	1:A:652:LEU:N	2.31	0.42
1:C:289:ILE:HG21	1:C:346:TRP:NE1	2.34	0.42
1:D:175:VAL:HA	1:D:176:PRO:HD3	1.86	0.42
1:D:188:GLU:HA	1:D:192:TYR:CE2	2.55	0.42
1:D:226:TRP:CE2	1:D:234:SER:HB3	2.53	0.42
1:D:373:PRO:HB3	1:D:404:ILE:HD11	2.02	0.42
1:E:245:LYS:NZ	1:F:514:LEU:HD23	2.34	0.42
1:H:705:ASN:CG	1:H:722:LYS:HB3	2.44	0.42
1:A:299:HIS:HB3	1:A:500:LEU:HD13	2.02	0.42
1:A:365:ARG:NH1	1:A:414:LYS:HA	2.33	0.42
1:A:455:VAL:O	1:A:455:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HD12	1:B:379:PRO:HD3	2.01	0.42
1:C:638:ILE:HG13	1:C:639:LEU:HD12	2.01	0.42
1:D:411:TYR:CD1	1:D:412:PRO:HA	2.54	0.42
1:D:439:PHE:CD1	1:D:439:PHE:C	2.98	0.42
1:E:365:ARG:NH1	1:E:414:LYS:HA	2.34	0.42
1:F:238:LYS:HD3	1:F:251:ALA:O	2.19	0.42
1:F:411:TYR:CD1	1:F:412:PRO:HA	2.54	0.42
1:G:383:LEU:HD22	1:G:391:LEU:HD12	2.01	0.42
1:H:269:ILE:HG13	1:H:293:THR:HG21	2.01	0.42
1:H:649:THR:HG22	1:H:693:ASN:O	2.20	0.42
1:A:378:LEU:HD12	1:A:379:PRO:HD3	2.02	0.42
1:A:548:THR:HA	1:A:575:TYR:CE1	2.55	0.42
1:A:725:LEU:C	1:A:726:ILE:HD12	2.45	0.42
1:B:377:VAL:HG12	1:B:378:LEU:N	2.34	0.42
1:C:383:LEU:HD22	1:C:391:LEU:HD12	2.01	0.42
1:C:515:GLU:OE1	1:C:518:LYS:NZ	2.49	0.42
1:D:649:THR:HG22	1:D:693:ASN:O	2.20	0.42
1:E:433:THR:HG22	1:E:434:MET:H	1.85	0.42
1:F:196:VAL:HG12	1:F:201:THR:HG22	2.01	0.42
1:G:179:ASP:HB3	1:G:224:GLU:C	2.44	0.42
1:G:299:HIS:HB3	1:G:500:LEU:HD13	2.02	0.42
1:H:274:ASN:N	1:H:274:ASN:HD22	2.16	0.42
1:A:440:LEU:HD23	1:A:440:LEU:HA	1.90	0.42
1:B:649:THR:HG22	1:B:693:ASN:O	2.20	0.42
1:E:184:PRO:HD2	1:E:187:LEU:HD12	2.01	0.42
1:F:301:SER:O	1:F:302:GLU:HG3	2.19	0.42
1:F:345:THR:HG22	1:F:347:ALA:H	1.84	0.42
1:G:185:ASP:O	1:G:189:VAL:HG23	2.19	0.42
1:G:435:ASN:OD1	1:G:435:ASN:C	2.63	0.42
1:G:698:VAL:HB	1:G:727:PHE:HB3	2.01	0.42
1:A:411:TYR:HA	1:A:412:PRO:HA	1.83	0.42
1:C:435:ASN:OD1	1:C:435:ASN:C	2.63	0.42
1:D:350:MET:HE2	1:D:352:LEU:HD11	2.02	0.42
1:E:455:VAL:HG13	1:E:455:VAL:O	2.19	0.42
1:H:179:ASP:HB3	1:H:224:GLU:C	2.45	0.42
1:A:334:ILE:CD1	1:A:442:LEU:HD11	2.50	0.42
1:B:417:ALA:HA	1:B:418:PRO:HD3	1.92	0.42
1:D:179:ASP:HB3	1:D:224:GLU:C	2.45	0.42
1:D:378:LEU:HD12	1:D:379:PRO:HD3	2.01	0.42
1:E:365:ARG:NH1	1:E:414:LYS:HD2	2.26	0.42
1:E:497:ASP:O	1:E:498:LEU:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:585:ALA:O	1:E:586:LYS:HB2	2.19	0.42
1:F:175:VAL:HA	1:F:176:PRO:HD3	1.86	0.42
1:F:350:MET:HE2	1:F:352:LEU:HD11	2.00	0.42
1:G:455:VAL:HG13	1:G:455:VAL:O	2.19	0.42
1:G:725:LEU:C	1:G:726:ILE:HD12	2.45	0.42
1:H:527:LEU:HB3	1:H:533:PHE:CD1	2.55	0.42
1:H:652:LEU:HD13	1:H:652:LEU:C	2.45	0.42
1:B:269:ILE:HG13	1:B:293:THR:HG21	2.02	0.41
1:B:287:ARG:O	1:B:350:MET:HA	2.20	0.41
1:B:350:MET:HE2	1:B:352:LEU:HD11	2.02	0.41
1:C:245:LYS:HB2	1:D:483:GLN:NE2	2.35	0.41
1:C:433:THR:HG22	1:C:434:MET:H	1.85	0.41
1:D:453:ASP:OD2	1:D:455:VAL:HG12	2.19	0.41
1:F:238:LYS:HB3	1:F:252:ARG:O	2.20	0.41
1:F:287:ARG:O	1:F:350:MET:HA	2.20	0.41
1:G:401:LEU:HD12	1:G:403:GLN:N	2.34	0.41
1:G:412:PRO:HD3	1:G:419:ILE:HG13	2.02	0.41
1:G:446:LYS:HD2	1:G:708:ILE:HB	2.01	0.41
1:G:548:THR:HA	1:G:575:TYR:CE1	2.55	0.41
1:H:226:TRP:CE2	1:H:234:SER:HB3	2.54	0.41
1:A:262:VAL:CG1	1:A:379:PRO:HG2	2.46	0.41
1:A:433:THR:HG22	1:A:434:MET:H	1.86	0.41
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.75	0.41
1:D:200:ARG:NH1	1:E:185:ASP:HB3	2.34	0.41
1:E:422:ASN:O	1:E:432:ILE:HG13	2.20	0.41
1:G:223:PRO:HD2	1:G:517:THR:HG22	2.02	0.41
1:G:372:ALA:HA	1:G:373:PRO:HD3	1.89	0.41
1:G:422:ASN:O	1:G:432:ILE:HG13	2.21	0.41
1:G:497:ASP:O	1:G:498:LEU:CB	2.68	0.41
1:H:505:ILE:CG2	1:H:521:MET:HE3	2.50	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.89	0.41
1:B:652:LEU:C	1:B:652:LEU:HD13	2.45	0.41
1:C:383:LEU:HD23	1:C:384:VAL:N	2.36	0.41
1:D:705:ASN:CG	1:D:722:LYS:HB3	2.45	0.41
1:F:372:ALA:HA	1:F:373:PRO:HD3	1.82	0.41
1:G:637:LYS:HE2	1:G:637:LYS:HB3	1.59	0.41
1:H:255:LEU:HD13	1:H:521:MET:HE2	2.02	0.41
1:A:395:LYS:HD2	1:A:395:LYS:O	2.19	0.41
1:B:301:SER:O	1:B:302:GLU:HG3	2.20	0.41
1:B:439:PHE:CD1	1:B:439:PHE:C	2.98	0.41
1:B:705:ASN:CG	1:B:722:LYS:HB3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:VAL:HG12	1:D:378:LEU:N	2.34	0.41
1:G:291:LYS:HD3	1:G:291:LYS:HA	1.80	0.41
1:B:179:ASP:HB3	1:B:224:GLU:C	2.45	0.41
1:D:430:THR:HA	1:D:431:PRO:HD3	1.87	0.41
1:D:585:ALA:O	1:D:586:LYS:HB2	2.20	0.41
1:E:299:HIS:HB3	1:E:500:LEU:HD13	2.02	0.41
1:F:439:PHE:CD1	1:F:439:PHE:C	2.98	0.41
1:G:638:ILE:HG13	1:G:639:LEU:HD12	2.02	0.41
1:H:238:LYS:HB3	1:H:252:ARG:O	2.20	0.41
1:C:243:ILE:HG12	1:C:244:ASP:N	2.36	0.41
1:C:291:LYS:HA	1:C:291:LYS:HD3	1.80	0.41
1:C:525:GLU:OE1	1:C:525:GLU:HA	2.20	0.41
1:E:365:ARG:NH2	1:E:416:LEU:O	2.47	0.41
1:E:446:LYS:HD2	1:E:708:ILE:HB	2.02	0.41
1:G:214:LYS:HE2	1:G:214:LYS:HB3	1.86	0.41
1:G:585:ALA:O	1:G:586:LYS:HB2	2.21	0.41
1:H:195:ASP:O	1:H:202:PHE:N	2.48	0.41
1:H:439:PHE:CD1	1:H:439:PHE:C	2.98	0.41
1:A:422:ASN:O	1:A:432:ILE:HG13	2.21	0.41
1:A:637:LYS:HB3	1:A:637:LYS:HE2	1.59	0.41
1:A:698:VAL:HB	1:A:727:PHE:HB3	2.01	0.41
1:B:253:HIS:HA	1:B:254:PRO:HD3	1.90	0.41
1:C:334:ILE:CD1	1:C:442:LEU:HD11	2.51	0.41
1:C:378:LEU:HD12	1:C:379:PRO:HD3	2.02	0.41
1:C:412:PRO:HD3	1:C:419:ILE:HG13	2.02	0.41
1:C:422:ASN:O	1:C:432:ILE:HG13	2.21	0.41
1:E:378:LEU:HA	1:E:379:PRO:HD3	1.86	0.41
1:F:427:PHE:HD2	1:F:429:SER:HG	1.68	0.41
1:G:378:LEU:HD12	1:G:379:PRO:HD3	2.02	0.41
1:G:411:TYR:HA	1:G:412:PRO:HA	1.83	0.41
1:G:525:GLU:OE1	1:G:525:GLU:HA	2.19	0.41
1:A:494:ASN:OD1	1:A:592:ARG:HA	2.21	0.41
1:B:404:ILE:HG12	1:B:405:LEU:N	2.36	0.41
1:B:505:ILE:CG2	1:B:521:MET:HE3	2.51	0.41
1:E:412:PRO:HD3	1:E:419:ILE:HG13	2.02	0.41
1:E:725:LEU:C	1:E:726:ILE:HD12	2.45	0.41
1:F:179:ASP:HB3	1:F:224:GLU:C	2.45	0.41
1:G:494:ASN:OD1	1:G:592:ARG:HA	2.21	0.41
1:H:175:VAL:HA	1:H:176:PRO:HD3	1.86	0.41
1:H:221:SER:HB2	1:H:228:THR:OG1	2.20	0.41
1:H:497:ASP:O	1:H:498:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:HA	1:A:291:LYS:HD3	1.79	0.41
1:A:446:LYS:HD2	1:A:708:ILE:HB	2.02	0.41
1:B:238:LYS:HB3	1:B:252:ARG:O	2.21	0.41
1:C:197:LYS:HB2	1:C:202:PHE:HE2	1.85	0.41
1:C:223:PRO:HD2	1:C:517:THR:HG22	2.03	0.41
1:C:239:VAL:O	1:D:513:PRO:HG2	2.19	0.41
1:C:698:VAL:HB	1:C:727:PHE:HB3	2.01	0.41
1:D:497:ASP:O	1:D:498:LEU:HB2	2.21	0.41
1:E:196:VAL:HG21	1:F:516:THR:HG21	2.02	0.41
1:E:255:LEU:HD21	1:E:519:PRO:HG2	2.02	0.41
1:E:258:ALA:HA	1:E:371:THR:OG1	2.21	0.41
1:F:373:PRO:HB3	1:F:404:ILE:HD11	2.03	0.41
1:F:379:PRO:HA	1:F:455:VAL:HG13	2.02	0.41
1:G:197:LYS:O	1:G:198:ASN:C	2.62	0.41
1:G:334:ILE:CD1	1:G:442:LEU:HD11	2.51	0.41
1:G:365:ARG:NH1	1:G:414:LYS:HA	2.34	0.41
1:C:262:VAL:CG1	1:C:379:PRO:HG2	2.45	0.41
1:C:299:HIS:HB3	1:C:500:LEU:HD13	2.02	0.41
1:D:255:LEU:HD13	1:D:521:MET:HE2	2.02	0.41
1:D:417:ALA:HA	1:D:418:PRO:HD3	1.92	0.41
1:D:652:LEU:HD13	1:D:652:LEU:C	2.45	0.41
1:E:649:THR:HG23	1:E:694:TYR:CE2	2.56	0.41
1:F:255:LEU:HD13	1:F:521:MET:HE2	2.03	0.41
1:G:262:VAL:CG1	1:G:379:PRO:HG2	2.44	0.41
1:G:433:THR:HG22	1:G:434:MET:H	1.85	0.41
1:H:379:PRO:HA	1:H:455:VAL:HG13	2.03	0.41
1:A:383:LEU:HD23	1:A:384:VAL:N	2.35	0.40
1:B:379:PRO:HA	1:B:455:VAL:HG13	2.02	0.40
1:D:243:ILE:HG12	1:D:244:ASP:N	2.36	0.40
1:F:440:LEU:HD23	1:F:440:LEU:HA	1.85	0.40
1:B:433:THR:HG22	1:B:434:MET:N	2.27	0.40
1:D:379:PRO:HA	1:D:455:VAL:HG13	2.02	0.40
1:E:435:ASN:OD1	1:E:435:ASN:C	2.64	0.40
1:F:187:LEU:HD23	1:F:187:LEU:HA	1.77	0.40
1:G:258:ALA:HA	1:G:371:THR:OG1	2.21	0.40
1:G:383:LEU:HD23	1:G:384:VAL:N	2.37	0.40
1:G:537:ASN:C	1:G:539:ASN:H	2.29	0.40
1:H:404:ILE:HG12	1:H:405:LEU:N	2.36	0.40
1:A:214:LYS:HE2	1:A:214:LYS:HB3	1.86	0.40
1:A:385:LEU:HD12	1:A:386:GLY:N	2.36	0.40
1:C:548:THR:HA	1:C:575:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:LEU:C	1:C:726:ILE:HD12	2.46	0.40
1:D:620:ILE:HB	1:D:628:LEU:O	2.22	0.40
1:F:246:ASN:CB	1:F:373:PRO:HG3	2.52	0.40
1:G:239:VAL:O	1:H:513:PRO:HG2	2.22	0.40
1:H:620:ILE:HB	1:H:628:LEU:O	2.22	0.40
1:B:434:MET:HG2	1:B:438:GLN:HB3	2.04	0.40
1:F:199:LYS:HA	1:F:199:LYS:HD2	1.75	0.40
1:F:505:ILE:CG2	1:F:521:MET:HE3	2.52	0.40
1:B:243:ILE:HG12	1:B:244:ASP:N	2.36	0.40
1:C:401:LEU:HD22	1:C:403:GLN:O	2.21	0.40
1:C:453:ASP:CG	1:C:455:VAL:HG12	2.46	0.40
1:D:404:ILE:HG12	1:D:405:LEU:N	2.37	0.40
1:F:649:THR:HG22	1:F:693:ASN:O	2.20	0.40
1:G:363:ASN:ND2	1:H:388:ASN:HD22	2.20	0.40
1:G:649:THR:HG23	1:G:694:TYR:CE2	2.56	0.40
1:H:246:ASN:CB	1:H:373:PRO:HG3	2.52	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	510/548 (93%)	450 (88%)	52 (10%)	8 (2%)	7	36
1	B	517/548 (94%)	448 (87%)	54 (10%)	15 (3%)	3	24
1	C	509/548 (93%)	446 (88%)	55 (11%)	8 (2%)	7	36
1	D	510/548 (93%)	449 (88%)	48 (9%)	13 (2%)	4	27
1	E	511/548 (93%)	447 (88%)	55 (11%)	9 (2%)	6	34
1	F	511/548 (93%)	446 (87%)	52 (10%)	13 (2%)	4	27
1	G	510/548 (93%)	448 (88%)	54 (11%)	8 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	510/548 (93%)	447 (88%)	51 (10%)	12 (2%)	4	28
All	All	4088/4384 (93%)	3581 (88%)	421 (10%)	86 (2%)	5	31

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	713	ASN
1	B	181	ASP
1	B	325	SER
1	B	326	ASN
1	B	398	GLU
1	B	446	LYS
1	B	683	ASP
1	C	713	ASN
1	D	181	ASP
1	D	398	GLU
1	D	446	LYS
1	D	683	ASP
1	E	713	ASN
1	F	181	ASP
1	F	398	GLU
1	F	446	LYS
1	F	683	ASP
1	G	713	ASN
1	H	181	ASP
1	H	398	GLU
1	H	446	LYS
1	H	683	ASP
1	A	415	ASN
1	B	238	LYS
1	B	413	SER
1	C	415	ASN
1	D	238	LYS
1	D	413	SER
1	E	415	ASN
1	F	413	SER
1	G	415	ASN
1	H	238	LYS
1	H	413	SER
1	A	197	LYS
1	B	424	GLN
1	B	664	ASN

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Mol	Chain	Res	Type
1	B	684	LYS
1	B	711	SER
1	C	197	LYS
1	D	424	GLN
1	D	664	ASN
1	D	684	LYS
1	D	711	SER
1	E	197	LYS
1	F	238	LYS
1	F	664	ASN
1	F	684	LYS
1	F	711	SER
1	G	197	LYS
1	H	424	GLN
1	H	664	ASN
1	H	684	LYS
1	H	711	SER
1	A	577	VAL
1	A	728	SER
1	C	577	VAL
1	C	728	SER
1	E	577	VAL
1	E	728	SER
1	F	424	GLN
1	G	577	VAL
1	G	728	SER
1	A	177	ASP
1	A	351	GLY
1	A	636	ARG
1	C	177	ASP
1	C	636	ARG
1	E	177	ASP
1	E	351	GLY
1	E	636	ARG
1	G	177	ASP
1	G	351	GLY
1	G	636	ARG
1	B	542	TYR
1	D	542	TYR
1	E	301	SER
1	F	542	TYR
1	C	351	GLY

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Mol	Chain	Res	Type
1	B	455	VAL
1	D	455	VAL
1	F	455	VAL
1	H	455	VAL
1	B	686	PRO
1	D	686	PRO
1	F	686	PRO
1	H	686	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	453/491 (92%)	440 (97%)	13 (3%)	37	67
1	B	450/491 (92%)	443 (98%)	7 (2%)	55	75
1	C	457/491 (93%)	445 (97%)	12 (3%)	40	69
1	D	452/491 (92%)	447 (99%)	5 (1%)	65	79
1	E	458/491 (93%)	446 (97%)	12 (3%)	40	69
1	F	460/491 (94%)	453 (98%)	7 (2%)	57	76
1	G	460/491 (94%)	447 (97%)	13 (3%)	38	68
1	H	465/491 (95%)	455 (98%)	10 (2%)	45	71
All	All	3655/3928 (93%)	3576 (98%)	79 (2%)	45	71

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	ARG
1	A	252	ARG
1	A	381	THR
1	A	390	THR
1	A	395	LYS
1	A	401	LEU
1	A	421	LEU

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Mol	Chain	Res	Type
1	A	433	THR
1	A	527	LEU
1	A	574	ILE
1	A	619	VAL
1	A	630	ASN
1	A	706	THR
1	B	196	VAL
1	B	404	ILE
1	B	405	LEU
1	B	419	ILE
1	B	498	LEU
1	B	527	LEU
1	B	639	LEU
1	C	242	ARG
1	C	252	ARG
1	C	381	THR
1	C	390	THR
1	C	401	LEU
1	C	421	LEU
1	C	433	THR
1	C	527	LEU
1	C	574	ILE
1	C	619	VAL
1	C	630	ASN
1	C	706	THR
1	D	404	ILE
1	D	419	ILE
1	D	498	LEU
1	D	527	LEU
1	D	639	LEU
1	E	200	ARG
1	E	242	ARG
1	E	252	ARG
1	E	381	THR
1	E	390	THR
1	E	421	LEU
1	E	433	THR
1	E	527	LEU
1	E	574	ILE
1	E	619	VAL
1	E	630	ASN
1	E	706	THR

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Mol	Chain	Res	Type
1	F	196	VAL
1	F	399	ASN
1	F	401	LEU
1	F	404	ILE
1	F	419	ILE
1	F	527	LEU
1	F	639	LEU
1	G	242	ARG
1	G	252	ARG
1	G	381	THR
1	G	390	THR
1	G	401	LEU
1	G	421	LEU
1	G	426	ASP
1	G	433	THR
1	G	527	LEU
1	G	574	ILE
1	G	619	VAL
1	G	630	ASN
1	G	706	THR
1	H	196	VAL
1	H	352	LEU
1	H	399	ASN
1	H	401	LEU
1	H	404	ILE
1	H	419	ILE
1	H	498	LEU
1	H	527	LEU
1	H	639	LEU
1	H	648	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
1	A	389	GLN
1	A	437	ASN
1	A	447	GLN
1	A	543	GLN
1	A	573	ASN
1	A	597	HIS
1	A	601	ASN

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Mol	Chain	Res	Type
1	A	709	ASN
1	B	274	ASN
1	B	422	ASN
1	B	483	GLN
1	B	537	ASN
1	B	539	ASN
1	B	541	GLN
1	B	543	GLN
1	B	597	HIS
1	C	336	HIS
1	C	363	ASN
1	C	389	GLN
1	C	437	ASN
1	C	447	GLN
1	C	543	GLN
1	C	573	ASN
1	C	597	HIS
1	C	601	ASN
1	C	709	ASN
1	D	422	ASN
1	D	454	GLN
1	D	458	ASN
1	D	483	GLN
1	D	485	GLN
1	D	537	ASN
1	D	541	GLN
1	D	543	GLN
1	D	597	HIS
1	E	336	HIS
1	E	363	ASN
1	E	389	GLN
1	E	437	ASN
1	E	447	GLN
1	E	543	GLN
1	E	573	ASN
1	E	597	HIS
1	E	601	ASN
1	E	709	ASN
1	F	399	ASN
1	F	422	ASN
1	F	483	GLN
1	F	537	ASN

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Mol	Chain	Res	Type
1	F	541	GLN
1	F	543	GLN
1	F	597	HIS
1	G	336	HIS
1	G	363	ASN
1	G	389	GLN
1	G	437	ASN
1	G	447	GLN
1	G	543	GLN
1	G	573	ASN
1	G	597	HIS
1	G	601	ASN
1	G	709	ASN
1	H	274	ASN
1	H	399	ASN
1	H	422	ASN
1	H	483	GLN
1	H	537	ASN
1	H	539	ASN
1	H	541	GLN
1	H	597	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/548 (94%)	-1.48	0 100 100	5, 45, 111, 207	0
1	B	523/548 (95%)	-1.38	0 100 100	4, 55, 140, 335	0
1	C	517/548 (94%)	-1.48	0 100 100	8, 46, 110, 234	0
1	D	518/548 (94%)	-1.39	0 100 100	8, 54, 136, 258	0
1	E	519/548 (94%)	-1.47	0 100 100	5, 46, 120, 198	0
1	F	519/548 (94%)	-1.40	0 100 100	5, 55, 142, 205	0
1	G	518/548 (94%)	-1.46	0 100 100	5, 46, 111, 264	0
1	H	518/548 (94%)	-1.39	0 100 100	6, 54, 135, 221	0
All	All	4150/4384 (94%)	-1.43	0 100 100	4, 50, 126, 335	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	736	1/1	1.00	0.01	35,35,35,35	0
2	CA	A	737	1/1	1.00	0.01	20,20,20,20	0
2	CA	B	736	1/1	1.00	0.02	56,56,56,56	0
2	CA	B	737	1/1	1.00	0.01	20,20,20,20	0
2	CA	C	736	1/1	1.00	0.01	33,33,33,33	0
2	CA	C	737	1/1	1.00	0.02	18,18,18,18	0
2	CA	D	736	1/1	1.00	0.01	44,44,44,44	0
2	CA	D	737	1/1	1.00	0.01	25,25,25,25	0
2	CA	E	736	1/1	1.00	0.01	38,38,38,38	0
2	CA	E	737	1/1	1.00	0.01	24,24,24,24	0
2	CA	F	736	1/1	1.00	0.02	47,47,47,47	0
2	CA	F	737	1/1	1.00	0.01	20,20,20,20	0
2	CA	G	736	1/1	1.00	0.01	40,40,40,40	0
2	CA	G	737	1/1	1.00	0.01	23,23,23,23	0
2	CA	H	736	1/1	1.00	0.01	37,37,37,37	0
2	CA	H	737	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.