Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:02 PM GMT

PDB ID	:	4NHG
Title	:	Crystal Structure of 2G12 IgG Dimer
Authors	:	Wu, Y.; West Jr., A.P.; Kim, H.J.; Thornton, M.E.; Ward, A.B.; Bjorkman, P.J.
Deposited on	:	2013-11-05
Resolution	:	8.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

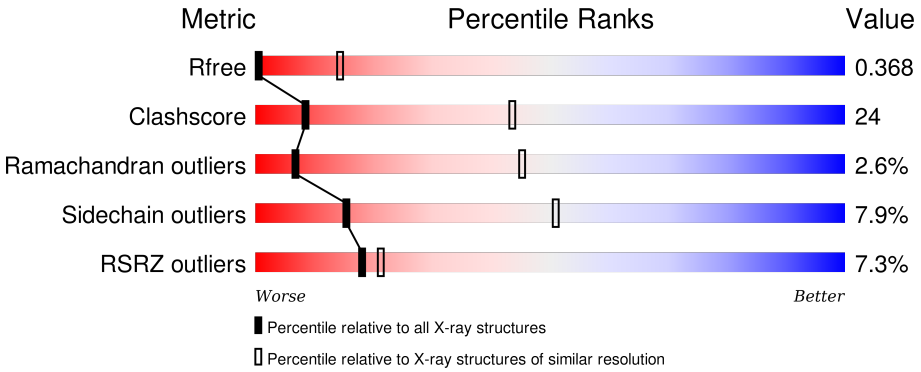
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 8.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	243	4% 53% 33% • 12%
1	D	243	2% 50% 33% 5% 12%
1	E	243	10% 50% 33% 5% 12%
1	H	243	2% 50% 35% • 12%
1	I	243	9% 50% 36% • 12%

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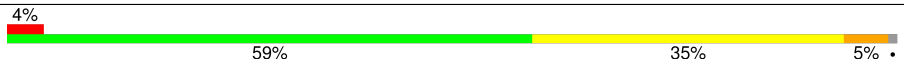
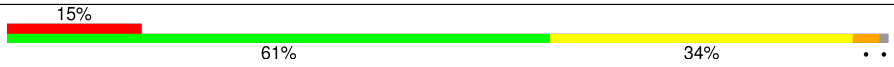
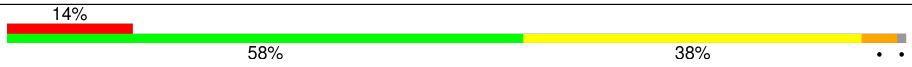
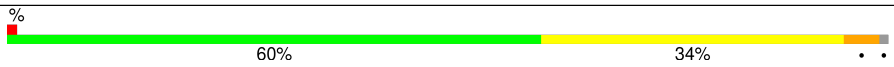
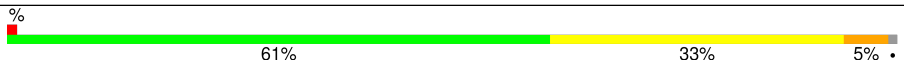
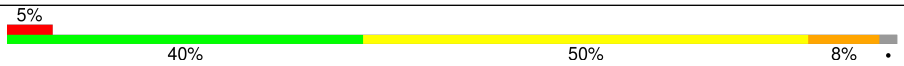
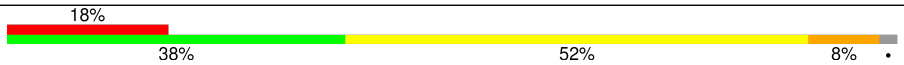
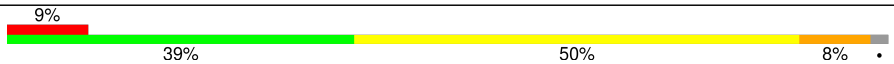
Mol	Chain	Length	Quality of chain
1	M	243	
2	B	213	
2	C	213	
2	F	213	
2	G	213	
2	K	213	
2	L	213	
3	J	211	
3	N	211	
3	O	211	
3	P	211	
3	X	211	
3	Y	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29250 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 2G12 IgG dimer heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	D	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			
1	E	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	I	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			
1	H	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	M	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			

- Molecule 2 is a protein called 2G12 IgG dimer light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	C	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	F	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	G	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	K	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	L	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			

- Molecule 3 is a protein called Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	N	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	X	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	Y	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	O	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	P	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	272	GLN	GLU	CONFLICT	UNP Q6PYX1
X	283	GLN	GLU	CONFLICT	UNP Q6PYX1
X	294	GLN	GLU	CONFLICT	UNP Q6PYX1
X	312	ASN	ASP	CONFLICT	UNP Q6PYX1
X	315	ASP	ASN	CONFLICT	UNP Q6PYX1
X	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
Y	272	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	283	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	294	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	312	ASN	ASP	CONFLICT	UNP Q6PYX1
Y	315	ASP	ASN	CONFLICT	UNP Q6PYX1
Y	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
J	272	GLN	GLU	CONFLICT	UNP Q6PYX1
J	283	GLN	GLU	CONFLICT	UNP Q6PYX1
J	294	GLN	GLU	CONFLICT	UNP Q6PYX1
J	312	ASN	ASP	CONFLICT	UNP Q6PYX1
J	315	ASP	ASN	CONFLICT	UNP Q6PYX1
J	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
N	272	GLN	GLU	CONFLICT	UNP Q6PYX1
N	283	GLN	GLU	CONFLICT	UNP Q6PYX1
N	294	GLN	GLU	CONFLICT	UNP Q6PYX1
N	312	ASN	ASP	CONFLICT	UNP Q6PYX1
N	315	ASP	ASN	CONFLICT	UNP Q6PYX1
N	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	272	GLN	GLU	CONFLICT	UNP Q6PYX1
O	283	GLN	GLU	CONFLICT	UNP Q6PYX1
O	294	GLN	GLU	CONFLICT	UNP Q6PYX1
O	312	ASN	ASP	CONFLICT	UNP Q6PYX1

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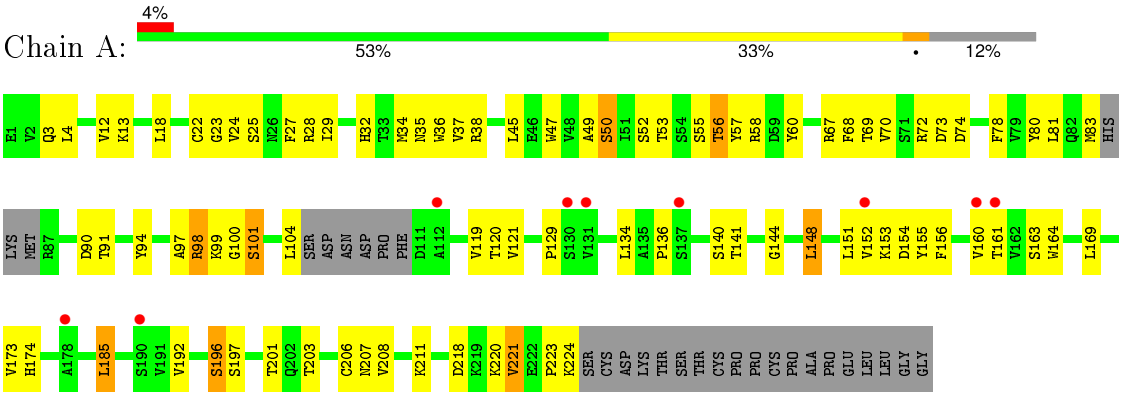
Chain	Residue	Modelled	Actual	Comment	Reference
O	315	ASP	ASN	CONFLICT	UNP Q6PYX1
O	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
P	272	GLN	GLU	CONFLICT	UNP Q6PYX1
P	283	GLN	GLU	CONFLICT	UNP Q6PYX1
P	294	GLN	GLU	CONFLICT	UNP Q6PYX1
P	312	ASN	ASP	CONFLICT	UNP Q6PYX1
P	315	ASP	ASN	CONFLICT	UNP Q6PYX1
P	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

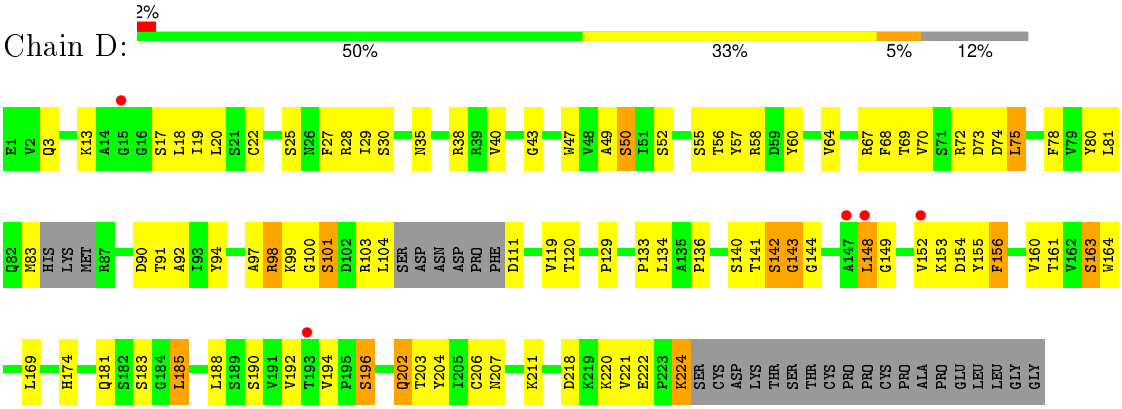
- Molecule 1: 2G12 IgG dimer heavy chain

Chain A:



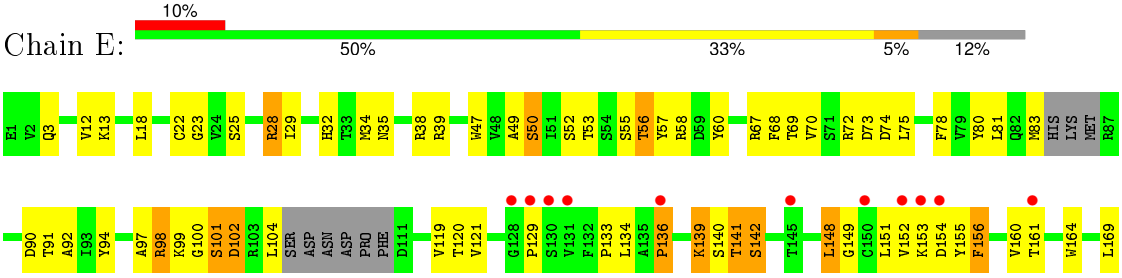
- Molecule 1: 2G12 IgG dimer heavy chain

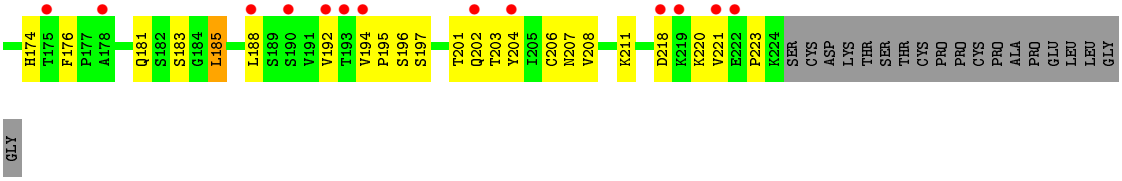
Chain D:



- Molecule 1: 2G12 IgG dimer heavy chain

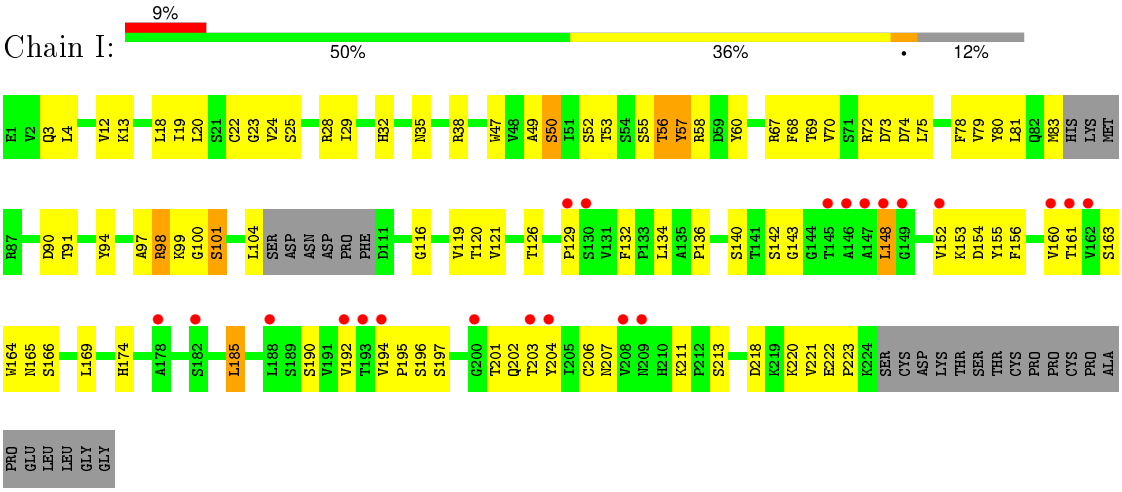
Chain E:





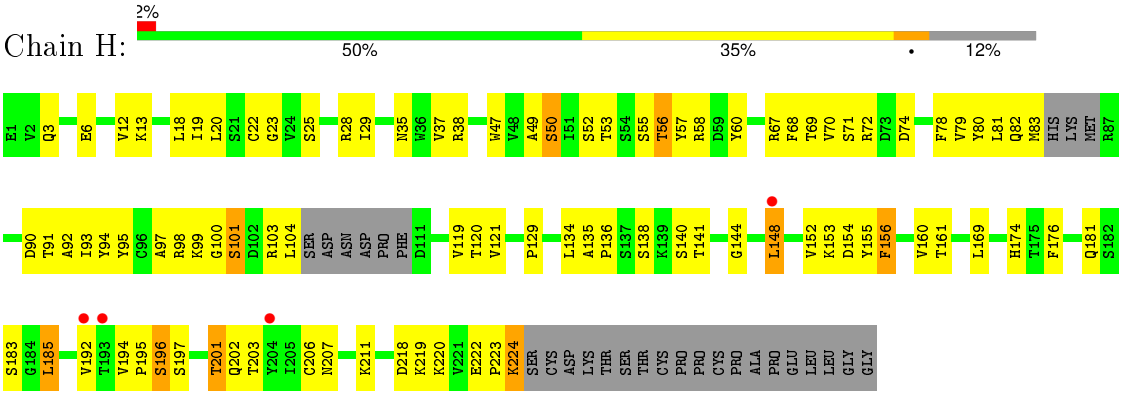
- Molecule 1: 2G12 IgG dimer heavy chain

Chain I:



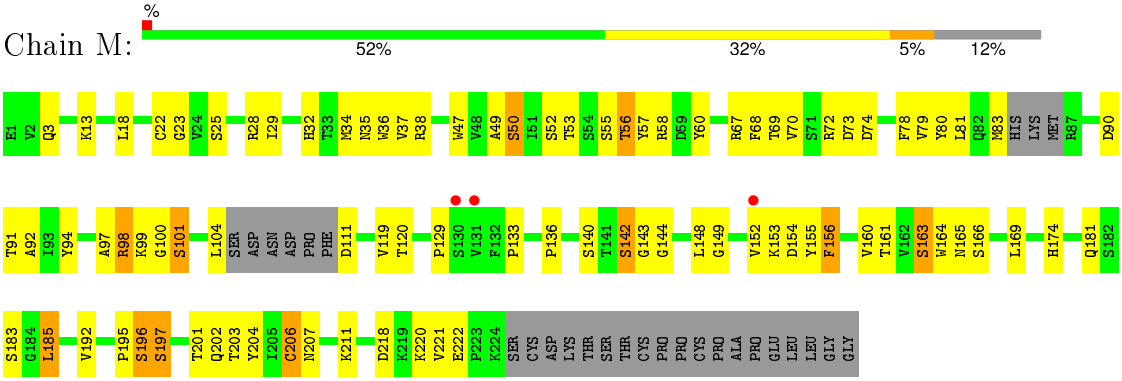
- Molecule 1: 2G12 IgG dimer heavy chain

Chain H:



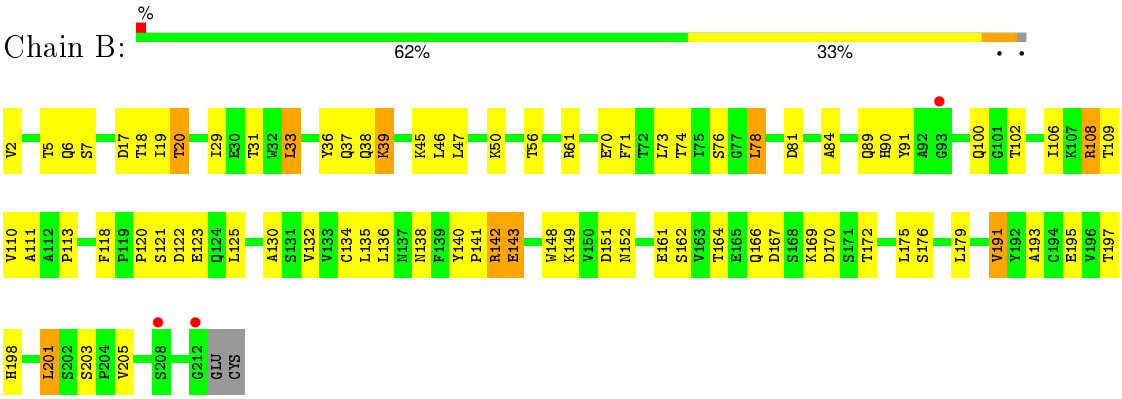
- Molecule 1: 2G12 IgG dimer heavy chain

Chain M:



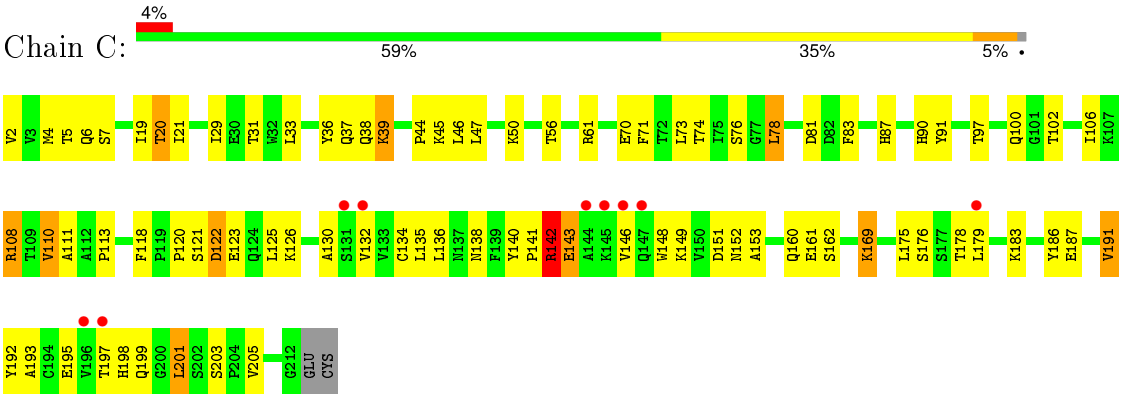
- Molecule 2: 2G12 IgG dimer light chain

Chain B:



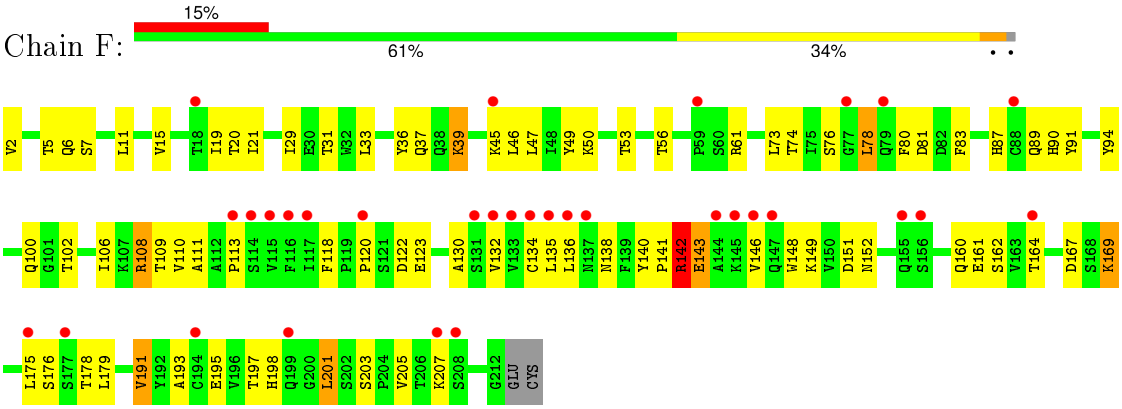
• Molecule 2: 2G12 IgG dimer light chain

Chain C:



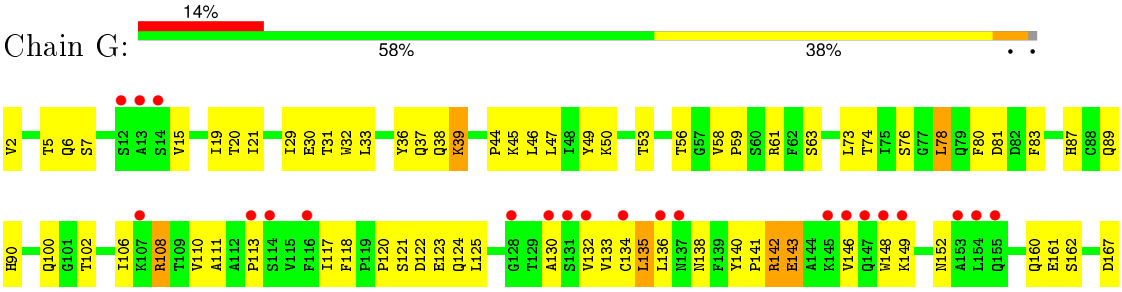
• Molecule 2: 2G12 IgG dimer light chain

Chain F:

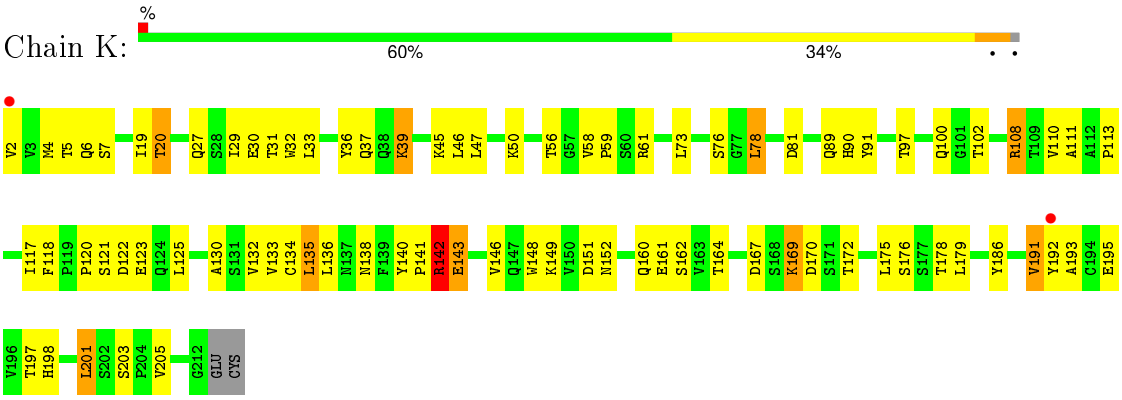


• Molecule 2: 2G12 IgG dimer light chain

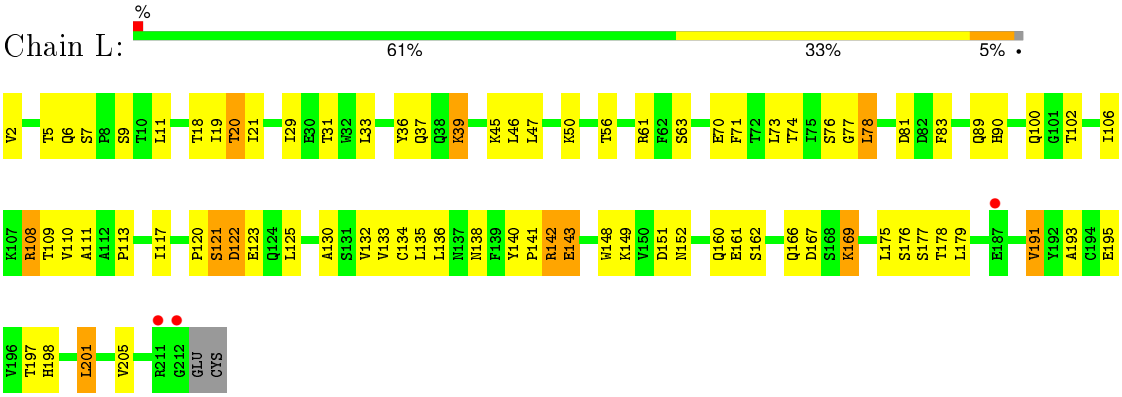
Chain G:



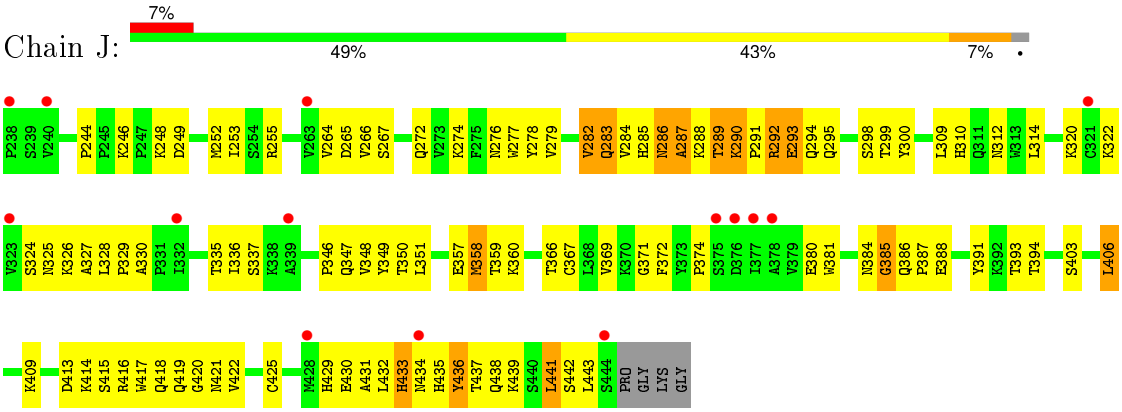
• Molecule 2: 2G12 IgG dimer light chain



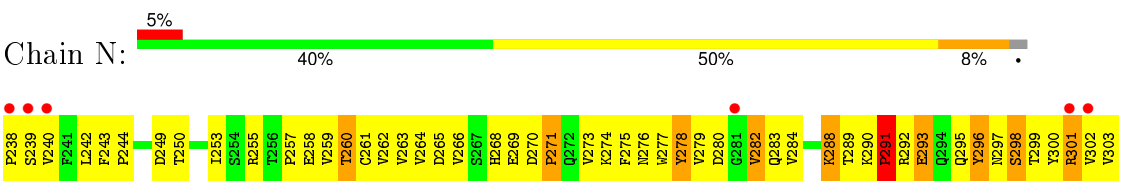
• Molecule 2: 2G12 IgG dimer light chain

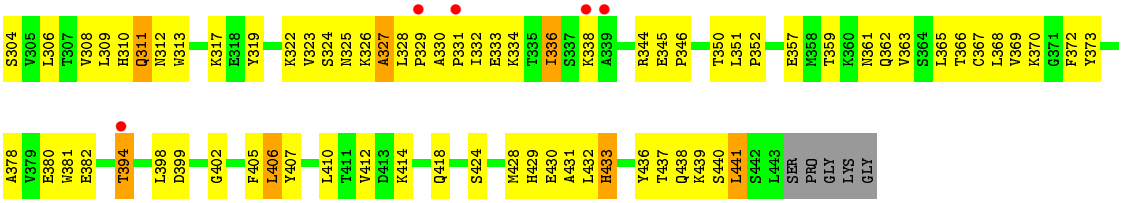


• Molecule 3: Hepatitis B virus receptor binding protein



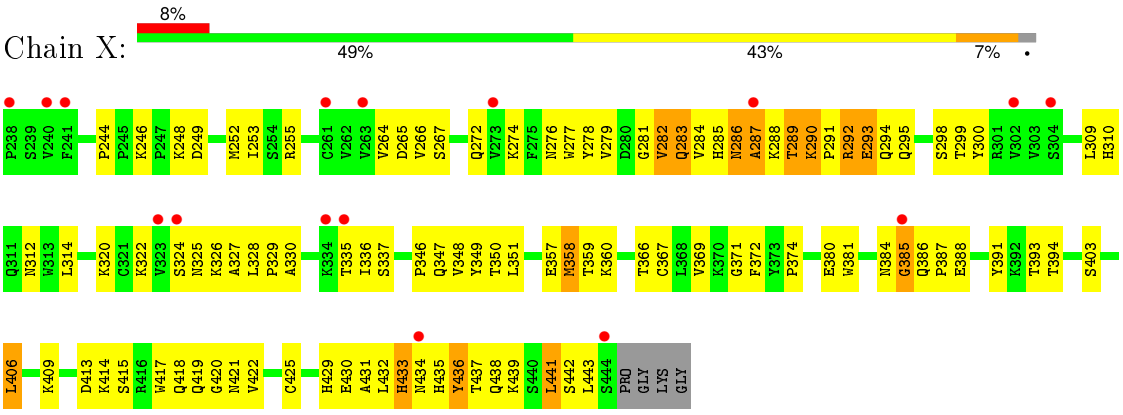
• Molecule 3: Hepatitis B virus receptor binding protein





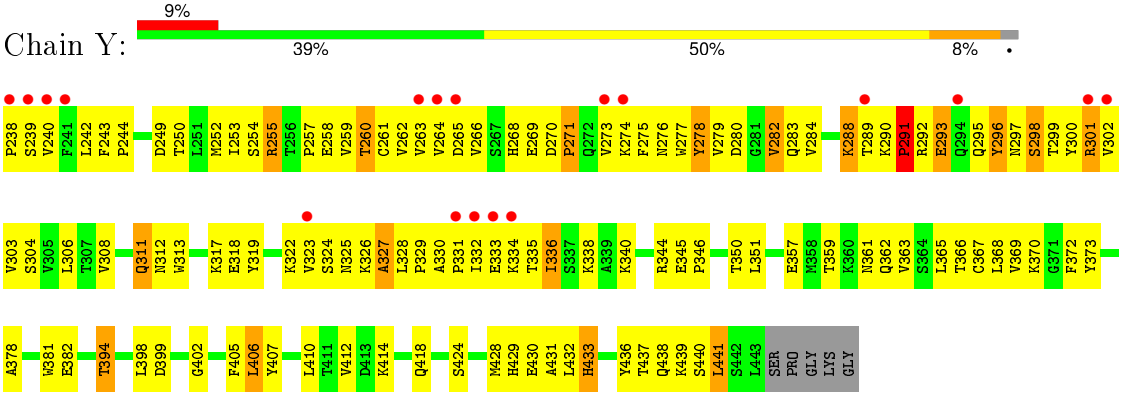
• Molecule 3: Hepatitis B virus receptor binding protein

Chain X:



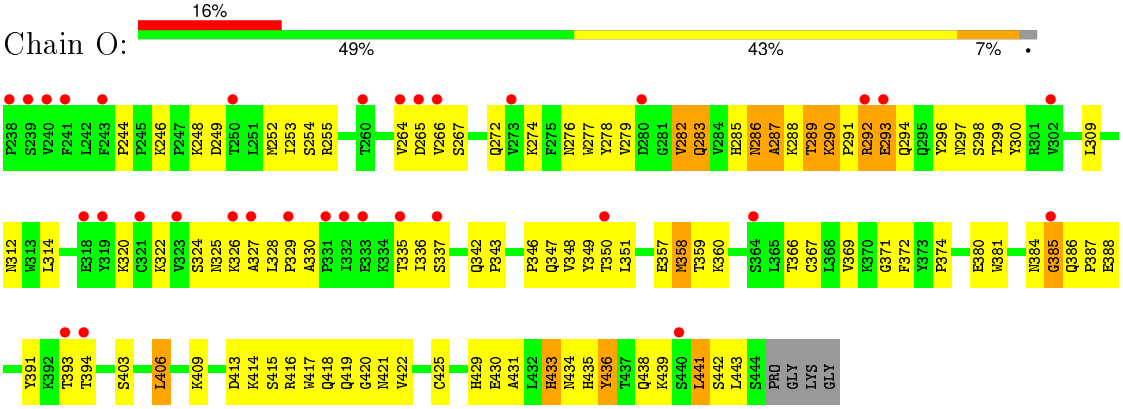
• Molecule 3: Hepatitis B virus receptor binding protein

Chain Y:



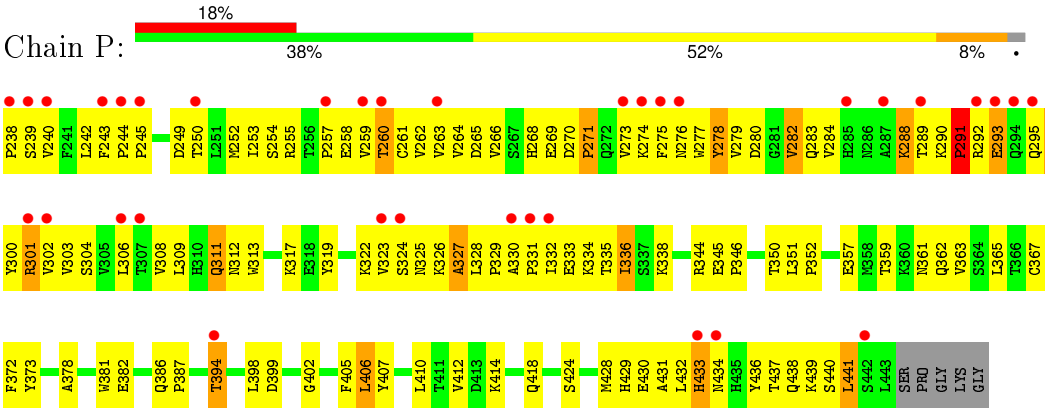
• Molecule 3: Hepatitis B virus receptor binding protein

Chain O:



• Molecule 3: Hepatitis B virus receptor binding protein

Chain P:


18%
38%
52%
8%
P238 S239 V240 P241 L242 F243 P244 P245 D249 T250 L251 M252 I253 S254 R255 T256 P257 E258 V259 T260 C261 V262 V263 V264 D265 V266 S267 H268 E269 D270 P271 Q272 V273 K274 F275 N276 W277 Y278 V279 D280 G281 V282 Q283 V284 H285 N286 A287 K288 T289 K290 P291 R292 E293 Q294 Q295 Y296 N297 S298 T299
Y300 R301 V302 V303 S304 V305 L306 T307 V308 L309 H310 Q311 N312 W313 K317 E318 Y319 K322 V323 S324 N325 K326 A327 L328 P329 A330 P331 I332 E333 K334 T335 I336 S337 K338 R344 E345 P346 T350 L351 P352 E357 M358 T359 K360 N361 Q362 V363 S364 L365 T366 C367 L368 V369 K370 G371
F372 Y373 A378 W381 E382 Q386 P387 T394 L398 D399 G402 F405 L406 Y407 L410 T411 V412 D413 K414 Q418 S424 M428 H429 E430 A431 L432 H433 N434 H435 Y436 T437 Q438 K439 S440 L441 S442 L443 SER PRO GLY LYS GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	246.25Å 246.25Å 657.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.75 – 8.00 39.75 – 7.43	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.75-8.00) 82.2 (39.75-7.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 7.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.359 , 0.369 0.352 , 0.368	Depositor DCC
R_{free} test set	1263 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	296.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 280.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 13337 reflections	Xtriage
F_o,F_c correlation	0.60	EDS
Total number of atoms	29250	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.69	1/1633 (0.1%)	0.95	4/2220 (0.2%)
1	D	0.63	0/1631	0.85	3/2214 (0.1%)
1	E	0.67	0/1633	0.93	4/2220 (0.2%)
1	H	0.63	0/1633	0.92	3/2220 (0.1%)
1	I	0.68	0/1631	0.83	3/2214 (0.1%)
1	M	0.68	2/1631 (0.1%)	0.85	3/2214 (0.1%)
2	B	0.63	0/1654	0.75	1/2246 (0.0%)
2	C	0.70	1/1654 (0.1%)	0.78	2/2246 (0.1%)
2	F	0.69	0/1654	0.77	2/2246 (0.1%)
2	G	0.69	1/1654 (0.1%)	0.77	1/2246 (0.0%)
2	K	0.63	0/1654	0.77	3/2246 (0.1%)
2	L	0.67	1/1654 (0.1%)	0.78	1/2246 (0.0%)
3	J	0.43	0/1706	0.68	0/2323
3	N	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	O	0.43	0/1706	0.68	0/2323
3	P	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	X	0.43	0/1706	0.68	0/2323
3	Y	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
All	All	0.60	9/29931 (0.0%)	0.78	36/40683 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
3	N	0	1
3	P	0	1
3	Y	0	1
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	433	HIS	CA-C	11.57	1.83	1.52
3	N	433	HIS	CA-C	11.50	1.82	1.52
3	P	433	HIS	CA-C	11.50	1.82	1.52
1	M	36	TRP	CB-CG	6.40	1.61	1.50
2	C	143	GLU	CB-CG	6.03	1.63	1.52
2	L	143	GLU	CB-CG	5.60	1.62	1.52
1	A	36	TRP	CB-CG	5.48	1.60	1.50
2	G	143	GLU	CB-CG	5.30	1.62	1.52
1	M	197	SER	CB-OG	-5.20	1.35	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	ARG	NE-CZ-NH1	-17.15	111.73	120.30
1	H	28	ARG	NE-CZ-NH1	-16.64	111.98	120.30
1	E	28	ARG	NE-CZ-NH1	-15.56	112.52	120.30
1	A	28	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	E	28	ARG	NE-CZ-NH2	13.74	127.17	120.30
1	H	28	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	D	28	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	M	28	ARG	NE-CZ-NH2	-11.26	114.67	120.30
2	G	135	LEU	CA-CB-CG	10.28	138.94	115.30
1	D	28	ARG	NE-CZ-NH1	10.17	125.38	120.30
2	F	135	LEU	CA-CB-CG	9.76	137.74	115.30
2	B	135	LEU	CA-CB-CG	9.65	137.50	115.30
1	I	28	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	C	135	LEU	CA-CB-CG	9.59	137.35	115.30
1	M	28	ARG	NE-CZ-NH1	9.35	124.98	120.30
2	K	135	LEU	CA-CB-CG	9.18	136.42	115.30
2	L	135	LEU	CA-CB-CG	9.13	136.30	115.30
1	I	28	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	E	28	ARG	CD-NE-CZ	8.21	135.09	123.60
1	A	28	ARG	CD-NE-CZ	7.90	134.66	123.60
1	H	28	ARG	CD-NE-CZ	7.30	133.82	123.60
3	N	433	HIS	CB-CA-C	-6.57	97.26	110.40
3	Y	433	HIS	CB-CA-C	-6.56	97.27	110.40
3	P	433	HIS	CB-CA-C	-6.54	97.33	110.40
3	Y	433	HIS	N-CA-C	-6.29	94.02	111.00
3	P	433	HIS	N-CA-C	-6.28	94.03	111.00
3	N	433	HIS	N-CA-C	-6.28	94.04	111.00
2	F	142	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	K	142	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	M	28	ARG	CD-NE-CZ	5.53	131.34	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	151	LEU	CA-CB-CG	5.46	127.86	115.30
2	C	142	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	I	28	ARG	CD-NE-CZ	5.18	130.85	123.60
1	D	28	ARG	CD-NE-CZ	5.11	130.75	123.60
2	K	169	LYS	CD-CE-NZ	5.01	123.23	111.70
1	A	151	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	139	LYS	Peptide
1	E	140	SER	Peptide
1	E	142	SER	Peptide
3	N	373	TYR	Sidechain
3	P	373	TYR	Sidechain
3	Y	373	TYR	Sidechain

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	1600	0	1581	73	0
1	D	1600	0	1579	96	11
1	E	1600	0	1581	72	0
1	H	1600	0	1580	78	2
1	I	1600	0	1578	78	0
1	M	1600	0	1579	85	0
2	B	1618	0	1580	49	23
2	C	1618	0	1580	54	0
2	F	1618	0	1580	69	0
2	G	1618	0	1580	58	2
2	K	1618	0	1580	54	0
2	L	1618	0	1580	57	19
3	J	1660	0	1632	99	60
3	N	1654	0	1627	114	37
3	O	1660	0	1630	93	19

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1654	0	1624	123	37
3	X	1660	0	1632	98	56
3	Y	1654	0	1627	118	37
All	All	29250	0	28730	1381	174

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 24.

All (1381) 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:D:103:ARG:C	2:F:50:LYS:HZ2	1.05	1.59
3:P:433:HIS:C	3:P:433:HIS:CA	1.82	1.45
3:N:433:HIS:C	3:N:433:HIS:CA	1.82	1.45
3:Y:433:HIS:C	3:Y:433:HIS:CA	1.83	1.45
1:D:103:ARG:CA	2:F:50:LYS:NZ	1.90	1.34
1:D:103:ARG:C	2:F:50:LYS:NZ	1.79	1.33
2:F:207:LYS:NZ	1:M:201:THR:HB	1.41	1.31
1:D:103:ARG:CA	2:F:50:LYS:HZ3	1.44	1.27
1:D:75:LEU:HD22	1:I:57:TYR:CZ	1.76	1.20
1:A:104:LEU:HD12	1:E:28:ARG:HG3	1.28	1.10
1:D:103:ARG:HA	2:F:50:LYS:NZ	1.53	1.09
3:P:266:VAL:HB	3:P:300:TYR:HB2	1.45	0.99
3:N:266:VAL:HB	3:N:300:TYR:HB2	1.45	0.99
3:Y:266:VAL:HB	3:Y:300:TYR:HB2	1.45	0.99
1:I:201:THR:HG1	1:I:202:GLN:N	1.62	0.96
1:H:174:HIS:NE2	2:K:138:ASN:OD1	1.99	0.96
1:A:174:HIS:NE2	2:B:138:ASN:OD1	2.00	0.94
1:D:103:ARG:HA	2:F:50:LYS:HZ3	0.76	0.92
3:X:272:GLN:HE22	3:X:326:LYS:HD2	1.35	0.92
3:O:272:GLN:HE22	3:O:326:LYS:HD2	1.35	0.91
2:F:207:LYS:HZ2	1:M:201:THR:HB	1.00	0.91
3:J:272:GLN:HE22	3:J:326:LYS:HD2	1.35	0.91
3:O:282:VAL:O	3:O:283:GLN:HB2	1.72	0.90
3:X:282:VAL:O	3:X:283:GLN:HB2	1.72	0.90
3:Y:311:GLN:H	3:Y:311:GLN:NE2	1.71	0.89
3:J:282:VAL:O	3:J:283:GLN:HB2	1.72	0.89
3:N:311:GLN:NE2	3:N:311:GLN:H	1.71	0.89
3:P:311:GLN:H	3:P:311:GLN:NE2	1.71	0.89
1:D:103:ARG:O	2:F:50:LYS:NZ	1.96	0.88
1:D:204:TYR:O	1:D:221:VAL:N	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:290:LYS:NZ	2:L:109:THR:HG21	1.90	0.86
1:E:174:HIS:NE2	2:F:138:ASN:OD1	2.08	0.85
3:N:328:LEU:HD21	3:N:332:ILE:HG13	1.59	0.84
1:A:197:SER:CB	3:X:295:GLN:HE22	1.90	0.84
2:F:207:LYS:NZ	1:M:201:THR:CB	2.35	0.84
3:Y:291:PRO:HB3	3:Y:304:SER:HA	1.60	0.84
1:I:148:LEU:HD13	1:I:221:VAL:HB	1.59	0.84
3:X:346:PRO:HB3	3:X:372:PHE:HB3	1.60	0.83
3:P:328:LEU:HD21	3:P:332:ILE:HG13	1.59	0.83
1:A:3:GLN:HB2	1:A:25:SER:HB2	1.58	0.83
3:P:243:PHE:HB2	3:P:260:THR:HG23	1.60	0.83
3:Y:328:LEU:HD21	3:Y:332:ILE:HG13	1.59	0.83
3:N:291:PRO:HB3	3:N:304:SER:HA	1.60	0.83
3:P:291:PRO:HB3	3:P:304:SER:HA	1.60	0.83
3:O:346:PRO:HB3	3:O:372:PHE:HB3	1.60	0.82
3:Y:243:PHE:HB2	3:Y:260:THR:HG23	1.60	0.82
2:F:207:LYS:HZ2	1:M:201:THR:CB	1.89	0.82
1:E:3:GLN:HB2	1:E:25:SER:HB2	1.61	0.82
1:D:3:GLN:HB2	1:D:25:SER:HB2	1.61	0.81
3:N:243:PHE:HB2	3:N:260:THR:HG23	1.60	0.81
3:J:314:LEU:HD22	3:J:430:GLU:HG3	1.62	0.81
3:J:346:PRO:HB3	3:J:372:PHE:HB3	1.60	0.81
1:H:90:ASP:O	1:H:94:TYR:OH	1.99	0.81
3:O:314:LEU:HD22	3:O:430:GLU:HG3	1.62	0.81
1:I:3:GLN:HB2	1:I:25:SER:HB2	1.60	0.81
1:M:3:GLN:HB2	1:M:25:SER:HB2	1.62	0.81
1:M:90:ASP:O	1:M:94:TYR:OH	1.99	0.80
1:E:90:ASP:O	1:E:94:TYR:OH	2.00	0.80
3:N:346:PRO:HB3	3:N:372:PHE:HB3	1.63	0.80
3:P:346:PRO:HB3	3:P:372:PHE:HB3	1.63	0.80
3:N:433:HIS:C	3:N:433:HIS:N	2.36	0.79
3:Y:429:HIS:HD2	3:Y:431:ALA:H	1.31	0.79
3:P:433:HIS:N	3:P:433:HIS:C	2.36	0.78
3:Y:346:PRO:HB3	3:Y:372:PHE:HB3	1.63	0.78
3:P:289:THR:HG22	3:P:290:LYS:H	1.48	0.78
3:N:429:HIS:HD2	3:N:431:ALA:H	1.31	0.78
3:O:291:PRO:C	3:O:292:ARG:HD2	2.03	0.78
3:X:291:PRO:C	3:X:292:ARG:HD2	2.03	0.78
1:E:207:ASN:ND2	1:E:218:ASP:OD2	2.17	0.78
3:Y:289:THR:HG22	3:Y:290:LYS:H	1.48	0.78
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ASN:ND2	1:A:218:ASP:OD2	2.16	0.78
3:X:314:LEU:HD22	3:X:430:GLU:HG3	1.62	0.78
3:P:263:VAL:O	3:P:301:ARG:HA	1.84	0.78
3:Y:433:HIS:C	3:Y:433:HIS:N	2.37	0.78
3:Y:263:VAL:O	3:Y:301:ARG:HA	1.84	0.78
3:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.78
1:E:39:ARG:HD2	2:G:38:GLN:HE22	1.47	0.78
1:D:75:LEU:HD22	1:I:57:TYR:CE1	2.19	0.77
3:N:433:HIS:C	3:N:433:HIS:CB	2.53	0.77
3:O:292:ARG:O	3:O:293:GLU:HB3	1.84	0.77
3:P:429:HIS:HD2	3:P:431:ALA:H	1.31	0.77
1:H:101:SER:HB2	1:H:104:LEU:H	1.47	0.77
3:J:292:ARG:O	3:J:293:GLU:HB3	1.85	0.76
1:I:207:ASN:ND2	1:I:218:ASP:OD2	2.19	0.76
3:P:433:HIS:CB	3:P:433:HIS:C	2.53	0.76
3:X:292:ARG:O	3:X:293:GLU:HB3	1.85	0.76
3:N:263:VAL:O	3:N:301:ARG:HA	1.84	0.76
3:P:429:HIS:CD2	3:P:431:ALA:H	2.03	0.76
3:Y:433:HIS:CB	3:Y:433:HIS:C	2.53	0.76
3:Y:429:HIS:CD2	3:Y:431:ALA:H	2.03	0.76
3:N:429:HIS:CD2	3:N:431:ALA:H	2.03	0.76
1:D:90:ASP:O	1:D:94:TYR:OH	2.03	0.76
3:Y:266:VAL:HB	3:Y:300:TYR:CB	2.15	0.75
3:O:272:GLN:NE2	3:O:326:LYS:HD2	2.01	0.75
3:N:266:VAL:HB	3:N:300:TYR:CB	2.15	0.75
1:D:75:LEU:HD13	1:I:57:TYR:CE1	2.22	0.75
3:P:266:VAL:HB	3:P:300:TYR:CB	2.15	0.75
3:J:272:GLN:NE2	3:J:326:LYS:HD2	2.01	0.75
1:M:91:THR:HG23	1:M:120:THR:HA	1.68	0.75
2:F:207:LYS:HZ3	1:M:201:THR:HB	1.46	0.75
1:D:91:THR:HG23	1:D:120:THR:HA	1.68	0.75
1:H:3:GLN:HB2	1:H:25:SER:HB2	1.66	0.75
3:X:429:HIS:CD2	3:X:431:ALA:H	2.05	0.75
1:D:75:LEU:HD22	1:I:57:TYR:CE2	2.20	0.74
3:N:328:LEU:HD12	3:N:329:PRO:HD2	1.69	0.74
3:J:429:HIS:CD2	3:J:431:ALA:H	2.05	0.74
1:H:207:ASN:ND2	1:H:218:ASP:OD2	2.20	0.74
3:P:365:LEU:HD12	3:P:410:LEU:HD23	1.69	0.74
1:H:224:LYS:HD2	1:H:224:LYS:N	2.03	0.74
3:N:365:LEU:HD12	3:N:410:LEU:HD23	1.69	0.74
3:O:429:HIS:CD2	3:O:431:ALA:H	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:272:GLN:NE2	3:X:326:LYS:HD2	2.01	0.74
1:I:152:VAL:HG11	1:I:160:VAL:HG11	1.69	0.73
3:Y:365:LEU:HD12	3:Y:410:LEU:HD23	1.69	0.73
3:J:295:GLN:OE1	1:M:195:PRO:HB3	1.89	0.73
1:A:197:SER:HB2	3:X:295:GLN:HE22	1.53	0.72
1:M:153:LYS:HG2	1:M:154:ASP:CG	2.10	0.72
3:Y:328:LEU:HD12	3:Y:329:PRO:HD2	1.69	0.72
1:H:18:LEU:HB3	1:H:83:MET:HE3	1.70	0.72
1:E:101:SER:HB2	1:E:104:LEU:H	1.54	0.72
1:A:153:LYS:HG2	1:A:154:ASP:CG	2.09	0.72
2:B:142:ARG:HG2	2:B:142:ARG:HH11	1.54	0.72
3:J:290:LYS:HZ2	2:L:109:THR:HG21	1.54	0.72
1:D:220:LYS:HE2	1:D:222:GLU:CD	2.10	0.72
3:P:328:LEU:HD12	3:P:329:PRO:HD2	1.69	0.72
3:J:295:GLN:NE2	1:M:197:SER:OG	2.23	0.72
1:A:197:SER:HB3	3:X:295:GLN:NE2	2.04	0.71
3:N:288:LYS:H	3:N:288:LYS:HD3	1.54	0.71
2:L:39:LYS:NZ	2:L:81:ASP:O	2.22	0.71
2:L:142:ARG:HH11	2:L:142:ARG:HG2	1.56	0.71
1:H:91:THR:HG23	1:H:120:THR:HA	1.71	0.71
1:D:153:LYS:HG2	1:D:154:ASP:CG	2.10	0.71
3:Y:288:LYS:H	3:Y:288:LYS:HD3	1.54	0.71
1:D:18:LEU:HB3	1:D:83:MET:HE3	1.73	0.71
3:P:288:LYS:H	3:P:288:LYS:HD3	1.54	0.71
1:H:153:LYS:HG2	1:H:154:ASP:CG	2.11	0.71
1:I:90:ASP:O	1:I:94:TYR:OH	2.05	0.70
2:G:142:ARG:HH11	2:G:142:ARG:HG2	1.55	0.70
2:G:143:GLU:OE2	2:G:143:GLU:N	2.24	0.70
3:J:290:LYS:HZ2	2:L:109:THR:CG2	2.05	0.70
2:G:39:LYS:NZ	2:G:81:ASP:O	2.20	0.70
3:J:290:LYS:NZ	2:L:109:THR:CG2	2.53	0.70
1:E:153:LYS:HG2	1:E:154:ASP:CG	2.13	0.70
1:M:207:ASN:ND2	1:M:218:ASP:OD2	2.25	0.69
3:X:422:VAL:HG22	3:X:442:SER:OG	1.92	0.69
3:J:252:MET:HB2	3:J:255:ARG:HG3	1.75	0.69
1:A:197:SER:HB3	3:X:295:GLN:HE22	1.56	0.69
1:I:204:TYR:O	1:I:221:VAL:N	2.26	0.69
2:C:136:LEU:HD13	2:C:175:LEU:HD22	1.75	0.69
1:A:101:SER:HB2	1:A:104:LEU:H	1.57	0.68
3:O:422:VAL:HG22	3:O:442:SER:OG	1.92	0.68
2:L:143:GLU:N	2:L:143:GLU:OE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:422:VAL:HG22	3:J:442:SER:OG	1.92	0.68
3:X:252:MET:HB2	3:X:255:ARG:HG3	1.75	0.68
1:A:90:ASP:O	1:A:94:TYR:OH	2.06	0.68
2:C:143:GLU:N	2:C:143:GLU:OE2	2.27	0.68
1:M:152:VAL:HG11	1:M:160:VAL:HG11	1.75	0.68
1:E:152:VAL:HG11	1:E:160:VAL:HG11	1.76	0.68
3:X:325:ASN:HD21	3:X:327:ALA:HB3	1.58	0.68
3:P:270:ASP:N	3:P:271:PRO:HD3	2.09	0.68
1:D:152:VAL:HG11	1:D:160:VAL:HG11	1.75	0.68
1:I:153:LYS:HG2	1:I:154:ASP:CG	2.15	0.67
3:O:252:MET:HB2	3:O:255:ARG:HG3	1.75	0.67
3:J:325:ASN:HD21	3:J:327:ALA:HB3	1.58	0.67
3:N:270:ASP:N	3:N:271:PRO:HD3	2.09	0.67
1:I:91:THR:HG23	1:I:120:THR:HA	1.76	0.67
3:O:418:GLN:HA	3:O:443:LEU:CD2	2.24	0.67
3:X:418:GLN:HA	3:X:443:LEU:CD2	2.24	0.67
3:O:325:ASN:HD21	3:O:327:ALA:HB3	1.58	0.67
1:E:136:PRO:HD3	1:E:148:LEU:HB3	1.77	0.67
2:F:142:ARG:HH11	2:F:142:ARG:HG2	1.60	0.67
3:J:429:HIS:HD2	3:J:431:ALA:H	1.42	0.67
2:C:39:LYS:NZ	2:C:81:ASP:O	2.21	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
1:A:152:VAL:HG11	1:A:160:VAL:HG11	1.75	0.67
1:A:203:THR:HB	1:A:220:LYS:HE3	1.77	0.67
1:D:75:LEU:HD13	1:I:57:TYR:HE1	1.58	0.66
3:Y:270:ASP:N	3:Y:271:PRO:HD3	2.09	0.66
1:D:207:ASN:ND2	1:D:218:ASP:OD2	2.29	0.66
3:X:350:THR:HB	3:X:441:LEU:HG	1.77	0.66
3:O:325:ASN:ND2	3:O:327:ALA:HB3	2.10	0.66
3:O:350:THR:HB	3:O:441:LEU:HG	1.77	0.66
1:I:201:THR:OG1	1:I:202:GLN:N	2.28	0.66
1:A:174:HIS:HE1	2:B:167:ASP:HB2	1.61	0.66
3:J:325:ASN:ND2	3:J:327:ALA:HB3	2.10	0.66
3:J:350:THR:HB	3:J:441:LEU:HG	1.77	0.66
2:K:142:ARG:HH11	2:K:142:ARG:HG2	1.59	0.66
1:D:202:GLN:O	1:D:203:THR:HA	1.96	0.66
3:X:325:ASN:ND2	3:X:327:ALA:HB3	2.11	0.66
1:H:152:VAL:HG11	1:H:160:VAL:HG11	1.77	0.66
3:O:429:HIS:HD2	3:O:431:ALA:H	1.42	0.65
1:M:201:THR:HG1	1:M:202:GLN:N	1.94	0.65
3:P:290:LYS:HE3	3:P:292:ARG:HH22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:LYS:NZ	2:F:195:GLU:OE1	2.27	0.65
2:F:143:GLU:OE2	2:F:143:GLU:N	2.30	0.65
1:D:154:ASP:HB3	1:D:185:LEU:HD23	1.79	0.65
3:J:279:VAL:O	3:J:282:VAL:HG13	1.97	0.64
3:O:328:LEU:HG	3:O:330:ALA:O	1.98	0.64
2:B:143:GLU:N	2:B:143:GLU:OE2	2.29	0.64
1:A:136:PRO:HD3	1:A:148:LEU:HB3	1.79	0.64
3:X:429:HIS:HD2	3:X:431:ALA:H	1.43	0.64
2:B:29:ILE:HG21	2:B:90:HIS:HD2	1.62	0.64
3:Y:332:ILE:HG22	3:Y:333:GLU:N	2.13	0.64
2:F:37:GLN:O	2:F:45:LYS:N	2.30	0.64
3:P:330:ALA:HB1	3:P:331:PRO:HD2	1.80	0.64
2:C:149:LYS:NZ	2:C:195:GLU:OE1	2.26	0.64
3:O:279:VAL:O	3:O:282:VAL:HG13	1.97	0.64
3:Y:290:LYS:HE3	3:Y:292:ARG:HH22	1.61	0.64
3:X:328:LEU:HG	3:X:330:ALA:O	1.98	0.64
3:X:288:LYS:HD2	3:X:288:LYS:H	1.63	0.64
2:G:149:LYS:NZ	2:G:195:GLU:OE1	2.26	0.64
3:J:288:LYS:H	3:J:288:LYS:HD2	1.63	0.63
3:O:288:LYS:H	3:O:288:LYS:HD2	1.63	0.63
1:E:174:HIS:HE1	2:F:167:ASP:HB2	1.62	0.63
3:N:332:ILE:HG22	3:N:333:GLU:N	2.13	0.63
3:P:332:ILE:HG22	3:P:333:GLU:N	2.13	0.63
3:N:290:LYS:HE3	3:N:292:ARG:HH22	1.61	0.63
2:K:143:GLU:OE2	2:K:143:GLU:N	2.31	0.63
1:I:101:SER:HB2	1:I:104:LEU:H	1.63	0.63
3:J:290:LYS:HZ3	2:L:109:THR:HG21	1.61	0.63
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.79	0.63
1:M:164:TRP:C	1:M:166:SER:H	2.02	0.63
3:J:328:LEU:HG	3:J:330:ALA:O	1.98	0.63
1:M:204:TYR:O	1:M:221:VAL:N	2.32	0.63
1:A:154:ASP:HB3	1:A:185:LEU:HD23	1.80	0.63
1:E:201:THR:OG1	1:E:202:GLN:N	2.31	0.63
3:J:290:LYS:NZ	2:L:109:THR:OG1	2.32	0.63
2:C:120:PRO:HG3	2:C:130:ALA:HB1	1.81	0.63
1:E:18:LEU:HB3	1:E:83:MET:HE3	1.79	0.63
3:X:279:VAL:O	3:X:282:VAL:HG13	1.97	0.63
1:I:148:LEU:HB2	1:I:221:VAL:HG11	1.80	0.63
3:Y:330:ALA:HB1	3:Y:331:PRO:HD2	1.79	0.62
1:A:34:MET:SD	1:A:98:ARG:HB2	2.39	0.62
1:H:174:HIS:HE1	2:K:167:ASP:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.81	0.62
2:C:61:ARG:HB2	2:C:76:SER:O	1.99	0.62
1:D:75:LEU:CD2	1:I:57:TYR:CE1	2.82	0.62
1:H:154:ASP:HB3	1:H:185:LEU:HD23	1.82	0.62
1:E:203:THR:HB	1:E:220:LYS:HE3	1.81	0.62
2:C:142:ARG:HH11	2:C:142:ARG:HG2	1.63	0.62
3:O:384:ASN:O	3:O:386:GLN:N	2.31	0.62
2:K:136:LEU:HD13	2:K:175:LEU:HD22	1.82	0.62
2:C:29:ILE:HG21	2:C:90:HIS:HD2	1.64	0.62
1:I:18:LEU:HB3	1:I:83:MET:HE3	1.81	0.62
2:G:136:LEU:HD13	2:G:175:LEU:HD22	1.80	0.62
2:K:61:ARG:HB2	2:K:76:SER:O	2.00	0.61
1:H:203:THR:HB	1:H:220:LYS:HE3	1.81	0.61
2:G:37:GLN:O	2:G:45:LYS:N	2.29	0.61
2:G:29:ILE:HG21	2:G:90:HIS:HD2	1.64	0.61
1:M:163:SER:O	1:M:207:ASN:N	2.32	0.61
2:F:151:ASP:HA	2:F:191:VAL:HG12	1.81	0.61
1:M:99:LYS:HG2	1:M:100:GLY:N	2.14	0.61
2:C:37:GLN:O	2:C:45:LYS:N	2.31	0.61
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.32	0.61
3:P:394:THR:HG23	3:P:407:TYR:O	2.01	0.61
3:J:384:ASN:O	3:J:386:GLN:N	2.31	0.61
2:G:36:TYR:HB2	2:G:87:HIS:HB2	1.81	0.61
1:A:91:THR:HG23	1:A:120:THR:HA	1.83	0.60
2:F:136:LEU:HD13	2:F:175:LEU:HD22	1.82	0.60
2:G:120:PRO:HG3	2:G:130:ALA:HB1	1.83	0.60
1:A:99:LYS:HG2	1:A:100:GLY:N	2.16	0.60
3:N:406:LEU:HD12	3:N:406:LEU:C	2.22	0.60
1:D:203:THR:HB	1:D:220:LYS:HE3	1.83	0.60
3:X:417:TRP:CH2	3:X:441:LEU:HD22	2.37	0.60
1:D:99:LYS:HG2	1:D:100:GLY:N	2.16	0.60
3:J:417:TRP:CH2	3:J:441:LEU:HD22	2.37	0.60
3:J:421:ASN:N	3:J:421:ASN:HD22	2.00	0.60
1:M:18:LEU:HB3	1:M:83:MET:HE3	1.83	0.60
3:Y:394:THR:HG23	3:Y:407:TYR:O	2.01	0.60
2:K:6:GLN:NE2	2:K:102:THR:OG1	2.35	0.60
3:X:384:ASN:O	3:X:386:GLN:N	2.31	0.60
2:B:37:GLN:O	2:B:45:LYS:N	2.29	0.60
3:P:406:LEU:HD12	3:P:406:LEU:C	2.22	0.60
3:N:325:ASN:HD22	3:N:326:LYS:H	1.51	0.59
1:I:154:ASP:HB3	1:I:185:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:ILE:HG21	2:F:90:HIS:HD2	1.66	0.59
3:P:274:LYS:HE2	3:P:276:ASN:HD21	1.67	0.59
3:O:417:TRP:CH2	3:O:441:LEU:HD22	2.37	0.59
2:K:149:LYS:NZ	2:K:195:GLU:OE1	2.36	0.59
3:Y:406:LEU:C	3:Y:406:LEU:HD12	2.22	0.59
1:M:101:SER:HB2	1:M:104:LEU:H	1.66	0.59
3:N:257:PRO:HB2	3:N:308:VAL:HB	1.84	0.59
1:A:197:SER:CB	3:X:295:GLN:NE2	2.62	0.59
1:I:60:TYR:OH	1:I:69:THR:HA	2.03	0.59
1:A:129:PRO:HB3	1:A:155:TYR:HB3	1.83	0.59
1:H:99:LYS:HG2	1:H:100:GLY:N	2.17	0.59
3:N:274:LYS:HE2	3:N:276:ASN:HD21	1.67	0.59
3:P:257:PRO:HB2	3:P:308:VAL:HB	1.84	0.59
2:L:120:PRO:HG3	2:L:130:ALA:HB1	1.85	0.59
3:Y:325:ASN:HD22	3:Y:326:LYS:H	1.51	0.59
1:H:72:ARG:NE	1:H:74:ASP:OD1	2.31	0.59
1:D:72:ARG:NE	1:D:74:ASP:OD1	2.30	0.59
1:E:154:ASP:HB3	1:E:185:LEU:HD23	1.84	0.59
1:D:148:LEU:HD13	1:D:221:VAL:HB	1.85	0.59
3:P:269:GLU:HG2	3:P:269:GLU:O	2.03	0.59
3:O:417:TRP:HH2	3:O:441:LEU:HD22	1.67	0.59
3:N:394:THR:HG23	3:N:407:TYR:O	2.01	0.59
2:K:37:GLN:O	2:K:45:LYS:N	2.33	0.59
2:L:29:ILE:HG21	2:L:90:HIS:HD2	1.67	0.59
3:O:421:ASN:N	3:O:421:ASN:HD22	2.00	0.59
3:P:296:TYR:CE1	3:P:301:ARG:HD3	2.38	0.59
1:A:18:LEU:HB3	1:A:83:MET:HE3	1.83	0.59
1:D:75:LEU:CD2	1:I:57:TYR:CZ	2.69	0.58
3:J:417:TRP:HH2	3:J:441:LEU:HD22	1.67	0.58
3:P:279:VAL:O	3:P:279:VAL:HG23	2.03	0.58
3:X:433:HIS:ND1	3:X:434:ASN:OD1	2.36	0.58
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
1:M:133:PRO:HB3	1:M:221:VAL:HG22	1.85	0.58
3:Y:265:ASP:HA	3:Y:299:THR:HB	1.85	0.58
3:O:276:ASN:HB2	3:O:322:LYS:HB3	1.86	0.58
3:Y:269:GLU:O	3:Y:269:GLU:HG2	2.03	0.58
1:H:222:GLU:HB2	1:H:223:PRO:HD2	1.84	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	0.58
3:P:265:ASP:HA	3:P:299:THR:HB	1.86	0.58
3:X:421:ASN:N	3:X:421:ASN:HD22	2.00	0.58
3:Y:296:TYR:CE1	3:Y:301:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:274:LYS:HE2	3:Y:276:ASN:HD21	1.67	0.58
2:G:201:LEU:HG	2:G:205:VAL:HG23	1.85	0.58
3:X:415:SER:O	3:X:419:GLN:HG3	2.04	0.58
3:J:286:ASN:O	3:J:287:ALA:HB2	2.03	0.58
2:B:136:LEU:HD13	2:B:175:LEU:HD22	1.83	0.58
3:Y:424:SER:OG	3:Y:438:GLN:HG2	2.04	0.58
3:N:288:LYS:HE2	3:N:306:LEU:HD11	1.86	0.58
3:X:417:TRP:HH2	3:X:441:LEU:HD22	1.67	0.58
1:H:201:THR:OG1	1:H:202:GLN:N	2.33	0.58
1:H:169:LEU:HD21	1:H:192:VAL:HG21	1.85	0.58
2:F:201:LEU:HG	2:F:205:VAL:HG23	1.86	0.58
1:E:91:THR:HG23	1:E:120:THR:HA	1.85	0.58
3:N:266:VAL:CB	3:N:300:TYR:HB2	2.28	0.58
3:O:286:ASN:O	3:O:287:ALA:HB2	2.03	0.58
1:M:164:TRP:O	1:M:166:SER:N	2.37	0.58
1:H:129:PRO:HB3	1:H:155:TYR:HB3	1.84	0.58
1:I:99:LYS:HG2	1:I:100:GLY:N	2.18	0.58
3:N:424:SER:OG	3:N:438:GLN:HG2	2.04	0.58
3:P:288:LYS:HE2	3:P:306:LEU:HD11	1.86	0.58
2:B:39:LYS:NZ	2:B:81:ASP:O	2.27	0.58
2:C:201:LEU:HG	2:C:205:VAL:HG23	1.85	0.58
3:J:415:SER:O	3:J:419:GLN:HG3	2.04	0.58
3:Y:288:LYS:HE2	3:Y:306:LEU:HD11	1.86	0.57
3:Y:257:PRO:HB2	3:Y:308:VAL:HB	1.85	0.57
3:N:296:TYR:CE1	3:N:301:ARG:HD3	2.38	0.57
3:P:325:ASN:HD22	3:P:326:LYS:H	1.51	0.57
2:C:19:ILE:HG12	2:C:78:LEU:HD11	1.86	0.57
1:I:203:THR:HB	1:I:220:LYS:HE3	1.85	0.57
2:G:118:PHE:CD2	1:I:134:LEU:HD13	2.39	0.57
1:M:73:ASP:N	1:M:78:PHE:O	2.37	0.57
3:X:286:ASN:O	3:X:287:ALA:HB2	2.03	0.57
1:M:154:ASP:HB3	1:M:185:LEU:HD23	1.86	0.57
2:K:91:TYR:HD1	1:M:99:LYS:NZ	2.03	0.57
3:O:415:SER:O	3:O:419:GLN:HG3	2.04	0.57
3:N:265:ASP:HA	3:N:299:THR:HB	1.85	0.57
2:L:136:LEU:HD13	2:L:175:LEU:HD22	1.86	0.57
2:L:149:LYS:NZ	2:L:195:GLU:OE1	2.33	0.57
3:O:433:HIS:ND1	3:O:434:ASN:OD1	2.35	0.57
3:Y:279:VAL:HG23	3:Y:279:VAL:O	2.03	0.57
1:D:35:ASN:O	1:D:97:ALA:N	2.37	0.57
1:D:75:LEU:CD1	1:I:57:TYR:CE1	2.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:SER:O	1:D:72:ARG:NH1	2.37	0.57
3:X:320:LYS:HG3	3:X:335:THR:HG22	1.87	0.57
3:J:433:HIS:ND1	3:J:434:ASN:OD1	2.36	0.57
3:O:320:LYS:HG3	3:O:335:THR:HG22	1.87	0.57
3:P:311:GLN:CD	3:P:311:GLN:H	2.08	0.57
3:P:424:SER:OG	3:P:438:GLN:HG2	2.04	0.57
2:K:29:ILE:HG21	2:K:90:HIS:HD2	1.69	0.57
3:N:328:LEU:HG	3:N:330:ALA:O	2.05	0.57
3:J:320:LYS:HG3	3:J:335:THR:HG22	1.87	0.56
3:J:276:ASN:HB2	3:J:322:LYS:HB3	1.86	0.56
3:P:439:LYS:HE3	3:P:440:SER:O	2.05	0.56
1:D:103:ARG:O	2:F:50:LYS:CE	2.53	0.56
1:A:153:LYS:HG2	1:A:154:ASP:OD2	2.06	0.56
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.87	0.56
1:D:144:GLY:O	1:D:196:SER:HB2	2.05	0.56
3:X:276:ASN:HB2	3:X:322:LYS:HB3	1.86	0.56
2:K:201:LEU:HG	2:K:205:VAL:HG23	1.87	0.56
2:G:6:GLN:NE2	2:G:102:THR:OG1	2.39	0.56
2:K:148:TRP:CE3	2:K:179:LEU:HD22	2.40	0.56
2:C:6:GLN:NE2	2:C:102:THR:OG1	2.38	0.56
3:N:311:GLN:CD	3:N:311:GLN:H	2.08	0.56
3:Y:325:ASN:ND2	3:Y:326:LYS:H	2.04	0.56
2:G:19:ILE:HG12	2:G:78:LEU:HD11	1.88	0.56
1:H:136:PRO:HD3	1:H:148:LEU:HB3	1.87	0.56
1:A:60:TYR:OH	1:A:69:THR:HA	2.04	0.56
3:N:301:ARG:HE	3:N:303:VAL:CG2	2.18	0.56
1:E:52:SER:O	1:E:72:ARG:NH1	2.37	0.56
3:Y:301:ARG:HE	3:Y:303:VAL:CG2	2.18	0.56
3:X:288:LYS:O	3:X:289:THR:O	2.24	0.56
3:P:328:LEU:HG	3:P:330:ALA:O	2.05	0.56
3:P:270:ASP:OD2	3:P:327:ALA:HB2	2.06	0.56
3:N:270:ASP:OD2	3:N:327:ALA:HB2	2.06	0.56
3:N:439:LYS:HE3	3:N:440:SER:O	2.05	0.56
3:Y:328:LEU:HG	3:Y:330:ALA:O	2.05	0.56
2:B:6:GLN:NE2	2:B:102:THR:OG1	2.38	0.56
3:Y:311:GLN:H	3:Y:311:GLN:CD	2.08	0.56
3:O:328:LEU:HD12	3:O:329:PRO:HD2	1.88	0.56
1:H:35:ASN:OD1	1:H:50:SER:HB2	2.06	0.56
1:A:104:LEU:HD12	1:E:28:ARG:CG	2.20	0.56
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
3:N:325:ASN:ND2	3:N:326:LYS:H	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:160:GLN:O	2:K:178:THR:N	2.36	0.56
1:D:129:PRO:HB3	1:D:155:TYR:HB3	1.87	0.56
2:F:120:PRO:HG3	2:F:130:ALA:HB1	1.87	0.56
1:D:38:ARG:HB3	1:D:94:TYR:CE2	2.41	0.55
2:L:160:GLN:O	2:L:178:THR:N	2.38	0.55
1:H:58:ARG:NH1	1:H:70:VAL:O	2.39	0.55
3:P:301:ARG:HE	3:P:303:VAL:CG2	2.18	0.55
3:O:288:LYS:O	3:O:289:THR:O	2.24	0.55
3:O:289:THR:O	3:O:290:LYS:HB2	2.07	0.55
3:J:289:THR:O	3:J:290:LYS:HB2	2.07	0.55
3:Y:266:VAL:CB	3:Y:300:TYR:HB2	2.28	0.55
1:D:164:TRP:HZ2	1:D:190:SER:O	1.90	0.55
1:D:169:LEU:HD21	1:D:192:VAL:HG21	1.88	0.55
2:F:142:ARG:NH1	2:F:142:ARG:HG2	2.22	0.55
3:J:328:LEU:HD12	3:J:329:PRO:HD2	1.88	0.55
1:D:60:TYR:OH	1:D:69:THR:HA	2.06	0.55
1:A:70:VAL:HA	1:A:80:TYR:O	2.06	0.55
3:P:325:ASN:ND2	3:P:326:LYS:H	2.04	0.55
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.89	0.55
1:M:60:TYR:OH	1:M:69:THR:HA	2.06	0.55
1:H:70:VAL:HA	1:H:80:TYR:O	2.06	0.55
1:D:101:SER:H	1:D:104:LEU:HD23	1.71	0.55
2:K:39:LYS:NZ	2:K:81:ASP:O	2.30	0.55
2:F:39:LYS:NZ	2:F:81:ASP:O	2.30	0.55
1:M:34:MET:SD	1:M:98:ARG:HB2	2.46	0.55
2:B:19:ILE:HG12	2:B:78:LEU:HD11	1.88	0.55
1:I:29:ILE:O	1:I:72:ARG:NH2	2.39	0.55
3:Y:439:LYS:HE3	3:Y:440:SER:O	2.05	0.55
3:X:289:THR:O	3:X:290:LYS:HB2	2.07	0.55
3:Y:270:ASP:OD2	3:Y:327:ALA:HB2	2.06	0.55
1:E:35:ASN:OD1	1:E:50:SER:HB2	2.07	0.55
2:L:167:ASP:HB2	1:M:174:HIS:HE1	1.71	0.55
1:A:47:TRP:NE1	1:A:49:ALA:O	2.40	0.55
1:H:94:TYR:CE1	1:H:119:VAL:HB	2.42	0.55
1:M:94:TYR:CE1	1:M:119:VAL:HB	2.42	0.55
3:O:414:LYS:HE2	3:O:418:GLN:NE2	2.22	0.55
3:P:238:PRO:CG	3:P:328:LEU:HD13	2.37	0.55
2:K:142:ARG:NH1	2:K:142:ARG:HG2	2.22	0.55
2:F:2:VAL:HG11	2:F:90:HIS:CD2	2.42	0.55
3:P:275:PHE:HE1	3:P:302:VAL:HG12	1.72	0.55
1:D:133:PRO:HG2	1:D:224:LYS:HZ1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.89	0.54
3:X:328:LEU:HD12	3:X:329:PRO:HD2	1.88	0.54
2:L:37:GLN:O	2:L:45:LYS:N	2.37	0.54
1:A:45:LEU:HG	2:C:87:HIS:CE1	2.43	0.54
1:M:70:VAL:HA	1:M:80:TYR:O	2.06	0.54
3:X:414:LYS:HE2	3:X:418:GLN:NE2	2.22	0.54
1:M:68:PHE:CD1	1:M:83:MET:HA	2.42	0.54
3:O:282:VAL:O	3:O:283:GLN:CB	2.52	0.54
3:Y:238:PRO:CG	3:Y:328:LEU:HD13	2.37	0.54
3:Y:240:VAL:O	3:Y:334:LYS:HE3	2.08	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
1:H:135:ALA:HB3	1:H:224:LYS:HD3	1.89	0.54
2:B:91:TYR:HD1	1:D:99:LYS:NZ	2.04	0.54
2:K:162:SER:HB3	2:K:176:SER:OG	2.07	0.54
3:P:240:VAL:O	3:P:334:LYS:HE3	2.08	0.54
3:N:262:VAL:HG13	3:N:303:VAL:HG22	1.90	0.54
3:J:414:LYS:O	3:J:418:GLN:HG3	2.08	0.54
3:J:414:LYS:HE2	3:J:418:GLN:NE2	2.22	0.54
2:L:31:THR:OG1	2:L:50:LYS:HE2	2.07	0.54
3:N:275:PHE:HE1	3:N:302:VAL:HG12	1.72	0.54
3:N:238:PRO:CG	3:N:328:LEU:HD13	2.37	0.54
3:O:414:LYS:O	3:O:418:GLN:HG3	2.08	0.54
1:D:103:ARG:O	2:F:50:LYS:CD	2.56	0.54
3:O:285:HIS:O	3:O:286:ASN:HB2	2.08	0.54
3:O:418:GLN:HA	3:O:443:LEU:HD22	1.90	0.54
2:L:6:GLN:NE2	2:L:102:THR:OG1	2.40	0.54
2:K:120:PRO:HG3	2:K:130:ALA:HB1	1.89	0.54
3:Y:289:THR:HG22	3:Y:290:LYS:N	2.22	0.54
3:X:418:GLN:HA	3:X:443:LEU:HD22	1.90	0.54
1:E:60:TYR:OH	1:E:69:THR:HA	2.08	0.54
1:E:99:LYS:HG2	1:E:100:GLY:N	2.23	0.54
3:P:351:LEU:C	3:P:441:LEU:HD11	2.28	0.54
2:L:162:SER:HB3	2:L:176:SER:OG	2.07	0.54
3:Y:275:PHE:HE1	3:Y:302:VAL:HG12	1.72	0.54
1:I:169:LEU:HD21	1:I:192:VAL:HG21	1.90	0.54
1:H:69:THR:C	1:H:81:LEU:HD12	2.28	0.53
1:H:153:LYS:HG2	1:H:154:ASP:OD2	2.08	0.53
3:X:414:LYS:O	3:X:418:GLN:HG3	2.08	0.53
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.90	0.53
1:I:22:CYS:O	1:I:78:PHE:HA	2.08	0.53
1:E:70:VAL:HA	1:E:80:TYR:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:TRP:NE1	1:M:49:ALA:O	2.41	0.53
3:Y:262:VAL:HG13	3:Y:303:VAL:HG22	1.90	0.53
3:X:285:HIS:O	3:X:286:ASN:HB2	2.08	0.53
2:B:142:ARG:HG2	2:B:142:ARG:NH1	2.18	0.53
3:Y:351:LEU:C	3:Y:441:LEU:HD11	2.28	0.53
3:N:351:LEU:C	3:N:441:LEU:HD11	2.28	0.53
3:P:322:LYS:HE3	3:P:333:GLU:OE2	2.08	0.53
1:H:101:SER:H	1:H:104:LEU:CD2	2.21	0.53
1:D:35:ASN:OD1	1:D:50:SER:HB2	2.08	0.53
3:P:266:VAL:CB	3:P:300:TYR:HB2	2.28	0.53
3:J:285:HIS:O	3:J:286:ASN:HB2	2.08	0.53
3:Y:322:LYS:HE3	3:Y:333:GLU:OE2	2.08	0.53
3:N:289:THR:HG22	3:N:290:LYS:N	2.21	0.53
2:L:142:ARG:CG	2:L:142:ARG:HH11	2.21	0.53
1:D:70:VAL:HA	1:D:80:TYR:O	2.09	0.53
1:M:220:LYS:C	1:M:221:VAL:HA	2.29	0.53
1:A:37:VAL:HG22	1:A:47:TRP:HA	1.90	0.53
3:X:351:LEU:HB2	3:X:366:THR:HB	1.90	0.53
1:I:72:ARG:NE	1:I:74:ASP:OD1	2.34	0.53
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.53
2:G:149:LYS:HB2	2:G:193:ALA:HB3	1.91	0.53
1:I:101:SER:OG	1:I:104:LEU:HA	2.09	0.53
2:F:160:GLN:O	2:F:178:THR:N	2.41	0.53
3:O:351:LEU:HB2	3:O:366:THR:HB	1.90	0.53
2:B:151:ASP:HA	2:B:191:VAL:HG12	1.90	0.53
1:A:22:CYS:O	1:A:78:PHE:HA	2.09	0.53
1:H:38:ARG:HB3	1:H:94:TYR:CE2	2.44	0.52
2:G:37:GLN:HB2	2:G:47:LEU:HD11	1.91	0.52
2:F:140:TYR:CD2	2:F:141:PRO:HA	2.44	0.52
3:Y:297:ASN:O	3:Y:298:SER:HB3	2.09	0.52
1:D:94:TYR:CE1	1:D:119:VAL:HB	2.44	0.52
3:J:418:GLN:HA	3:J:443:LEU:HD22	1.90	0.52
2:B:201:LEU:HG	2:B:205:VAL:HG23	1.90	0.52
3:P:262:VAL:HG13	3:P:303:VAL:HG22	1.90	0.52
1:E:101:SER:H	1:E:104:LEU:HD23	1.75	0.52
1:H:29:ILE:O	1:H:72:ARG:NH2	2.43	0.52
1:M:35:ASN:O	1:M:97:ALA:N	2.42	0.52
3:J:384:ASN:OD1	3:J:385:GLY:N	2.41	0.52
3:N:312:ASN:ND2	3:N:317:LYS:HD2	2.24	0.52
2:L:142:ARG:NH1	2:L:142:ARG:HG2	2.19	0.52
1:D:101:SER:HB2	1:D:104:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:N	1:A:78:PHE:O	2.40	0.52
1:A:164:TRP:CH2	1:A:221:VAL:HG21	2.45	0.52
3:X:283:GLN:C	3:X:285:HIS:N	2.62	0.52
2:G:160:GLN:O	2:G:178:THR:N	2.40	0.52
3:Y:312:ASN:ND2	3:Y:317:LYS:HD2	2.24	0.52
1:A:52:SER:O	1:A:72:ARG:NH1	2.42	0.52
1:I:35:ASN:OD1	1:I:50:SER:HB2	2.10	0.52
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.52
2:F:149:LYS:HB2	2:F:193:ALA:HB3	1.91	0.52
1:M:203:THR:HG21	1:M:220:LYS:HZ1	1.75	0.52
1:M:35:ASN:OD1	1:M:50:SER:HB2	2.09	0.52
1:M:129:PRO:HB3	1:M:155:TYR:HB3	1.90	0.52
1:E:47:TRP:NE1	1:E:49:ALA:O	2.43	0.52
2:C:138:ASN:OD1	1:D:174:HIS:NE2	2.43	0.52
2:G:148:TRP:CE3	2:G:179:LEU:HD22	2.45	0.52
2:F:148:TRP:CE3	2:F:179:LEU:HD22	2.44	0.52
1:A:134:LEU:HD13	2:B:118:PHE:CD2	2.45	0.52
2:B:142:ARG:HH11	2:B:142:ARG:CG	2.21	0.52
3:X:384:ASN:OD1	3:X:385:GLY:N	2.41	0.52
2:G:21:ILE:HG12	2:G:102:THR:HG21	1.91	0.52
2:K:151:ASP:HA	2:K:191:VAL:HG12	1.91	0.52
2:C:186:TYR:HA	2:C:192:TYR:OH	2.10	0.52
3:J:436:TYR:CD1	3:J:436:TYR:C	2.84	0.52
1:D:153:LYS:HG2	1:D:154:ASP:OD1	2.10	0.52
3:J:351:LEU:HB2	3:J:366:THR:HB	1.90	0.52
3:Y:296:TYR:HE1	3:Y:301:ARG:HD3	1.74	0.51
3:J:393:THR:HG22	3:J:394:THR:O	2.10	0.51
3:P:312:ASN:ND2	3:P:317:LYS:HD2	2.24	0.51
3:X:393:THR:HG22	3:X:394:THR:O	2.10	0.51
1:D:149:GLY:O	1:D:221:VAL:HG21	2.10	0.51
3:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
3:P:325:ASN:ND2	3:P:326:LYS:N	2.59	0.51
1:D:153:LYS:HG2	1:D:154:ASP:OD2	2.10	0.51
1:I:101:SER:H	1:I:104:LEU:HD23	1.76	0.51
1:D:69:THR:C	1:D:81:LEU:HD12	2.31	0.51
1:A:169:LEU:HD21	1:A:192:VAL:HG21	1.91	0.51
1:M:53:THR:O	1:M:56:THR:OG1	2.28	0.51
1:E:134:LEU:HD13	2:F:118:PHE:CD2	2.46	0.51
2:G:61:ARG:HB2	2:G:76:SER:O	2.10	0.51
3:X:429:HIS:O	3:X:435:HIS:HA	2.11	0.51
1:E:164:TRP:CZ2	1:E:192:VAL:HG12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASP:HB3	2:F:94:TYR:HE1	1.74	0.51
1:H:35:ASN:O	1:H:97:ALA:N	2.41	0.51
1:D:58:ARG:NH1	1:D:70:VAL:O	2.43	0.51
2:C:140:TYR:CD2	2:C:141:PRO:HA	2.45	0.51
2:G:31:THR:OG1	2:G:50:LYS:HE2	2.10	0.51
2:L:5:THR:HG23	2:L:100:GLN:HE22	1.75	0.51
3:Y:291:PRO:CB	3:Y:304:SER:HA	2.37	0.51
3:P:291:PRO:CB	3:P:304:SER:HA	2.37	0.51
1:I:94:TYR:CE1	1:I:119:VAL:HB	2.46	0.51
1:M:52:SER:O	1:M:72:ARG:NH1	2.43	0.51
2:G:167:ASP:HB2	1:I:174:HIS:HE1	1.75	0.51
3:P:297:ASN:O	3:P:298:SER:HB3	2.09	0.51
1:D:202:GLN:HB2	1:D:204:TYR:CZ	2.45	0.51
3:Y:291:PRO:HB3	3:Y:304:SER:CA	2.37	0.51
3:Y:325:ASN:ND2	3:Y:326:LYS:N	2.59	0.51
3:X:350:THR:HB	3:X:441:LEU:CG	2.40	0.51
1:A:35:ASN:O	1:A:97:ALA:N	2.44	0.51
3:X:436:TYR:CD1	3:X:436:TYR:C	2.84	0.51
1:E:72:ARG:NE	1:E:74:ASP:OD1	2.33	0.51
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.93	0.51
3:J:429:HIS:O	3:J:435:HIS:HA	2.11	0.51
3:O:429:HIS:O	3:O:435:HIS:HA	2.11	0.51
3:P:249:ASP:O	3:P:257:PRO:HG3	2.11	0.51
1:D:29:ILE:O	1:D:72:ARG:NH2	2.44	0.51
2:G:113:PRO:HD3	2:G:198:HIS:CG	2.46	0.51
3:O:393:THR:HG22	3:O:394:THR:O	2.10	0.51
3:X:418:GLN:C	3:X:420:GLY:H	2.15	0.51
3:J:418:GLN:C	3:J:420:GLY:H	2.15	0.51
3:O:350:THR:HB	3:O:441:LEU:CG	2.40	0.51
1:I:68:PHE:CD1	1:I:83:MET:HA	2.46	0.51
2:C:140:TYR:CG	2:C:141:PRO:HA	2.45	0.51
2:L:73:LEU:HD12	2:L:74:THR:H	1.76	0.51
2:L:19:ILE:HG12	2:L:78:LEU:HD11	1.91	0.51
3:O:384:ASN:OD1	3:O:385:GLY:N	2.41	0.51
2:G:113:PRO:HD2	2:G:201:LEU:HD22	1.93	0.51
1:I:70:VAL:HA	1:I:80:TYR:O	2.10	0.51
3:Y:378:ALA:HB3	3:Y:428:MET:HB2	1.92	0.51
1:H:134:LEU:HD13	2:K:118:PHE:CD2	2.46	0.51
2:G:142:ARG:NH1	2:G:142:ARG:HG2	2.20	0.50
3:O:443:LEU:HG	3:O:443:LEU:O	2.11	0.50
3:Y:261:CYS:HB2	3:Y:277:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:144:GLY:O	1:M:196:SER:HB2	2.10	0.50
1:E:94:TYR:CE1	1:E:119:VAL:HB	2.46	0.50
3:X:360:LYS:O	3:X:414:LYS:HD2	2.11	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.50
1:M:23:GLY:HA2	1:M:78:PHE:CD2	2.46	0.50
1:A:35:ASN:OD1	1:A:50:SER:HB2	2.11	0.50
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.50
1:H:68:PHE:CD1	1:H:83:MET:HA	2.47	0.50
3:N:249:ASP:O	3:N:257:PRO:HG3	2.11	0.50
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.50
2:G:36:TYR:CE1	2:G:46:LEU:HD13	2.46	0.50
3:Y:249:ASP:C	3:Y:257:PRO:HG3	2.32	0.50
2:F:36:TYR:HE2	2:F:89:GLN:HB3	1.76	0.50
3:X:294:GLN:O	3:X:300:TYR:CD1	2.65	0.50
1:D:38:ARG:HD3	1:D:94:TYR:CE2	2.46	0.50
1:M:195:PRO:C	1:M:197:SER:H	2.14	0.50
1:M:153:LYS:HG2	1:M:154:ASP:OD1	2.11	0.50
3:O:418:GLN:C	3:O:420:GLY:H	2.15	0.50
1:I:220:LYS:HE2	1:I:222:GLU:HG3	1.93	0.50
3:O:360:LYS:O	3:O:414:LYS:HD2	2.11	0.50
1:E:169:LEU:HD21	1:E:192:VAL:HG21	1.93	0.50
1:M:133:PRO:HB2	1:M:221:VAL:HG13	1.92	0.50
3:P:278:TYR:CD1	3:P:278:TYR:N	2.79	0.50
3:P:249:ASP:C	3:P:257:PRO:HG3	2.32	0.50
1:I:52:SER:O	1:I:72:ARG:NH1	2.44	0.50
2:L:148:TRP:CE3	2:L:179:LEU:HD22	2.47	0.50
1:M:169:LEU:HD21	1:M:192:VAL:HG21	1.94	0.50
3:N:432:LEU:CD1	3:N:437:THR:HG22	2.42	0.50
2:C:148:TRP:CE3	2:C:179:LEU:HD22	2.46	0.50
3:J:283:GLN:C	3:J:285:HIS:N	2.63	0.50
3:N:291:PRO:HB3	3:N:304:SER:CA	2.37	0.50
2:F:21:ILE:HG12	2:F:102:THR:HG21	1.92	0.50
3:O:294:GLN:O	3:O:300:TYR:CD1	2.65	0.50
3:Y:292:ARG:O	3:Y:293:GLU:HB3	2.12	0.50
3:P:332:ILE:CG2	3:P:333:GLU:N	2.74	0.50
3:P:406:LEU:HD12	3:P:406:LEU:O	2.12	0.50
1:A:67:ARG:C	1:A:68:PHE:HD1	2.15	0.50
3:Y:249:ASP:O	3:Y:257:PRO:HG3	2.10	0.50
3:N:378:ALA:HB3	3:N:428:MET:HB2	1.92	0.50
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:P:432:LEU:CD1	3:P:437:THR:HG22	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:289:THR:HG22	3:P:290:LYS:N	2.21	0.50
3:J:380:GLU:O	3:J:425:CYS:HA	2.12	0.50
3:P:250:THR:HG22	3:P:257:PRO:HB3	1.94	0.50
1:E:34:MET:SD	1:E:98:ARG:HB2	2.52	0.50
2:F:140:TYR:CG	2:F:141:PRO:HA	2.47	0.50
2:L:121:SER:O	2:L:125:LEU:HB2	2.11	0.50
3:O:436:TYR:C	3:O:436:TYR:CD1	2.84	0.50
1:D:73:ASP:N	1:D:78:PHE:O	2.44	0.50
3:N:332:ILE:CG2	3:N:333:GLU:N	2.74	0.49
3:P:291:PRO:HB3	3:P:304:SER:CA	2.37	0.49
1:H:38:ARG:NH1	1:H:90:ASP:HA	2.27	0.49
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	0.49
3:X:409:LYS:HB2	3:Y:407:TYR:OH	2.12	0.49
3:Y:406:LEU:HD12	3:Y:406:LEU:O	2.12	0.49
3:N:250:THR:HG22	3:N:257:PRO:HB3	1.94	0.49
3:N:278:TYR:N	3:N:278:TYR:CD1	2.79	0.49
1:M:58:ARG:NH1	1:M:70:VAL:O	2.44	0.49
1:D:92:ALA:N	1:D:119:VAL:O	2.44	0.49
3:J:443:LEU:HG	3:J:443:LEU:O	2.11	0.49
3:O:380:GLU:O	3:O:425:CYS:HA	2.12	0.49
3:P:378:ALA:HB3	3:P:428:MET:HB2	1.92	0.49
1:H:92:ALA:HB3	1:H:94:TYR:CE1	2.47	0.49
3:O:292:ARG:O	3:O:293:GLU:CB	2.58	0.49
1:E:67:ARG:C	1:E:68:PHE:HD1	2.15	0.49
3:Y:278:TYR:N	3:Y:278:TYR:CD1	2.79	0.49
3:Y:350:THR:HB	3:Y:441:LEU:HG	1.95	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	0.49
3:O:357:GLU:C	3:O:359:THR:H	2.15	0.49
3:J:357:GLU:C	3:J:359:THR:H	2.15	0.49
3:P:296:TYR:HE1	3:P:301:ARG:HD3	1.74	0.49
3:X:278:TYR:HB2	3:X:320:LYS:HB3	1.95	0.49
3:Y:332:ILE:CG2	3:Y:333:GLU:N	2.74	0.49
1:I:47:TRP:NE1	1:I:49:ALA:O	2.45	0.49
1:I:129:PRO:HB3	1:I:155:TYR:HB3	1.93	0.49
3:N:292:ARG:O	3:N:293:GLU:HB3	2.12	0.49
3:X:443:LEU:HG	3:X:443:LEU:O	2.11	0.49
1:M:164:TRP:CE2	1:M:206:CYS:HB2	2.47	0.49
3:X:357:GLU:C	3:X:359:THR:H	2.15	0.49
3:O:246:LYS:HB2	3:O:249:ASP:OD2	2.12	0.49
1:I:12:VAL:O	1:I:121:VAL:HA	2.13	0.49
2:F:19:ILE:HG12	2:F:78:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:278:TYR:HB2	3:J:320:LYS:HB3	1.94	0.49
1:E:58:ARG:NH1	1:E:70:VAL:O	2.44	0.49
3:X:246:LYS:HB2	3:X:249:ASP:OD2	2.12	0.49
2:K:19:ILE:HG12	2:K:78:LEU:HD11	1.94	0.49
2:B:5:THR:HG23	2:B:100:GLN:HE22	1.77	0.49
1:H:38:ARG:HD3	1:H:94:TYR:CE2	2.48	0.49
2:G:142:ARG:HH11	2:G:142:ARG:CG	2.22	0.49
2:G:138:ASN:OD1	1:I:174:HIS:NE2	2.45	0.49
3:Y:432:LEU:CD1	3:Y:437:THR:HG22	2.42	0.49
3:P:398:LEU:HD11	3:P:402:GLY:HA2	1.95	0.49
3:Y:369:VAL:O	3:Y:405:PHE:HA	2.13	0.49
3:X:380:GLU:O	3:X:425:CYS:HA	2.12	0.49
3:P:369:VAL:O	3:P:405:PHE:HA	2.12	0.49
2:K:117:ILE:HG13	2:K:133:VAL:O	2.12	0.49
2:G:5:THR:HG23	2:G:100:GLN:HE22	1.77	0.49
3:O:283:GLN:CD	3:O:287:ALA:HB2	2.33	0.49
1:H:38:ARG:HB3	1:H:94:TYR:CD2	2.48	0.49
3:N:406:LEU:HD12	3:N:406:LEU:O	2.12	0.49
3:N:249:ASP:C	3:N:257:PRO:HG3	2.32	0.49
2:G:83:PHE:CE1	2:G:106:ILE:HG12	2.48	0.49
1:I:101:SER:H	1:I:104:LEU:CD2	2.26	0.49
3:O:409:LYS:HB2	3:P:407:TYR:OH	2.12	0.49
1:M:101:SER:H	1:M:104:LEU:HD23	1.77	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	0.49
3:Y:250:THR:HG22	3:Y:257:PRO:HB3	1.94	0.49
1:I:23:GLY:HA2	1:I:78:PHE:CD2	2.48	0.49
1:E:23:GLY:HA2	1:E:78:PHE:CD2	2.48	0.49
3:X:283:GLN:CD	3:X:287:ALA:HB2	2.34	0.49
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.49
1:H:60:TYR:OH	1:H:69:THR:HA	2.13	0.49
3:Y:398:LEU:HD11	3:Y:402:GLY:HA2	1.95	0.49
1:A:53:THR:O	1:A:56:THR:OG1	2.31	0.49
3:P:261:CYS:HB2	3:P:277:TRP:CZ2	2.47	0.49
3:O:388:GLU:OE2	3:O:416:ARG:NH2	2.42	0.49
3:N:311:GLN:N	3:N:311:GLN:NE2	2.53	0.48
1:H:69:THR:O	1:H:81:LEU:HD12	2.13	0.48
1:E:153:LYS:HG2	1:E:154:ASP:OD2	2.13	0.48
3:O:248:LYS:O	3:O:255:ARG:HD3	2.13	0.48
1:H:176:PHE:CD1	2:K:176:SER:HB3	2.48	0.48
1:E:73:ASP:N	1:E:78:PHE:O	2.42	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:248:LYS:O	3:X:255:ARG:HD3	2.13	0.48
1:H:202:GLN:O	1:H:203:THR:HA	2.12	0.48
2:G:31:THR:O	2:G:50:LYS:HA	2.13	0.48
2:L:201:LEU:HG	2:L:205:VAL:HG23	1.95	0.48
3:X:277:TRP:O	3:X:283:GLN:HB3	2.13	0.48
1:A:38:ARG:HB3	1:A:94:TYR:CE2	2.48	0.48
3:J:350:THR:HB	3:J:441:LEU:CG	2.40	0.48
1:M:22:CYS:O	1:M:78:PHE:HA	2.12	0.48
2:L:140:TYR:CG	2:L:141:PRO:HA	2.48	0.48
1:A:197:SER:HB3	3:X:295:GLN:CD	2.34	0.48
3:P:292:ARG:O	3:P:293:GLU:HB3	2.12	0.48
3:X:292:ARG:O	3:X:293:GLU:CB	2.58	0.48
2:C:149:LYS:HB2	2:C:193:ALA:HB3	1.94	0.48
1:E:68:PHE:CD1	1:E:83:MET:HA	2.48	0.48
1:I:67:ARG:C	1:I:68:PHE:HD1	2.17	0.48
1:A:69:THR:C	1:A:81:LEU:HD12	2.33	0.48
3:X:266:VAL:O	3:X:300:TYR:HB2	2.13	0.48
1:H:47:TRP:NE1	1:H:49:ALA:O	2.46	0.48
2:G:2:VAL:HG11	2:G:90:HIS:CD2	2.48	0.48
1:I:35:ASN:O	1:I:97:ALA:N	2.45	0.48
1:M:29:ILE:O	1:M:72:ARG:NH2	2.46	0.48
3:J:277:TRP:O	3:J:283:GLN:HB3	2.13	0.48
1:A:32:HIS:ND1	1:A:98:ARG:HG3	2.29	0.48
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.48
3:O:266:VAL:O	3:O:300:TYR:HB2	2.13	0.48
2:B:20:THR:HG22	2:B:73:LEU:O	2.13	0.48
2:L:61:ARG:HB2	2:L:76:SER:O	2.14	0.48
3:O:278:TYR:HB2	3:O:320:LYS:HB3	1.95	0.48
3:J:248:LYS:O	3:J:255:ARG:HD3	2.13	0.48
1:I:153:LYS:HG2	1:I:154:ASP:OD2	2.13	0.48
2:K:91:TYR:CD1	1:M:99:LYS:NZ	2.81	0.48
3:P:259:VAL:HG23	3:P:308:VAL:CG2	2.43	0.48
3:P:350:THR:HB	3:P:441:LEU:HG	1.95	0.48
1:M:72:ARG:NE	1:M:74:ASP:OD1	2.36	0.48
2:F:108:ARG:NH1	2:F:111:ALA:HB2	2.28	0.48
3:N:369:VAL:O	3:N:405:PHE:HA	2.12	0.48
3:P:244:PRO:HB3	3:P:336:ILE:HD11	1.95	0.48
1:M:92:ALA:N	1:M:119:VAL:O	2.46	0.48
3:X:358:MET:O	3:X:414:LYS:HE3	2.14	0.48
2:G:149:LYS:HZ1	2:G:195:GLU:CD	2.13	0.48
1:I:101:SER:N	1:I:104:LEU:HD23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:118:PHE:CG	1:I:134:LEU:HB3	2.49	0.48
2:B:140:TYR:CG	2:B:141:PRO:HA	2.49	0.48
2:G:162:SER:HB3	2:G:176:SER:OG	2.13	0.48
3:J:246:LYS:HB2	3:J:249:ASP:OD2	2.12	0.48
2:G:169:LYS:HB3	2:G:169:LYS:NZ	2.29	0.48
3:O:277:TRP:O	3:O:283:GLN:HB3	2.13	0.48
3:X:371:GLY:HA2	3:X:403:SER:OG	2.14	0.48
3:O:283:GLN:C	3:O:285:HIS:N	2.63	0.48
3:Y:311:GLN:N	3:Y:311:GLN:NE2	2.53	0.48
1:M:149:GLY:O	1:M:221:VAL:HG21	2.14	0.48
2:C:142:ARG:HG2	2:C:142:ARG:NH1	2.28	0.48
2:L:21:ILE:HG12	2:L:102:THR:HG21	1.95	0.48
3:P:312:ASN:HB3	3:P:319:TYR:OH	2.14	0.48
3:Y:244:PRO:HB3	3:Y:336:ILE:HD11	1.95	0.48
3:J:388:GLU:OE1	3:J:388:GLU:HA	2.14	0.48
3:X:388:GLU:OE1	3:X:388:GLU:HA	2.14	0.48
1:D:38:ARG:HB3	1:D:94:TYR:CD2	2.49	0.47
1:D:92:ALA:HB3	1:D:94:TYR:CE1	2.48	0.47
1:H:69:THR:O	1:H:81:LEU:HA	2.13	0.47
3:O:358:MET:O	3:O:414:LYS:HE3	2.14	0.47
3:X:414:LYS:HG2	3:X:418:GLN:NE2	2.29	0.47
1:E:164:TRP:CH2	1:E:192:VAL:HG12	2.49	0.47
3:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.47
3:J:414:LYS:HG2	3:J:418:GLN:NE2	2.29	0.47
3:N:259:VAL:HG23	3:N:308:VAL:CG2	2.43	0.47
2:C:201:LEU:HB3	2:C:203:SER:O	2.14	0.47
3:J:371:GLY:HA2	3:J:403:SER:OG	2.14	0.47
3:J:292:ARG:O	3:J:293:GLU:CB	2.58	0.47
3:O:414:LYS:HG2	3:O:418:GLN:NE2	2.29	0.47
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
3:Y:312:ASN:HB3	3:Y:319:TYR:OH	2.14	0.47
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.49	0.47
2:C:169:LYS:NZ	2:C:169:LYS:HB3	2.29	0.47
3:J:266:VAL:O	3:J:300:TYR:HB2	2.13	0.47
3:J:388:GLU:OE2	3:J:416:ARG:NH2	2.42	0.47
2:L:151:ASP:HA	2:L:191:VAL:HG12	1.95	0.47
2:L:169:LYS:NZ	2:L:169:LYS:HB3	2.29	0.47
3:X:282:VAL:O	3:X:283:GLN:CB	2.52	0.47
3:X:288:LYS:H	3:X:288:LYS:CD	2.27	0.47
2:F:142:ARG:CG	2:F:142:ARG:HH11	2.26	0.47
1:H:52:SER:O	1:H:72:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.47
3:Y:259:VAL:HG23	3:Y:308:VAL:CG2	2.43	0.47
1:A:23:GLY:HA2	1:A:78:PHE:CD2	2.50	0.47
1:D:67:ARG:C	1:D:68:PHE:HD1	2.18	0.47
1:E:102:ASP:OD1	1:E:102:ASP:N	2.47	0.47
1:H:153:LYS:HG2	1:H:154:ASP:OD1	2.14	0.47
1:M:203:THR:HG21	1:M:220:LYS:NZ	2.30	0.47
1:M:101:SER:OG	1:M:104:LEU:HA	2.14	0.47
2:C:113:PRO:HD3	2:C:198:HIS:CG	2.50	0.47
3:P:275:PHE:HZ	3:P:302:VAL:O	1.98	0.47
1:D:98:ARG:NH2	1:D:111:ASP:OD2	2.35	0.47
1:H:174:HIS:HB3	2:K:164:THR:HG21	1.97	0.47
3:J:288:LYS:H	3:J:288:LYS:CD	2.27	0.47
3:N:322:LYS:HG3	3:N:333:GLU:HG2	1.97	0.47
1:M:153:LYS:HG2	1:M:154:ASP:OD2	2.14	0.47
1:H:67:ARG:C	1:H:68:PHE:HD1	2.18	0.47
2:B:29:ILE:HG21	2:B:90:HIS:CD2	2.47	0.47
1:I:68:PHE:HB3	1:I:81:LEU:HD11	1.95	0.47
3:P:308:VAL:HG11	3:P:313:TRP:HB2	1.97	0.47
2:K:4:MET:HG2	2:K:97:THR:HG23	1.95	0.47
1:H:134:LEU:HB3	2:K:118:PHE:CG	2.49	0.47
2:F:6:GLN:NE2	2:F:102:THR:OG1	2.48	0.47
3:P:432:LEU:HD22	3:P:437:THR:HB	1.97	0.47
2:F:11:LEU:HD22	2:F:19:ILE:HD12	1.97	0.47
2:K:113:PRO:HD3	2:K:198:HIS:CG	2.49	0.47
2:K:121:SER:O	2:K:125:LEU:HB2	2.14	0.47
2:C:162:SER:HB3	2:C:176:SER:OG	2.15	0.47
2:B:61:ARG:HB2	2:B:76:SER:O	2.15	0.47
3:X:438:GLN:O	3:X:439:LYS:HD3	2.15	0.47
3:N:244:PRO:HB3	3:N:336:ILE:HD11	1.95	0.47
2:F:167:ASP:OD2	2:F:169:LYS:HG3	2.15	0.47
3:Y:322:LYS:HG3	3:Y:333:GLU:HG2	1.97	0.47
1:M:203:THR:HB	1:M:220:LYS:HE3	1.96	0.47
2:L:20:THR:HG22	2:L:73:LEU:O	2.14	0.47
2:C:31:THR:O	2:C:50:LYS:HA	2.14	0.47
3:O:289:THR:CG2	3:O:290:LYS:N	2.78	0.47
1:I:53:THR:O	1:I:56:THR:OG1	2.32	0.47
3:Y:275:PHE:HZ	3:Y:302:VAL:O	1.97	0.47
2:C:118:PHE:CD2	1:D:134:LEU:HD13	2.50	0.47
1:I:126:THR:HB	1:I:213:SER:HB3	1.97	0.47
1:H:68:PHE:O	1:H:69:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:164:TRP:C	1:M:166:SER:N	2.67	0.47
1:A:99:LYS:NZ	2:C:91:TYR:CD1	2.83	0.47
3:Y:279:VAL:O	3:Y:282:VAL:HG22	2.15	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
3:P:368:LEU:HD12	3:P:369:VAL:H	1.79	0.47
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
3:P:322:LYS:HG3	3:P:333:GLU:HG2	1.97	0.46
1:M:92:ALA:HB3	1:M:94:TYR:CE1	2.50	0.46
3:P:279:VAL:O	3:P:282:VAL:HG22	2.15	0.46
3:Y:308:VAL:HG11	3:Y:313:TRP:HB2	1.97	0.46
2:L:31:THR:O	2:L:50:LYS:HA	2.15	0.46
2:K:108:ARG:NH1	2:K:111:ALA:HB2	2.30	0.46
1:H:19:ILE:C	1:H:20:LEU:HD23	2.36	0.46
3:O:438:GLN:O	3:O:439:LYS:HD3	2.15	0.46
3:Y:300:TYR:HB3	3:Y:301:ARG:H	1.37	0.46
1:M:101:SER:H	1:M:104:LEU:CD2	2.28	0.46
3:N:278:TYR:CE2	3:N:284:VAL:HG22	2.50	0.46
3:P:261:CYS:HB2	3:P:277:TRP:CH2	2.50	0.46
2:K:36:TYR:HE2	2:K:89:GLN:HB3	1.81	0.46
2:B:36:TYR:CE1	2:B:46:LEU:HD13	2.51	0.46
3:O:371:GLY:HA2	3:O:403:SER:OG	2.14	0.46
2:C:5:THR:HG23	2:C:100:GLN:HE22	1.80	0.46
1:H:101:SER:OG	1:H:104:LEU:HA	2.15	0.46
3:J:421:ASN:N	3:J:421:ASN:ND2	2.64	0.46
3:N:308:VAL:HG11	3:N:313:TRP:HB2	1.97	0.46
3:O:421:ASN:N	3:O:421:ASN:ND2	2.64	0.46
1:A:68:PHE:CD1	1:A:83:MET:HA	2.51	0.46
1:I:220:LYS:HE2	1:I:222:GLU:CG	2.46	0.46
1:D:69:THR:O	1:D:81:LEU:HD12	2.15	0.46
3:O:388:GLU:OE1	3:O:388:GLU:HA	2.14	0.46
2:G:146:VAL:HB	2:G:161:GLU:OE2	2.15	0.46
2:B:148:TRP:CE3	2:B:179:LEU:HD22	2.51	0.46
3:X:289:THR:CG2	3:X:290:LYS:N	2.78	0.46
3:X:421:ASN:N	3:X:421:ASN:ND2	2.64	0.46
2:B:201:LEU:HB3	2:B:203:SER:O	2.16	0.46
3:Y:361:ASN:ND2	3:Y:362:GLN:HG3	2.31	0.46
2:F:83:PHE:CE1	2:F:106:ILE:HG12	2.51	0.46
3:P:300:TYR:O	3:P:301:ARG:HB2	2.16	0.46
3:X:286:ASN:O	3:X:287:ALA:CB	2.63	0.46
1:H:103:ARG:O	1:H:104:LEU:HB2	2.15	0.46
1:D:154:ASP:HA	1:D:185:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LYS:HB2	2:B:193:ALA:HB3	1.96	0.46
2:G:36:TYR:HE2	2:G:89:GLN:HB3	1.81	0.46
3:P:278:TYR:CE2	3:P:284:VAL:HG22	2.50	0.46
1:E:29:ILE:O	1:E:72:ARG:NH2	2.48	0.46
1:I:52:SER:OG	1:I:56:THR:N	2.49	0.46
3:N:432:LEU:HD11	3:N:437:THR:HG22	1.98	0.46
2:B:140:TYR:CD2	2:B:141:PRO:HA	2.50	0.46
2:B:31:THR:O	2:B:50:LYS:HA	2.15	0.46
2:L:2:VAL:HG11	2:L:90:HIS:CD2	2.51	0.46
2:B:113:PRO:HD3	2:B:198:HIS:CG	2.50	0.46
3:Y:261:CYS:HB2	3:Y:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD11	3:Y:437:THR:HG22	1.98	0.46
2:B:162:SER:HB3	2:B:176:SER:OG	2.16	0.46
3:N:361:ASN:ND2	3:N:362:GLN:HG3	2.31	0.46
2:K:140:TYR:CG	2:K:141:PRO:HA	2.50	0.46
3:Y:278:TYR:CE2	3:Y:284:VAL:HG22	2.50	0.46
1:M:22:CYS:N	1:M:79:VAL:O	2.48	0.46
1:H:144:GLY:O	1:H:196:SER:HB2	2.15	0.46
3:O:265:ASP:HA	3:O:299:THR:HB	1.98	0.46
3:O:288:LYS:CD	3:O:288:LYS:H	2.27	0.46
1:H:92:ALA:N	1:H:119:VAL:O	2.47	0.46
3:N:275:PHE:HZ	3:N:302:VAL:O	1.98	0.46
3:N:368:LEU:HD12	3:N:369:VAL:H	1.79	0.46
3:J:289:THR:CG2	3:J:290:LYS:N	2.78	0.46
1:E:153:LYS:HG2	1:E:154:ASP:OD1	2.15	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD22	3:Y:437:THR:HB	1.97	0.46
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.46
3:P:344:ARG:O	3:P:372:PHE:HA	2.16	0.46
2:K:146:VAL:HB	2:K:161:GLU:OE2	2.16	0.46
3:P:432:LEU:HD11	3:P:437:THR:HG22	1.98	0.46
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.46
1:H:22:CYS:O	1:H:78:PHE:HA	2.15	0.46
3:N:300:TYR:O	3:N:301:ARG:CB	2.64	0.45
3:N:344:ARG:O	3:N:372:PHE:HA	2.16	0.45
1:I:69:THR:C	1:I:81:LEU:HD12	2.36	0.45
2:F:113:PRO:HD2	2:F:201:LEU:HD22	1.98	0.45
3:P:439:LYS:HA	3:P:439:LYS:HD2	1.81	0.45
3:Y:368:LEU:HD12	3:Y:369:VAL:H	1.79	0.45
2:C:36:TYR:CE1	2:C:46:LEU:HD13	2.50	0.45
2:L:106:ILE:O	2:L:166:GLN:NE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:HB3	2:B:164:THR:HG21	1.98	0.45
1:M:69:THR:C	1:M:81:LEU:HD12	2.36	0.45
2:C:121:SER:O	2:C:125:LEU:HB2	2.16	0.45
3:P:433:HIS:CA	3:P:434:ASN:N	2.69	0.45
1:H:135:ALA:CB	1:H:224:LYS:HD3	2.47	0.45
1:A:94:TYR:CE1	1:A:119:VAL:HB	2.51	0.45
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.98	0.45
2:L:83:PHE:CE1	2:L:106:ILE:HG12	2.52	0.45
1:A:101:SER:H	1:A:104:LEU:HD23	1.82	0.45
3:P:300:TYR:O	3:P:301:ARG:CB	2.65	0.45
3:Y:300:TYR:O	3:Y:301:ARG:HB2	2.16	0.45
3:P:311:GLN:N	3:P:311:GLN:NE2	2.53	0.45
2:K:142:ARG:HH11	2:K:142:ARG:CG	2.25	0.45
1:M:32:HIS:ND1	1:M:98:ARG:HG3	2.31	0.45
2:G:124:GLN:NE2	1:I:132:PHE:CE2	2.85	0.45
3:P:361:ASN:ND2	3:P:362:GLN:HG3	2.31	0.45
3:O:286:ASN:O	3:O:287:ALA:CB	2.63	0.45
3:J:278:TYR:N	3:J:278:TYR:CD1	2.85	0.45
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
1:E:69:THR:C	1:E:81:LEU:HD12	2.37	0.45
3:Y:279:VAL:O	3:Y:280:ASP:HB2	2.16	0.45
1:A:29:ILE:O	1:A:72:ARG:NH2	2.49	0.45
3:Y:242:LEU:HD13	3:Y:336:ILE:HG22	1.98	0.45
2:F:162:SER:HB3	2:F:176:SER:OG	2.16	0.45
3:X:265:ASP:HA	3:X:299:THR:HB	1.98	0.45
2:F:5:THR:HG23	2:F:100:GLN:HE22	1.81	0.45
1:H:53:THR:O	1:H:56:THR:OG1	2.34	0.45
3:Y:290:LYS:HE3	3:Y:292:ARG:HH12	1.82	0.45
1:E:32:HIS:ND1	1:E:98:ARG:HG3	2.31	0.45
1:A:72:ARG:NE	1:A:74:ASP:OD1	2.38	0.45
1:D:22:CYS:O	1:D:78:PHE:HA	2.16	0.45
3:O:342:GLN:HA	3:O:343:PRO:HD3	1.83	0.45
2:C:146:VAL:HB	2:C:161:GLU:OE2	2.17	0.45
3:J:244:PRO:HB3	3:J:336:ILE:HD13	1.99	0.45
3:N:326:LYS:C	3:N:328:LEU:H	2.20	0.45
3:Y:344:ARG:O	3:Y:372:PHE:HA	2.16	0.45
3:P:406:LEU:CD1	3:P:406:LEU:C	2.85	0.45
1:M:101:SER:N	1:M:104:LEU:HD23	2.31	0.45
3:N:279:VAL:O	3:N:280:ASP:HB2	2.17	0.45
3:N:265:ASP:HA	3:N:299:THR:CB	2.47	0.45
1:D:101:SER:N	1:D:104:LEU:HD23	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TRP:CZ3	1:A:221:VAL:HG21	2.52	0.45
2:F:36:TYR:CE1	2:F:46:LEU:HD13	2.52	0.45
2:K:31:THR:O	2:K:50:LYS:HA	2.16	0.45
1:E:101:SER:N	1:E:104:LEU:HD23	2.32	0.45
1:E:101:SER:OG	1:E:104:LEU:HA	2.17	0.45
3:P:269:GLU:C	3:P:271:PRO:HD3	2.36	0.45
3:Y:406:LEU:C	3:Y:406:LEU:CD1	2.84	0.45
2:C:113:PRO:HD2	2:C:201:LEU:HD22	1.99	0.45
1:D:101:SER:H	1:D:104:LEU:CD2	2.29	0.45
2:B:31:THR:OG1	2:B:50:LYS:HE2	2.15	0.45
2:K:140:TYR:CD2	2:K:141:PRO:HA	2.52	0.45
1:E:195:PRO:C	1:E:197:SER:H	2.20	0.45
1:I:164:TRP:HZ2	1:I:190:SER:O	1.99	0.45
2:G:108:ARG:NH1	2:G:111:ALA:HB2	2.32	0.45
2:F:31:THR:OG1	2:F:50:LYS:HE2	2.15	0.45
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	0.45
3:Y:300:TYR:O	3:Y:301:ARG:CB	2.65	0.45
3:Y:301:ARG:HG2	3:Y:303:VAL:HG23	1.99	0.45
1:E:101:SER:H	1:E:104:LEU:CD2	2.29	0.45
3:P:279:VAL:O	3:P:280:ASP:HB2	2.17	0.45
3:Y:265:ASP:HA	3:Y:299:THR:CB	2.47	0.45
2:F:113:PRO:HD3	2:F:198:HIS:CG	2.52	0.45
3:Y:323:VAL:HG12	3:Y:324:SER:N	2.32	0.45
2:F:31:THR:O	2:F:50:LYS:HA	2.16	0.45
1:A:101:SER:H	1:A:104:LEU:CD2	2.30	0.45
3:P:290:LYS:HE3	3:P:292:ARG:HH12	1.82	0.45
1:E:3:GLN:HB2	1:E:25:SER:CB	2.41	0.45
3:N:406:LEU:CD1	3:N:406:LEU:C	2.85	0.45
3:X:266:VAL:HB	3:X:300:TYR:HB2	1.98	0.45
3:N:323:VAL:HG12	3:N:324:SER:N	2.32	0.45
1:E:133:PRO:HB3	1:E:221:VAL:HG22	1.99	0.45
3:J:286:ASN:O	3:J:287:ALA:CB	2.63	0.44
3:N:238:PRO:CB	3:N:328:LEU:HD13	2.47	0.44
3:O:346:PRO:CB	3:O:372:PHE:HB3	2.39	0.44
1:E:38:ARG:HB3	1:E:94:TYR:CE2	2.52	0.44
3:Y:345:GLU:HA	3:Y:431:ALA:HB3	1.99	0.44
1:D:91:THR:HG23	1:D:120:THR:HG22	1.99	0.44
3:O:374:PRO:O	3:O:429:HIS:HE1	2.00	0.44
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.98	0.44
3:P:238:PRO:CB	3:P:328:LEU:HD13	2.47	0.44
1:E:148:LEU:HD12	1:E:164:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:149:LYS:HB2	2:K:193:ALA:HB3	1.99	0.44
1:H:192:VAL:HG22	1:H:194:VAL:HG13	2.00	0.44
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.32	0.44
3:X:244:PRO:HB3	3:X:336:ILE:HD13	1.99	0.44
2:F:61:ARG:HB2	2:F:76:SER:O	2.17	0.44
3:Y:238:PRO:CB	3:Y:328:LEU:HD13	2.47	0.44
3:X:291:PRO:O	3:X:292:ARG:HD2	2.17	0.44
3:P:265:ASP:HA	3:P:299:THR:CB	2.47	0.44
3:P:242:LEU:HD13	3:P:336:ILE:HG22	1.98	0.44
1:A:12:VAL:O	1:A:121:VAL:HA	2.17	0.44
3:J:347:GLN:NE2	3:J:349:TYR:OH	2.51	0.44
3:P:239:SER:HB3	3:P:264:VAL:CG2	2.47	0.44
3:X:287:ALA:O	3:X:288:LYS:C	2.56	0.44
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.44
3:P:345:GLU:HA	3:P:431:ALA:HB3	1.99	0.44
2:K:27:GLN:O	2:K:29:ILE:HG23	2.17	0.44
1:D:64:VAL:HB	1:D:68:PHE:CD2	2.53	0.44
1:D:192:VAL:HG22	1:D:194:VAL:HG13	1.99	0.44
3:N:345:GLU:HA	3:N:431:ALA:HB3	1.98	0.44
1:A:153:LYS:HG2	1:A:154:ASP:OD1	2.16	0.44
3:Y:269:GLU:C	3:Y:271:PRO:HD3	2.36	0.44
2:C:2:VAL:HG11	2:C:90:HIS:CD2	2.53	0.44
1:I:58:ARG:NH1	1:I:70:VAL:O	2.49	0.44
2:F:36:TYR:HB2	2:F:87:HIS:HB2	1.99	0.44
3:O:266:VAL:HB	3:O:300:TYR:HB2	1.98	0.44
2:G:124:GLN:HB2	1:I:132:PHE:CD1	2.52	0.44
3:J:309:LEU:O	3:J:312:ASN:N	2.51	0.44
3:O:347:GLN:NE2	3:O:349:TYR:OH	2.51	0.44
3:X:309:LEU:O	3:X:312:ASN:N	2.51	0.44
3:X:278:TYR:HA	3:X:282:VAL:O	2.18	0.44
3:J:287:ALA:O	3:J:288:LYS:C	2.56	0.44
3:P:326:LYS:C	3:P:328:LEU:H	2.20	0.44
3:J:346:PRO:CB	3:J:372:PHE:HB3	2.39	0.44
1:H:18:LEU:CB	1:H:83:MET:HE3	2.43	0.44
3:J:248:LYS:NZ	3:J:380:GLU:OE2	2.47	0.44
3:J:264:VAL:O	3:J:265:ASP:HB2	2.18	0.44
2:K:30:GLU:HB2	2:K:32:TRP:CD1	2.53	0.44
3:Y:239:SER:HB3	3:Y:264:VAL:CG2	2.47	0.44
3:P:363:VAL:HG22	3:P:412:VAL:O	2.18	0.44
3:X:278:TYR:N	3:X:278:TYR:CD1	2.85	0.44
1:E:174:HIS:HB3	2:F:164:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
1:H:92:ALA:HB3	1:H:94:TYR:CZ	2.53	0.44
3:O:291:PRO:O	3:O:292:ARG:HD2	2.18	0.44
1:D:92:ALA:HB3	1:D:94:TYR:CZ	2.53	0.44
2:F:149:LYS:HZ1	2:F:195:GLU:CD	2.18	0.44
3:P:278:TYR:HE2	3:P:284:VAL:HG22	1.83	0.44
1:A:69:THR:O	1:A:81:LEU:HD12	2.18	0.44
1:D:69:THR:O	1:D:81:LEU:HA	2.18	0.44
3:P:323:VAL:HG12	3:P:324:SER:N	2.32	0.44
1:D:188:LEU:O	1:D:188:LEU:HD12	2.17	0.44
3:Y:363:VAL:HG22	3:Y:412:VAL:O	2.18	0.44
3:N:301:ARG:HG2	3:N:303:VAL:HG23	1.99	0.44
3:Y:278:TYR:HE2	3:Y:284:VAL:HG22	1.83	0.44
3:Y:439:LYS:HA	3:Y:439:LYS:HD2	1.82	0.44
1:E:194:VAL:HG21	1:E:204:TYR:CZ	2.53	0.44
1:E:12:VAL:O	1:E:121:VAL:HA	2.18	0.44
1:M:185:LEU:HA	1:M:185:LEU:HD12	1.78	0.44
1:H:23:GLY:HA2	1:H:78:PHE:CD2	2.52	0.44
3:O:309:LEU:O	3:O:312:ASN:N	2.51	0.44
2:B:108:ARG:NH1	2:B:111:ALA:HB2	2.33	0.44
2:L:117:ILE:HG13	2:L:133:VAL:O	2.17	0.44
1:A:38:ARG:HD3	1:A:94:TYR:CE2	2.53	0.43
3:N:278:TYR:HE2	3:N:284:VAL:HG22	1.83	0.43
1:E:35:ASN:O	1:E:97:ALA:N	2.48	0.43
1:H:22:CYS:N	1:H:79:VAL:O	2.51	0.43
3:N:363:VAL:HG22	3:N:412:VAL:O	2.18	0.43
3:O:244:PRO:HB3	3:O:336:ILE:HD13	1.99	0.43
3:O:296:TYR:HB3	3:O:297:ASN:H	1.56	0.43
3:O:278:TYR:CD1	3:O:278:TYR:N	2.85	0.43
1:M:68:PHE:HB3	1:M:81:LEU:HD11	2.00	0.43
3:P:242:LEU:HA	3:P:242:LEU:HD23	1.86	0.43
2:L:70:GLU:HG3	2:L:71:PHE:N	2.32	0.43
3:O:278:TYR:HA	3:O:282:VAL:O	2.18	0.43
3:Y:326:LYS:C	3:Y:328:LEU:H	2.20	0.43
1:E:136:PRO:HG2	1:E:223:PRO:HG3	1.99	0.43
1:A:69:THR:O	1:A:81:LEU:HA	2.18	0.43
1:I:22:CYS:N	1:I:79:VAL:O	2.47	0.43
2:K:186:TYR:HA	2:K:192:TYR:OH	2.18	0.43
2:K:170:ASP:OD1	2:K:172:THR:OG1	2.19	0.43
3:X:347:GLN:NE2	3:X:349:TYR:OH	2.50	0.43
2:F:207:LYS:HZ3	1:M:201:THR:CB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:374:PRO:O	3:X:429:HIS:HE1	2.00	0.43
2:C:136:LEU:HB2	2:C:175:LEU:HB3	1.99	0.43
1:E:68:PHE:HB3	1:E:81:LEU:HD11	2.00	0.43
1:M:98:ARG:NH2	1:M:111:ASP:OD2	2.37	0.43
1:E:22:CYS:O	1:E:78:PHE:HA	2.18	0.43
3:O:264:VAL:O	3:O:265:ASP:HB2	2.18	0.43
2:G:121:SER:O	2:G:125:LEU:HB2	2.19	0.43
2:L:113:PRO:HD3	2:L:198:HIS:CG	2.52	0.43
1:H:101:SER:H	1:H:104:LEU:HD22	1.83	0.43
1:I:60:TYR:CE2	1:I:69:THR:HA	2.54	0.43
3:P:258:GLU:HA	3:P:308:VAL:HG23	1.99	0.43
3:N:351:LEU:HA	3:N:352:PRO:HD3	1.91	0.43
3:X:348:VAL:O	3:X:439:LYS:HG3	2.19	0.43
3:Y:338:LYS:NZ	3:Y:430:GLU:OE2	2.52	0.43
3:N:239:SER:HB3	3:N:264:VAL:CG2	2.47	0.43
3:P:338:LYS:NZ	3:P:430:GLU:OE2	2.52	0.43
2:K:20:THR:HG22	2:K:73:LEU:O	2.19	0.43
3:P:325:ASN:HD22	3:P:326:LYS:N	2.15	0.43
1:A:154:ASP:HA	1:A:185:LEU:HB3	2.01	0.43
1:D:156:PHE:HB3	1:D:185:LEU:HD12	2.00	0.43
2:K:2:VAL:HG11	2:K:90:HIS:CD2	2.53	0.43
2:L:63:SER:O	2:L:74:THR:N	2.52	0.43
3:Y:252:MET:SD	3:Y:428:MET:HE3	2.58	0.43
2:B:36:TYR:HE2	2:B:89:GLN:HB3	1.83	0.43
2:K:31:THR:OG1	2:K:50:LYS:HE2	2.18	0.43
1:E:181:GLN:C	1:E:183:SER:H	2.21	0.43
3:P:414:LYS:O	3:P:418:GLN:HG3	2.19	0.43
1:I:194:VAL:HG21	1:I:204:TYR:CZ	2.54	0.43
3:J:374:PRO:O	3:J:429:HIS:HE1	2.00	0.43
2:G:161:GLU:HA	2:G:176:SER:O	2.18	0.43
2:C:83:PHE:CE1	2:C:106:ILE:HG12	2.53	0.43
2:B:121:SER:O	2:B:125:LEU:HB2	2.18	0.43
3:N:414:LYS:O	3:N:418:GLN:HG3	2.19	0.43
1:A:3:GLN:HB2	1:A:25:SER:CB	2.41	0.43
1:M:38:ARG:HB3	1:M:94:TYR:CE2	2.54	0.43
1:M:67:ARG:C	1:M:68:PHE:HD1	2.22	0.43
1:I:222:GLU:HA	1:I:223:PRO:HD3	1.86	0.43
1:A:27:PHE:CE1	1:A:29:ILE:HG22	2.53	0.43
3:J:348:VAL:O	3:J:439:LYS:HG3	2.19	0.43
1:I:163:SER:O	1:I:164:TRP:CD1	2.71	0.43
2:C:20:THR:HG22	2:C:73:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:238:PRO:HB2	3:N:328:LEU:HD13	2.01	0.43
3:X:346:PRO:CB	3:X:372:PHE:HB3	2.39	0.43
1:H:60:TYR:CE2	1:H:69:THR:HA	2.53	0.43
2:C:4:MET:HG2	2:C:97:THR:HG23	1.99	0.43
2:G:201:LEU:HB3	2:G:203:SER:O	2.19	0.43
2:L:149:LYS:HB2	2:L:193:ALA:HB3	2.00	0.43
2:F:146:VAL:HB	2:F:161:GLU:OE2	2.18	0.43
2:G:49:TYR:CE2	2:G:53:THR:HB	2.54	0.43
1:D:103:ARG:N	2:F:50:LYS:NZ	2.60	0.43
3:O:287:ALA:O	3:O:288:LYS:C	2.56	0.43
3:Y:291:PRO:O	3:Y:292:ARG:HB3	2.19	0.43
1:D:18:LEU:CB	1:D:83:MET:HE3	2.47	0.43
3:Y:258:GLU:HA	3:Y:308:VAL:HG23	1.99	0.43
2:L:161:GLU:HA	2:L:176:SER:O	2.18	0.43
2:C:186:TYR:HA	2:C:192:TYR:HH	1.83	0.43
3:X:264:VAL:O	3:X:265:ASP:HB2	2.18	0.43
2:C:108:ARG:NH1	2:C:111:ALA:HB2	2.34	0.43
1:A:144:GLY:O	1:A:196:SER:HB2	2.19	0.43
3:P:386:GLN:HA	3:P:387:PRO:HD3	1.76	0.43
2:B:70:GLU:HG3	2:B:71:PHE:N	2.33	0.43
3:P:266:VAL:HB	3:P:300:TYR:CD2	2.54	0.42
3:P:301:ARG:HG2	3:P:303:VAL:HG23	1.99	0.42
1:D:194:VAL:HG21	1:D:204:TYR:CZ	2.54	0.42
2:L:167:ASP:CB	1:M:174:HIS:HE1	2.32	0.42
2:K:161:GLU:HA	2:K:176:SER:O	2.19	0.42
3:N:338:LYS:NZ	3:N:430:GLU:OE2	2.52	0.42
1:D:19:ILE:C	1:D:20:LEU:HD23	2.39	0.42
3:N:266:VAL:HB	3:N:300:TYR:CD2	2.54	0.42
1:D:149:GLY:O	1:D:221:VAL:HG11	2.18	0.42
2:F:201:LEU:HB3	2:F:203:SER:O	2.19	0.42
3:P:368:LEU:HD12	3:P:369:VAL:N	2.34	0.42
2:B:161:GLU:HA	2:B:176:SER:O	2.19	0.42
2:F:161:GLU:HA	2:F:176:SER:O	2.19	0.42
3:Y:266:VAL:HB	3:Y:300:TYR:CD2	2.54	0.42
3:P:291:PRO:O	3:P:292:ARG:HB3	2.19	0.42
2:G:29:ILE:HG21	2:G:90:HIS:CD2	2.50	0.42
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.42
1:M:69:THR:O	1:M:81:LEU:HD12	2.20	0.42
1:M:37:VAL:HG22	1:M:47:TRP:HA	2.01	0.42
3:O:348:VAL:O	3:O:439:LYS:HG3	2.19	0.42
2:B:38:GLN:O	2:B:84:ALA:HB1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:36:TYR:HE2	2:L:89:GLN:HB3	1.85	0.42
3:O:274:LYS:HE2	3:O:324:SER:HB2	2.02	0.42
1:H:156:PHE:CD1	1:H:156:PHE:C	2.92	0.42
3:Y:296:TYR:OH	3:Y:301:ARG:NH1	2.46	0.42
2:K:91:TYR:HD1	1:M:99:LYS:HZ3	1.66	0.42
1:A:58:ARG:NH1	1:A:70:VAL:O	2.52	0.42
1:I:164:TRP:O	1:I:166:SER:N	2.53	0.42
1:A:101:SER:N	1:A:104:LEU:HD23	2.34	0.42
3:J:291:PRO:O	3:J:292:ARG:HD2	2.17	0.42
1:H:68:PHE:HB3	1:H:81:LEU:HD11	2.01	0.42
1:D:153:LYS:NZ	1:D:181:GLN:OE1	2.23	0.42
2:F:29:ILE:HG21	2:F:90:HIS:CD2	2.52	0.42
3:N:258:GLU:HA	3:N:308:VAL:HG23	1.99	0.42
3:Y:368:LEU:HD12	3:Y:369:VAL:N	2.34	0.42
3:X:336:ILE:HG12	3:X:337:SER:N	2.35	0.42
3:O:336:ILE:HG12	3:O:337:SER:N	2.35	0.42
3:Y:357:GLU:C	3:Y:359:THR:H	2.23	0.42
3:Y:414:LYS:O	3:Y:418:GLN:HG3	2.18	0.42
3:P:296:TYR:OH	3:P:301:ARG:NH1	2.46	0.42
3:X:283:GLN:C	3:X:285:HIS:H	2.23	0.42
1:A:197:SER:HB3	3:X:295:GLN:OE1	2.20	0.42
1:E:38:ARG:HD3	1:E:94:TYR:CE2	2.55	0.42
1:A:185:LEU:HA	1:A:185:LEU:HD12	1.78	0.42
1:D:185:LEU:HD12	1:D:185:LEU:HA	1.76	0.42
1:A:38:ARG:NH1	1:A:90:ASP:HA	2.34	0.42
3:X:384:ASN:CG	3:X:385:GLY:H	2.22	0.42
1:D:74:ASP:HB3	2:F:94:TYR:CE1	2.54	0.42
2:F:91:TYR:HD1	1:I:99:LYS:NZ	2.17	0.42
3:N:368:LEU:HD12	3:N:369:VAL:N	2.34	0.42
2:C:160:GLN:O	2:C:178:THR:N	2.44	0.42
3:O:369:VAL:HB	3:O:406:LEU:HD12	2.02	0.42
2:G:63:SER:O	2:G:74:THR:N	2.50	0.42
1:E:152:VAL:HG22	1:E:208:VAL:HG21	2.01	0.42
1:I:153:LYS:HG2	1:I:154:ASP:OD1	2.20	0.42
2:C:21:ILE:HG12	2:C:102:THR:HG21	2.02	0.42
3:J:391:TYR:CD2	3:J:391:TYR:C	2.93	0.42
3:P:238:PRO:HB2	3:P:328:LEU:HD13	2.01	0.42
3:Y:238:PRO:HB2	3:Y:328:LEU:HD13	2.01	0.42
1:H:38:ARG:HA	1:H:93:ILE:O	2.19	0.42
1:M:38:ARG:HD3	1:M:94:TYR:CE2	2.55	0.42
1:E:149:GLY:HA2	1:E:164:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:TYR:CE2	1:E:69:THR:HA	2.54	0.42
3:J:336:ILE:HG12	3:J:337:SER:N	2.35	0.42
1:E:53:THR:O	1:E:56:THR:OG1	2.38	0.42
3:J:369:VAL:HB	3:J:406:LEU:HD12	2.02	0.42
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42
1:D:220:LYS:HE2	1:D:222:GLU:OE1	2.19	0.42
3:Y:328:LEU:HD12	3:Y:329:PRO:CD	2.47	0.42
1:H:101:SER:N	1:H:104:LEU:HD22	2.35	0.42
3:X:369:VAL:HB	3:X:406:LEU:HD12	2.02	0.42
1:I:32:HIS:ND1	1:I:98:ARG:HG3	2.35	0.42
1:A:38:ARG:HB3	1:A:94:TYR:CD2	2.55	0.42
2:L:29:ILE:HG21	2:L:90:HIS:CD2	2.53	0.42
3:N:350:THR:HB	3:N:441:LEU:CD1	2.50	0.42
3:J:367:CYS:HB2	3:J:381:TRP:CH2	2.55	0.42
1:H:6:GLU:OE1	1:H:95:TYR:HA	2.20	0.42
2:K:58:VAL:HA	2:K:59:PRO:HD3	1.91	0.42
3:J:274:LYS:HE2	3:J:324:SER:HB2	2.01	0.42
3:X:391:TYR:C	3:X:391:TYR:CD2	2.92	0.42
1:I:195:PRO:C	1:I:197:SER:H	2.23	0.42
2:C:4:MET:SD	2:C:90:HIS:HB2	2.59	0.41
3:Y:276:ASN:HB3	3:Y:278:TYR:CE1	2.56	0.41
2:L:138:ASN:OD1	1:M:174:HIS:NE2	2.52	0.41
2:L:161:GLU:HG2	2:L:177:SER:HB2	2.02	0.41
1:D:40:VAL:O	1:D:43:GLY:N	2.45	0.41
3:O:367:CYS:HB2	3:O:381:TRP:CH2	2.55	0.41
3:P:296:TYR:HB3	3:P:297:ASN:H	1.34	0.41
3:J:282:VAL:O	3:J:283:GLN:CB	2.52	0.41
1:E:38:ARG:NH1	1:E:90:ASP:HA	2.35	0.41
3:X:314:LEU:HD23	3:X:314:LEU:HA	1.87	0.41
1:D:181:GLN:C	1:D:183:SER:H	2.23	0.41
3:N:268:HIS:O	3:N:271:PRO:CG	2.68	0.41
3:Y:268:HIS:O	3:Y:271:PRO:CG	2.68	0.41
1:D:163:SER:OG	1:D:207:ASN:HB2	2.20	0.41
2:G:133:VAL:HG21	1:I:134:LEU:HD21	2.01	0.41
3:P:350:THR:HB	3:P:441:LEU:CD1	2.50	0.41
1:D:47:TRP:NE1	1:D:49:ALA:O	2.53	0.41
2:F:49:TYR:CE2	2:F:53:THR:HB	2.55	0.41
2:G:58:VAL:HA	2:G:59:PRO:HD3	1.97	0.41
2:C:183:LYS:HE2	2:C:187:GLU:OE1	2.20	0.41
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	0.41
1:M:38:ARG:HB3	1:M:94:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
1:A:99:LYS:HZ3	2:C:91:TYR:HD1	1.68	0.41
3:P:276:ASN:HB3	3:P:278:TYR:CE1	2.55	0.41
1:M:23:GLY:HA2	1:M:78:PHE:CE2	2.54	0.41
1:H:176:PHE:CE1	2:K:176:SER:HB3	2.55	0.41
1:A:173:VAL:HG22	1:A:192:VAL:HB	2.01	0.41
2:L:11:LEU:HD22	2:L:19:ILE:HD12	2.02	0.41
3:O:391:TYR:C	3:O:391:TYR:CD2	2.92	0.41
3:O:328:LEU:HD12	3:O:329:PRO:CD	2.50	0.41
1:D:30:SER:HB3	1:D:74:ASP:HB3	2.01	0.41
2:K:36:TYR:CE1	2:K:46:LEU:HD13	2.55	0.41
1:I:4:LEU:HG	1:I:24:VAL:HG12	2.02	0.41
1:E:188:LEU:HD12	1:E:188:LEU:O	2.20	0.41
2:B:138:ASN:C	2:B:172:THR:HB	2.41	0.41
2:G:38:GLN:HA	2:G:44:PRO:HA	2.02	0.41
1:H:68:PHE:HA	1:H:82:GLN:O	2.20	0.41
3:P:268:HIS:O	3:P:271:PRO:CG	2.68	0.41
3:O:386:GLN:HA	3:O:387:PRO:HD3	1.88	0.41
3:X:386:GLN:HG3	3:X:387:PRO:HD2	2.02	0.41
3:Y:350:THR:HB	3:Y:441:LEU:CD1	2.50	0.41
2:B:113:PRO:HD2	2:B:201:LEU:HD22	2.03	0.41
2:G:73:LEU:HD12	2:G:74:THR:H	1.84	0.41
3:O:283:GLN:C	3:O:285:HIS:H	2.23	0.41
1:A:160:VAL:HG13	1:A:208:VAL:HG13	2.02	0.41
3:O:384:ASN:CG	3:O:385:GLY:H	2.22	0.41
2:G:167:ASP:CG	1:I:174:HIS:HE1	2.23	0.41
2:C:110:VAL:HG13	2:C:199:GLN:HG2	2.02	0.41
3:X:367:CYS:HB2	3:X:381:TRP:CH2	2.55	0.41
1:M:181:GLN:C	1:M:183:SER:H	2.24	0.41
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
1:H:219:LYS:HE2	1:H:219:LYS:HB2	1.91	0.41
2:L:5:THR:CG2	2:L:100:GLN:HE22	2.33	0.41
3:Y:335:THR:O	3:Y:336:ILE:HB	2.21	0.41
2:B:106:ILE:O	2:B:166:GLN:NE2	2.48	0.41
2:G:15:VAL:HG21	2:G:80:PHE:CZ	2.56	0.41
2:C:38:GLN:HA	2:C:44:PRO:HA	2.03	0.41
3:X:274:LYS:HE2	3:X:324:SER:HB2	2.02	0.41
2:B:2:VAL:HG11	2:B:90:HIS:CD2	2.56	0.41
2:L:100:GLN:N	2:L:100:GLN:OE1	2.44	0.41
2:G:140:TYR:CG	2:G:141:PRO:HA	2.56	0.41
3:Y:367:CYS:HB2	3:Y:381:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:151:ASP:HA	2:C:191:VAL:HG12	2.02	0.41
1:I:94:TYR:O	1:I:116:GLY:HA2	2.20	0.41
3:O:252:MET:HB2	3:O:255:ARG:CG	2.49	0.41
1:H:160:VAL:HG12	1:H:160:VAL:O	2.20	0.41
2:C:149:LYS:HA	2:C:153:ALA:O	2.21	0.41
3:O:386:GLN:HG3	3:O:387:PRO:HD2	2.02	0.41
3:J:386:GLN:HG3	3:J:387:PRO:HD2	2.02	0.41
3:X:386:GLN:HA	3:X:387:PRO:HD3	1.88	0.41
2:K:4:MET:SD	2:K:90:HIS:HB2	2.61	0.41
2:K:201:LEU:HB3	2:K:203:SER:O	2.20	0.41
1:M:34:MET:O	1:M:50:SER:HA	2.19	0.41
1:E:34:MET:O	1:E:50:SER:HA	2.21	0.41
2:L:167:ASP:CG	1:M:174:HIS:CE1	2.94	0.41
3:P:273:VAL:HB	3:P:302:VAL:HG21	2.03	0.41
3:N:273:VAL:HB	3:N:302:VAL:HG21	2.03	0.41
3:P:350:THR:HB	3:P:441:LEU:CG	2.51	0.41
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	0.41
3:Y:351:LEU:HB2	3:Y:366:THR:HB	2.03	0.41
2:G:30:GLU:HB2	2:G:32:TRP:CD1	2.56	0.41
1:H:195:PRO:C	1:H:197:SER:H	2.23	0.41
3:P:357:GLU:C	3:P:359:THR:H	2.23	0.41
2:C:70:GLU:HG3	2:C:71:PHE:N	2.35	0.41
1:H:12:VAL:O	1:H:121:VAL:HA	2.20	0.41
3:J:283:GLN:C	3:J:285:HIS:H	2.23	0.41
1:D:17:SER:HA	1:D:83:MET:O	2.21	0.41
3:X:328:LEU:HD12	3:X:329:PRO:CD	2.50	0.41
3:P:308:VAL:HG12	3:P:309:LEU:N	2.36	0.41
3:Y:273:VAL:HB	3:Y:302:VAL:HG21	2.03	0.41
1:I:73:ASP:N	1:I:78:PHE:O	2.50	0.41
2:L:122:ASP:HA	2:L:125:LEU:HB3	2.03	0.41
2:B:33:LEU:HA	2:B:89:GLN:O	2.21	0.41
2:G:186:TYR:HA	2:G:192:TYR:OH	2.20	0.41
2:F:73:LEU:HD12	2:F:74:THR:H	1.85	0.41
1:D:164:TRP:HH2	1:D:221:VAL:HG21	1.85	0.40
1:M:38:ARG:NH1	1:M:90:ASP:HA	2.35	0.40
1:A:152:VAL:HG22	1:A:208:VAL:HG21	2.03	0.40
3:P:245:PRO:HB3	3:P:258:GLU:H	1.87	0.40
1:D:27:PHE:CE1	1:D:29:ILE:HG22	2.57	0.40
3:N:351:LEU:HB2	3:N:366:THR:HB	2.03	0.40
2:C:122:ASP:O	2:C:126:LYS:HB2	2.20	0.40
1:A:4:LEU:HG	1:A:24:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:289:THR:HG22	3:O:290:LYS:N	2.36	0.40
3:X:289:THR:HG22	3:X:290:LYS:N	2.37	0.40
1:E:176:PHE:CD2	2:F:164:THR:HG23	2.56	0.40
1:D:156:PHE:C	1:D:156:PHE:CD1	2.94	0.40
2:C:61:ARG:O	2:C:76:SER:N	2.36	0.40
3:N:308:VAL:HG12	3:N:309:LEU:N	2.37	0.40
3:N:276:ASN:HB3	3:N:278:TYR:CE1	2.56	0.40
2:G:117:ILE:HG13	2:G:133:VAL:O	2.21	0.40
2:F:108:ARG:HD3	2:F:109:THR:N	2.35	0.40
3:Y:242:LEU:HD23	3:Y:242:LEU:HA	1.85	0.40
2:C:73:LEU:HD12	2:C:74:THR:H	1.86	0.40
2:L:36:TYR:CE1	2:L:46:LEU:HD13	2.56	0.40
1:E:156:PHE:C	1:E:156:PHE:CD1	2.94	0.40
2:C:149:LYS:HZ1	2:C:195:GLU:CD	2.18	0.40
3:J:328:LEU:HA	3:J:329:PRO:HD3	1.94	0.40
3:P:350:THR:HB	3:P:441:LEU:HD12	2.03	0.40
2:B:73:LEU:HD12	2:B:74:THR:H	1.86	0.40
3:P:335:THR:O	3:P:336:ILE:HB	2.21	0.40
2:B:108:ARG:HD3	2:B:109:THR:N	2.36	0.40
3:P:367:CYS:HB2	3:P:381:TRP:CZ2	2.56	0.40
1:E:101:SER:CB	1:E:104:LEU:H	2.29	0.40
2:B:91:TYR:CD1	1:D:99:LYS:NZ	2.86	0.40
1:M:69:THR:O	1:M:81:LEU:HA	2.20	0.40
1:H:58:ARG:NH1	1:H:71:SER:OG	2.52	0.40
1:E:181:GLN:C	1:E:183:SER:N	2.75	0.40
1:H:181:GLN:C	1:H:183:SER:H	2.24	0.40
3:X:432:LEU:HD22	3:X:437:THR:HB	2.04	0.40
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.23	0.40
1:D:220:LYS:HE2	1:D:222:GLU:OE2	2.21	0.40
1:E:38:ARG:HB2	1:E:92:ALA:CB	2.52	0.40
1:I:38:ARG:NH1	1:I:90:ASP:HA	2.37	0.40
2:K:29:ILE:HG21	2:K:90:HIS:CD2	2.54	0.40
3:P:351:LEU:HA	3:P:352:PRO:HD3	1.91	0.40
2:G:167:ASP:CG	1:I:174:HIS:CE1	2.95	0.40
2:K:5:THR:HG23	2:K:100:GLN:HE22	1.86	0.40
1:I:19:ILE:C	1:I:20:LEU:HD23	2.41	0.40
3:J:432:LEU:HD22	3:J:437:THR:HB	2.04	0.40
2:F:15:VAL:HG21	2:F:80:PHE:CZ	2.56	0.40
1:M:156:PHE:CD1	1:M:156:PHE:C	2.94	0.40

All (174) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:252:MET:O	3:Y:253:ILE:CG1[12_555]	0.41	1.79
3:J:252:MET:O	3:X:253:ILE:CD1[12_545]	0.48	1.72
3:O:253:ILE:CA	3:O:253:ILE:CB[10_444]	0.59	1.61
3:J:253:ILE:CD1	3:X:252:MET:O[12_545]	0.66	1.54
3:Y:253:ILE:CA	3:Y:253:ILE:CA[12_555]	0.70	1.50
2:B:18:THR:CA	3:J:285:HIS:ND1[12_545]	0.71	1.49
2:B:18:THR:CA	3:J:285:HIS:CE1[12_545]	0.71	1.49
3:J:253:ILE:CG1	3:X:252:MET:C[12_545]	0.73	1.47
3:X:284:VAL:CG1	2:L:18:THR:CG2[12_545]	0.86	1.34
3:J:253:ILE:CG1	3:X:253:ILE:N[12_545]	0.87	1.33
3:Y:253:ILE:CA	3:Y:253:ILE:C[12_555]	0.87	1.33
3:O:253:ILE:CB	3:O:253:ILE:CB[10_444]	0.96	1.24
3:N:310:HIS:CD2	3:P:253:ILE:CD1[6_445]	1.05	1.15
3:N:380:GLU:OE1	3:P:433:HIS:NE2[6_445]	1.05	1.15
3:X:285:HIS:CG	2:L:18:THR:OG1[12_545]	1.10	1.10
3:J:253:ILE:CD1	3:X:252:MET:C[12_545]	1.17	1.03
3:Y:382:GLU:OE2	3:Y:433:HIS:CG[12_555]	1.19	1.01
3:Y:253:ILE:CG2	3:Y:255:ARG:N[12_555]	1.20	1.00
3:J:253:ILE:CB	3:X:253:ILE:N[12_545]	1.20	1.00
3:O:253:ILE:CD1	3:O:254:SER:N[10_444]	1.22	0.98
2:B:18:THR:C	3:J:285:HIS:ND1[12_545]	1.25	0.95
3:N:253:ILE:CG2	3:P:253:ILE:C[6_445]	1.25	0.95
2:B:18:THR:N	3:J:285:HIS:CG[12_545]	1.25	0.95
3:N:253:ILE:N	3:P:253:ILE:N[6_445]	1.28	0.92
3:N:380:GLU:OE1	3:P:433:HIS:CE1[6_445]	1.30	0.90
3:X:285:HIS:ND1	2:L:18:THR:OG1[12_545]	1.30	0.90
1:D:143:GLY:O	3:Y:280:ASP:CG[8_555]	1.31	0.89
2:B:18:THR:OG1	3:J:285:HIS:CD2[12_545]	1.32	0.88
3:Y:382:GLU:OE2	3:Y:433:HIS:CB[12_555]	1.32	0.88
2:B:18:THR:N	3:J:285:HIS:ND1[12_545]	1.33	0.87
3:N:253:ILE:CG2	3:P:253:ILE:CA[6_445]	1.34	0.86
3:N:433:HIS:CG	3:P:382:GLU:OE2[6_445]	1.35	0.85
3:X:283:GLN:N	2:L:18:THR:O[12_545]	1.35	0.85
1:D:143:GLY:O	3:Y:280:ASP:OD1[8_555]	1.35	0.85
1:D:143:GLY:O	3:Y:280:ASP:OD2[8_555]	1.35	0.85
1:D:143:GLY:C	3:Y:280:ASP:OD2[8_555]	1.35	0.85
3:J:253:ILE:N	3:X:253:ILE:CG1[12_545]	1.36	0.84
3:N:253:ILE:CB	3:P:253:ILE:CA[6_445]	1.37	0.83
3:Y:253:ILE:N	3:Y:253:ILE:N[12_555]	1.37	0.83
1:D:144:GLY:N	3:Y:280:ASP:OD2[8_555]	1.37	0.83
3:J:253:ILE:CA	3:X:253:ILE:CG1[12_545]	1.39	0.81
3:O:253:ILE:CA	3:O:253:ILE:CG2[10_444]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:253:ILE:CG1	3:O:254:SER:N[10_444]	1.41	0.79
3:N:253:ILE:CA	3:P:253:ILE:N[6_445]	1.41	0.79
3:J:252:MET:C	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:N:253:ILE:CA	3:P:253:ILE:CA[6_445]	1.42	0.78
3:J:252:MET:O	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:N:253:ILE:CG1	3:P:252:MET:C[6_445]	1.44	0.76
3:Y:253:ILE:CG2	3:Y:254:SER:C[12_555]	1.45	0.75
3:X:281:GLY:O	2:L:20:THR:OG1[12_545]	1.45	0.75
3:J:253:ILE:CA	3:X:253:ILE:CA[12_545]	1.46	0.74
3:J:310:HIS:NE2	3:X:253:ILE:CG2[12_545]	1.46	0.74
3:O:253:ILE:C	3:O:253:ILE:CG2[10_444]	1.47	0.73
1:D:144:GLY:CA	3:Y:280:ASP:OD2[8_555]	1.48	0.72
3:O:253:ILE:O	3:O:253:ILE:CG2[10_444]	1.48	0.72
3:Y:253:ILE:C	3:Y:253:ILE:CB[12_555]	1.48	0.72
3:Y:436:TYR:CD1	3:Y:436:TYR:CD1[12_555]	1.48	0.72
3:J:253:ILE:CB	3:X:253:ILE:CA[12_545]	1.49	0.71
3:J:253:ILE:CG1	3:X:252:MET:O[12_545]	1.50	0.70
3:N:310:HIS:CD2	3:P:253:ILE:CG1[6_445]	1.50	0.70
3:N:253:ILE:CB	3:P:253:ILE:N[6_445]	1.51	0.69
3:O:253:ILE:C	3:O:253:ILE:CG1[10_444]	1.51	0.69
2:B:18:THR:CA	3:J:285:HIS:NE2[12_545]	1.51	0.69
3:N:310:HIS:NE2	3:P:253:ILE:CD1[6_445]	1.51	0.69
3:O:253:ILE:CA	3:O:253:ILE:CG1[10_444]	1.54	0.66
3:J:253:ILE:CA	3:X:253:ILE:CB[12_545]	1.55	0.65
2:B:18:THR:CA	3:J:285:HIS:CG[12_545]	1.57	0.63
3:Y:252:MET:C	3:Y:253:ILE:CG1[12_555]	1.58	0.62
3:X:285:HIS:NE2	2:L:77:GLY:N[12_545]	1.58	0.62
3:Y:253:ILE:N	3:Y:254:SER:N[12_555]	1.60	0.60
3:Y:382:GLU:OE2	3:Y:433:HIS:CD2[12_555]	1.60	0.60
3:J:436:TYR:CD1	3:X:436:TYR:CE1[12_545]	1.61	0.59
1:D:142:SER:CB	3:Y:318:GLU:OE2[8_555]	1.62	0.58
3:N:436:TYR:CD1	3:P:436:TYR:CD1[6_445]	1.62	0.58
3:N:433:HIS:CD2	3:P:382:GLU:OE2[6_445]	1.65	0.55
3:N:253:ILE:C	3:P:253:ILE:CG2[6_445]	1.65	0.55
3:N:253:ILE:CG1	3:P:252:MET:O[6_445]	1.66	0.54
3:J:252:MET:C	3:X:253:ILE:CD1[12_545]	1.67	0.53
3:X:285:HIS:CB	2:L:18:THR:OG1[12_545]	1.67	0.53
3:J:310:HIS:CE1	3:X:253:ILE:CG2[12_545]	1.68	0.52
3:J:253:ILE:CB	3:X:252:MET:C[12_545]	1.69	0.51
2:B:18:THR:CB	3:J:285:HIS:CG[12_545]	1.69	0.51
2:B:18:THR:N	3:J:285:HIS:CD2[12_545]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:380:GLU:OE1	3:X:433:HIS:NE2[12_545]	1.71	0.49
3:X:285:HIS:ND1	2:L:18:THR:CB[12_545]	1.71	0.49
3:Y:253:ILE:N	3:Y:253:ILE:CA[12_555]	1.71	0.49
3:N:253:ILE:CA	3:P:253:ILE:CB[6_445]	1.72	0.48
3:J:253:ILE:CA	3:X:253:ILE:N[12_545]	1.72	0.48
2:B:18:THR:C	3:J:285:HIS:CE1[12_545]	1.73	0.47
3:N:253:ILE:CA	3:P:253:ILE:CG2[6_445]	1.73	0.47
3:O:253:ILE:C	3:O:253:ILE:CB[10_444]	1.73	0.47
3:J:436:TYR:CD1	3:X:436:TYR:CD1[12_545]	1.74	0.46
3:O:253:ILE:C	3:O:253:ILE:CD1[10_444]	1.75	0.45
3:N:253:ILE:CG2	3:P:252:MET:O[6_445]	1.75	0.45
3:Y:252:MET:O	3:Y:253:ILE:CD1[12_555]	1.75	0.45
3:O:253:ILE:N	3:O:253:ILE:CB[10_444]	1.75	0.45
3:O:253:ILE:N	3:O:253:ILE:CG1[10_444]	1.75	0.45
3:N:253:ILE:O	3:P:253:ILE:CG2[6_445]	1.76	0.44
3:N:253:ILE:CD1	3:P:252:MET:O[6_445]	1.77	0.43
3:X:285:HIS:ND1	2:L:18:THR:CA[12_545]	1.77	0.43
3:X:284:VAL:CB	2:L:18:THR:CG2[12_545]	1.78	0.42
3:Y:253:ILE:CA	3:Y:254:SER:N[12_555]	1.78	0.42
3:X:281:GLY:O	2:L:20:THR:N[12_545]	1.78	0.42
2:B:18:THR:CB	3:J:285:HIS:ND1[12_545]	1.79	0.41
3:Y:252:MET:O	3:Y:253:ILE:CB[12_555]	1.79	0.41
1:D:143:GLY:C	3:Y:280:ASP:CG[8_555]	1.80	0.40
3:J:253:ILE:CG2	3:X:310:HIS:NE2[12_545]	1.80	0.40
2:B:18:THR:N	3:J:285:HIS:CE1[12_545]	1.81	0.39
3:J:253:ILE:C	3:X:253:ILE:CG1[12_545]	1.83	0.37
3:J:253:ILE:CG1	3:X:253:ILE:CA[12_545]	1.84	0.36
2:B:18:THR:O	3:J:285:HIS:ND1[12_545]	1.84	0.36
3:X:285:HIS:N	2:L:18:THR:CB[12_545]	1.84	0.36
2:B:18:THR:CB	3:J:285:HIS:CD2[12_545]	1.85	0.35
3:N:253:ILE:CB	3:P:252:MET:C[6_445]	1.85	0.35
3:N:253:ILE:CG2	3:P:253:ILE:N[6_445]	1.86	0.34
3:N:310:HIS:NE2	3:P:253:ILE:CB[6_445]	1.86	0.34
3:Y:253:ILE:N	3:Y:253:ILE:C[12_555]	1.87	0.33
3:N:433:HIS:CB	3:P:382:GLU:OE2[6_445]	1.87	0.33
2:B:18:THR:CA	3:J:285:HIS:CD2[12_545]	1.89	0.31
2:B:18:THR:CG2	3:J:284:VAL:CG1[12_545]	1.90	0.30
3:J:253:ILE:CG2	3:X:253:ILE:CA[12_545]	1.91	0.29
3:Y:253:ILE:C	3:Y:253:ILE:CG2[12_555]	1.91	0.29
3:Y:253:ILE:O	3:Y:253:ILE:CB[12_555]	1.92	0.28
3:Y:253:ILE:CA	3:Y:253:ILE:O[12_555]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:253:ILE:CG2	3:P:254:SER:N[6_445]	1.93	0.27
3:N:310:HIS:NE2	3:P:253:ILE:CG1[6_445]	1.93	0.27
3:J:253:ILE:N	3:X:253:ILE:N[12_545]	1.93	0.27
3:Y:436:TYR:CD1	3:Y:436:TYR:CE1[12_555]	1.93	0.27
1:D:143:GLY:C	3:Y:280:ASP:OD1[8_555]	1.95	0.25
3:X:283:GLN:CA	2:L:18:THR:O[12_545]	1.96	0.24
3:N:253:ILE:CD1	3:P:249:ASP:O[6_445]	1.96	0.24
3:O:253:ILE:N	3:O:253:ILE:CD1[10_444]	1.97	0.23
3:X:285:HIS:N	2:L:18:THR:OG1[12_545]	1.97	0.23
3:Y:253:ILE:CA	3:Y:253:ILE:CB[12_555]	1.97	0.23
2:B:18:THR:N	3:J:285:HIS:NE2[12_545]	1.98	0.22
1:D:141:THR:CG2	3:Y:340:LYS:NZ[8_555]	1.99	0.21
3:Y:253:ILE:O	3:Y:253:ILE:CG2[12_555]	2.00	0.20
2:B:18:THR:OG1	3:J:285:HIS:NE2[12_545]	2.00	0.20
3:J:252:MET:SD	3:X:434:ASN:ND2[12_545]	2.00	0.20
3:N:253:ILE:CG2	3:P:252:MET:C[6_445]	2.01	0.19
2:B:18:THR:CB	3:J:285:HIS:CE1[12_545]	2.01	0.19
3:N:253:ILE:CB	3:P:252:MET:O[6_445]	2.01	0.19
2:B:18:THR:OG1	3:J:285:HIS:CG[12_545]	2.03	0.17
3:O:253:ILE:CG2	3:O:253:ILE:CG2[10_444]	2.03	0.17
2:B:18:THR:CB	3:J:285:HIS:NE2[12_545]	2.04	0.16
3:N:253:ILE:CG1	3:P:253:ILE:N[6_445]	2.04	0.16
3:J:253:ILE:CD1	3:X:252:MET:CA[12_545]	2.04	0.16
3:O:252:MET:CE	3:O:434:ASN:ND2[10_444]	2.04	0.16
3:O:253:ILE:CB	3:O:253:ILE:CG2[10_444]	2.05	0.15
3:X:285:HIS:CE1	2:L:77:GLY:N[12_545]	2.06	0.14
3:J:436:TYR:CE1	3:X:436:TYR:CD1[12_545]	2.06	0.14
3:X:281:GLY:O	2:L:20:THR:CB[12_545]	2.06	0.14
3:X:285:HIS:CA	2:L:18:THR:OG1[12_545]	2.07	0.13
3:N:253:ILE:CG2	3:P:253:ILE:O[6_445]	2.07	0.13
3:J:253:ILE:N	3:X:253:ILE:CB[12_545]	2.08	0.12
1:D:142:SER:CA	3:Y:318:GLU:OE2[8_555]	2.08	0.12
3:J:310:HIS:CD2	3:X:253:ILE:CG2[12_545]	2.08	0.12
3:Y:249:ASP:O	3:Y:253:ILE:CD1[12_555]	2.09	0.11
3:X:285:HIS:NE2	2:L:76:SER:C[12_545]	2.09	0.11
3:N:382:GLU:OE2	3:P:433:HIS:CB[6_445]	2.10	0.10
2:B:17:ASP:O	3:J:285:HIS:NE2[12_545]	2.10	0.10
3:J:253:ILE:CG1	3:X:252:MET:CA[12_545]	2.10	0.10
3:J:436:TYR:CE1	3:X:436:TYR:CE1[12_545]	2.11	0.09
3:O:253:ILE:CB	3:O:253:ILE:CG1[10_444]	2.11	0.09
3:O:253:ILE:CA	3:O:253:ILE:CA[10_444]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:253:ILE:CG2	3:X:310:HIS:CD2[12_545]	2.12	0.08
3:J:380:GLU:OE1	3:X:433:HIS:CE1[12_545]	2.12	0.08
3:N:380:GLU:CD	3:P:433:HIS:NE2[6_445]	2.14	0.06
2:G:50:LYS:NZ	1:H:103:ARG:C[8_445]	2.15	0.05
2:G:50:LYS:NZ	1:H:103:ARG:CA[8_445]	2.16	0.04
3:N:436:TYR:CE1	3:P:436:TYR:O[6_445]	2.17	0.03
3:Y:382:GLU:CD	3:Y:433:HIS:CD2[12_555]	2.17	0.03
3:J:253:ILE:CB	3:X:252:MET:O[12_545]	2.18	0.02
3:X:284:VAL:CA	2:L:18:THR:CG2[12_545]	2.19	0.01

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	207/243 (85%)	184 (89%)	19 (9%)	4 (2%)	10 52
1	D	204/243 (84%)	185 (91%)	15 (7%)	4 (2%)	9 51
1	E	207/243 (85%)	186 (90%)	18 (9%)	3 (1%)	14 58
1	H	207/243 (85%)	187 (90%)	16 (8%)	4 (2%)	10 52
1	I	204/243 (84%)	182 (89%)	17 (8%)	5 (2%)	7 46
1	M	204/243 (84%)	186 (91%)	13 (6%)	5 (2%)	7 46
2	B	209/213 (98%)	187 (90%)	21 (10%)	1 (0%)	34 77
2	C	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	34 77
2	F	209/213 (98%)	184 (88%)	24 (12%)	1 (0%)	34 77
2	G	209/213 (98%)	186 (89%)	22 (10%)	1 (0%)	34 77
2	K	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	34 77
2	L	209/213 (98%)	186 (89%)	21 (10%)	2 (1%)	19 65
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2 29
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	P	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
3	X	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	29
3	Y	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	31
All	All	3714/4002 (93%)	3276 (88%)	343 (9%)	95 (3%)	7	45

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	A	141	THR
1	A	223	PRO
1	D	136	PRO
1	D	140	SER
1	D	142	SER
1	E	141	THR
1	I	136	PRO
1	I	140	SER
1	I	142	SER
3	J	283	GLN
3	J	287	ALA
3	J	289	THR
3	J	433	HIS
3	N	298	SER
3	N	301	ARG
3	X	283	GLN
3	X	287	ALA
3	X	289	THR
3	X	433	HIS
3	Y	298	SER
3	Y	301	ARG
1	H	138	SER
1	H	140	SER
1	H	141	THR
1	M	136	PRO
1	M	140	SER
1	M	142	SER
1	M	165	ASN
3	O	283	GLN
3	O	287	ALA
3	O	289	THR

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Mol	Chain	Res	Type
3	O	433	HIS
3	P	298	SER
3	P	301	ARG
1	E	142	SER
2	F	110	VAL
2	G	110	VAL
1	I	165	ASN
3	J	267	SER
3	J	298	SER
3	N	271	PRO
3	X	267	SER
3	X	298	SER
3	Y	271	PRO
1	H	201	THR
3	O	267	SER
3	O	298	SER
3	P	271	PRO
3	J	293	GLU
3	N	282	VAL
3	N	291	PRO
3	N	293	GLU
3	X	293	GLU
3	Y	282	VAL
3	Y	291	PRO
3	Y	293	GLU
2	K	110	VAL
3	O	293	GLU
3	P	282	VAL
3	P	291	PRO
3	P	293	GLU
2	B	110	VAL
2	C	110	VAL
3	J	286	ASN
3	J	358	MET
3	J	385	GLY
3	N	283	GLN
3	N	295	GLN
3	X	286	ASN
3	X	358	MET
3	X	385	GLY
3	Y	283	GLN
3	Y	295	GLN

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Mol	Chain	Res	Type
3	O	286	ASN
3	O	358	MET
3	O	385	GLY
3	P	283	GLN
3	P	295	GLN
1	A	201	THR
1	E	136	PRO
1	I	143	GLY
3	N	336	ILE
3	Y	336	ILE
2	L	110	VAL
2	L	121	SER
3	P	327	ALA
3	P	336	ILE
3	N	327	ALA
3	Y	327	ALA
1	D	143	GLY
3	J	290	LYS
3	X	290	LYS
3	O	290	LYS
1	M	143	GLY

5.3.2 Protein sidechains (i)

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	180/205 (88%)	163 (91%)	17 (9%)	11 42
1	D	180/205 (88%)	162 (90%)	18 (10%)	9 38
1	E	180/205 (88%)	162 (90%)	18 (10%)	9 38
1	H	180/205 (88%)	165 (92%)	15 (8%)	14 49
1	I	180/205 (88%)	165 (92%)	15 (8%)	14 49
1	M	180/205 (88%)	163 (91%)	17 (9%)	11 42
2	B	182/184 (99%)	164 (90%)	18 (10%)	10 39
2	C	182/184 (99%)	165 (91%)	17 (9%)	11 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	182/184 (99%)	164 (90%)	18 (10%)	10 39
2	G	182/184 (99%)	164 (90%)	18 (10%)	10 39
2	K	182/184 (99%)	163 (90%)	19 (10%)	9 36
2	L	182/184 (99%)	164 (90%)	18 (10%)	10 39
3	J	193/196 (98%)	187 (97%)	6 (3%)	47 77
3	N	192/196 (98%)	180 (94%)	12 (6%)	22 59
3	O	193/196 (98%)	187 (97%)	6 (3%)	47 77
3	P	192/196 (98%)	180 (94%)	12 (6%)	22 59
3	X	193/196 (98%)	187 (97%)	6 (3%)	47 77
3	Y	192/196 (98%)	180 (94%)	12 (6%)	22 59
All	All	3327/3510 (95%)	3065 (92%)	262 (8%)	15 51

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	50	SER
1	A	55	SER
1	A	56	THR
1	A	57	TYR
1	A	98	ARG
1	A	101	SER
1	A	148	LEU
1	A	156	PHE
1	A	161	THR
1	A	163	SER
1	A	185	LEU
1	A	196	SER
1	A	206	CYS
1	A	211	LYS
1	A	221	VAL
1	A	224	LYS
2	B	7	SER
2	B	20	THR
2	B	33	LEU
2	B	39	LYS
2	B	56	THR
2	B	78	LEU

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Mol	Chain	Res	Type
2	B	108	ARG
2	B	122	ASP
2	B	123	GLU
2	B	132	VAL
2	B	134	CYS
2	B	142	ARG
2	B	143	GLU
2	B	152	ASN
2	B	169	LYS
2	B	191	VAL
2	B	197	THR
2	B	201	LEU
2	C	7	SER
2	C	20	THR
2	C	33	LEU
2	C	39	LYS
2	C	56	THR
2	C	78	LEU
2	C	108	ARG
2	C	122	ASP
2	C	123	GLU
2	C	132	VAL
2	C	134	CYS
2	C	142	ARG
2	C	152	ASN
2	C	169	LYS
2	C	191	VAL
2	C	197	THR
2	C	201	LEU
1	D	13	LYS
1	D	50	SER
1	D	55	SER
1	D	56	THR
1	D	57	TYR
1	D	75	LEU
1	D	98	ARG
1	D	101	SER
1	D	148	LEU
1	D	156	PHE
1	D	161	THR
1	D	163	SER
1	D	185	LEU

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Mol	Chain	Res	Type
1	D	196	SER
1	D	202	GLN
1	D	206	CYS
1	D	211	LYS
1	D	224	LYS
1	E	13	LYS
1	E	50	SER
1	E	55	SER
1	E	56	THR
1	E	57	TYR
1	E	75	LEU
1	E	98	ARG
1	E	101	SER
1	E	102	ASP
1	E	139	LYS
1	E	141	THR
1	E	148	LEU
1	E	156	PHE
1	E	161	THR
1	E	185	LEU
1	E	196	SER
1	E	206	CYS
1	E	211	LYS
2	F	7	SER
2	F	20	THR
2	F	33	LEU
2	F	39	LYS
2	F	56	THR
2	F	78	LEU
2	F	108	ARG
2	F	122	ASP
2	F	123	GLU
2	F	132	VAL
2	F	134	CYS
2	F	142	ARG
2	F	143	GLU
2	F	152	ASN
2	F	169	LYS
2	F	191	VAL
2	F	197	THR
2	F	201	LEU
2	G	7	SER

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Mol	Chain	Res	Type
2	G	20	THR
2	G	33	LEU
2	G	39	LYS
2	G	56	THR
2	G	78	LEU
2	G	108	ARG
2	G	122	ASP
2	G	123	GLU
2	G	132	VAL
2	G	134	CYS
2	G	135	LEU
2	G	142	ARG
2	G	152	ASN
2	G	169	LYS
2	G	191	VAL
2	G	197	THR
2	G	201	LEU
1	I	13	LYS
1	I	50	SER
1	I	55	SER
1	I	56	THR
1	I	57	TYR
1	I	75	LEU
1	I	98	ARG
1	I	101	SER
1	I	148	LEU
1	I	156	PHE
1	I	161	THR
1	I	185	LEU
1	I	196	SER
1	I	206	CYS
1	I	211	LYS
3	J	282	VAL
3	J	292	ARG
3	J	406	LEU
3	J	413	ASP
3	J	436	TYR
3	J	441	LEU
3	N	255	ARG
3	N	260	THR
3	N	278	TYR
3	N	288	LYS

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Mol	Chain	Res	Type
3	N	291	PRO
3	N	296	TYR
3	N	311	GLN
3	N	370	LYS
3	N	394	THR
3	N	399	ASP
3	N	406	LEU
3	N	441	LEU
3	X	282	VAL
3	X	292	ARG
3	X	406	LEU
3	X	413	ASP
3	X	436	TYR
3	X	441	LEU
3	Y	255	ARG
3	Y	260	THR
3	Y	278	TYR
3	Y	288	LYS
3	Y	291	PRO
3	Y	296	TYR
3	Y	311	GLN
3	Y	370	LYS
3	Y	394	THR
3	Y	399	ASP
3	Y	406	LEU
3	Y	441	LEU
1	H	13	LYS
1	H	50	SER
1	H	55	SER
1	H	56	THR
1	H	57	TYR
1	H	98	ARG
1	H	101	SER
1	H	148	LEU
1	H	156	PHE
1	H	161	THR
1	H	185	LEU
1	H	196	SER
1	H	206	CYS
1	H	211	LYS
1	H	224	LYS
2	K	7	SER

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Mol	Chain	Res	Type
2	K	20	THR
2	K	33	LEU
2	K	39	LYS
2	K	56	THR
2	K	78	LEU
2	K	108	ARG
2	K	122	ASP
2	K	123	GLU
2	K	132	VAL
2	K	134	CYS
2	K	135	LEU
2	K	142	ARG
2	K	143	GLU
2	K	152	ASN
2	K	169	LYS
2	K	191	VAL
2	K	197	THR
2	K	201	LEU
2	L	7	SER
2	L	9	SER
2	L	20	THR
2	L	33	LEU
2	L	39	LYS
2	L	56	THR
2	L	78	LEU
2	L	108	ARG
2	L	122	ASP
2	L	123	GLU
2	L	132	VAL
2	L	134	CYS
2	L	142	ARG
2	L	152	ASN
2	L	169	LYS
2	L	191	VAL
2	L	197	THR
2	L	201	LEU
1	M	13	LYS
1	M	50	SER
1	M	55	SER
1	M	56	THR
1	M	57	TYR
1	M	98	ARG

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Mol	Chain	Res	Type
1	M	101	SER
1	M	142	SER
1	M	148	LEU
1	M	156	PHE
1	M	161	THR
1	M	163	SER
1	M	185	LEU
1	M	196	SER
1	M	206	CYS
1	M	211	LYS
1	M	222	GLU
3	O	282	VAL
3	O	292	ARG
3	O	406	LEU
3	O	413	ASP
3	O	436	TYR
3	O	441	LEU
3	P	255	ARG
3	P	260	THR
3	P	278	TYR
3	P	288	LYS
3	P	291	PRO
3	P	296	TYR
3	P	311	GLN
3	P	370	LYS
3	P	394	THR
3	P	399	ASP
3	P	406	LEU
3	P	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	GLN
2	B	90	HIS
2	C	87	HIS
2	C	90	HIS
2	F	90	HIS
2	G	6	GLN
2	G	38	GLN
2	G	87	HIS
2	G	90	HIS

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Mol	Chain	Res	Type
3	J	272	GLN
3	J	283	GLN
3	J	311	GLN
3	J	325	ASN
3	J	347	GLN
3	J	361	ASN
3	J	390	ASN
3	J	418	GLN
3	J	419	GLN
3	J	421	ASN
3	J	429	HIS
3	N	272	GLN
3	N	276	ASN
3	N	283	GLN
3	N	286	ASN
3	N	311	GLN
3	N	312	ASN
3	N	325	ASN
3	N	342	GLN
3	N	361	ASN
3	N	389	ASN
3	N	390	ASN
3	N	419	GLN
3	N	429	HIS
3	N	434	ASN
3	N	438	GLN
3	X	272	GLN
3	X	283	GLN
3	X	311	GLN
3	X	325	ASN
3	X	347	GLN
3	X	361	ASN
3	X	390	ASN
3	X	418	GLN
3	X	419	GLN
3	X	421	ASN
3	X	429	HIS
3	Y	272	GLN
3	Y	276	ASN
3	Y	283	GLN
3	Y	286	ASN
3	Y	311	GLN

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Mol	Chain	Res	Type
3	Y	312	ASN
3	Y	325	ASN
3	Y	342	GLN
3	Y	361	ASN
3	Y	389	ASN
3	Y	390	ASN
3	Y	419	GLN
3	Y	429	HIS
3	Y	434	ASN
3	Y	438	GLN
2	K	87	HIS
2	K	90	HIS
2	K	137	ASN
2	L	90	HIS
2	L	199	GLN
3	O	272	GLN
3	O	283	GLN
3	O	311	GLN
3	O	325	ASN
3	O	347	GLN
3	O	361	ASN
3	O	390	ASN
3	O	418	GLN
3	O	419	GLN
3	O	421	ASN
3	O	429	HIS
3	P	272	GLN
3	P	276	ASN
3	P	283	GLN
3	P	286	ASN
3	P	311	GLN
3	P	312	ASN
3	P	325	ASN
3	P	342	GLN
3	P	361	ASN
3	P	389	ASN
3	P	390	ASN
3	P	419	GLN
3	P	429	HIS
3	P	434	ASN
3	P	438	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	209/243 (86%)	0.33	9 (4%) 39 37	114, 118, 126, 134	0
1	D	207/243 (85%)	0.29	5 (2%) 62 58	113, 118, 125, 139	0
1	E	209/243 (86%)	0.81	24 (11%) 6 12	178, 182, 190, 198	0
1	H	209/243 (86%)	0.26	4 (1%) 70 65	96, 100, 107, 115	0
1	I	207/243 (85%)	0.67	22 (10%) 8 13	177, 182, 189, 203	0
1	M	207/243 (85%)	0.17	3 (1%) 78 72	94, 100, 107, 121	0
2	B	211/213 (99%)	0.12	3 (1%) 78 72	113, 118, 124, 139	0
2	C	211/213 (99%)	0.29	9 (4%) 39 37	113, 118, 123, 143	0
2	F	211/213 (99%)	0.94	32 (15%) 3 9	177, 182, 188, 203	0
2	G	211/213 (99%)	0.90	29 (13%) 4 10	177, 182, 187, 207	0
2	K	211/213 (99%)	0.29	2 (0%) 85 81	94, 100, 105, 120	0
2	L	211/213 (99%)	0.25	3 (1%) 78 72	94, 100, 105, 124	0
3	J	207/211 (98%)	0.61	14 (6%) 20 23	176, 176, 176, 176	0
3	N	206/211 (97%)	0.63	11 (5%) 30 31	179, 179, 179, 179	0
3	O	207/211 (98%)	1.00	33 (15%) 3 8	274, 274, 274, 274	0
3	P	206/211 (97%)	1.02	38 (18%) 2 7	277, 277, 277, 277	0
3	X	207/211 (98%)	0.54	16 (7%) 16 20	167, 167, 167, 167	0
3	Y	206/211 (97%)	0.59	18 (8%) 13 17	171, 171, 171, 171	0
All	All	3753/4002 (93%)	0.54	275 (7%) 18 21	94, 167, 277, 277	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	6.7
3	O	238	PRO	6.0
1	E	193	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	190	SER	5.4
1	I	152	VAL	5.2
1	E	130	SER	5.0
3	Y	239	SER	4.9
3	P	273	VAL	4.6
2	G	134	CYS	4.5
1	M	130	SER	4.5
3	Y	302	VAL	4.4
3	Y	333	GLU	4.2
3	O	265	ASP	4.2
2	C	145	LYS	4.2
2	G	147	GLN	4.2
3	P	302	VAL	4.0
1	I	161	THR	4.0
1	I	129	PRO	4.0
2	F	114	SER	4.0
1	E	131	VAL	3.9
3	O	239	SER	3.9
1	E	152	VAL	3.9
1	E	222	GLU	3.8
1	D	152	VAL	3.8
2	F	116	PHE	3.7
3	Y	240	VAL	3.7
1	E	194	VAL	3.7
3	O	393	THR	3.6
2	C	197	THR	3.6
3	P	293	GLU	3.6
1	I	182	SER	3.6
3	X	302	VAL	3.6
1	I	160	VAL	3.5
2	F	132	VAL	3.5
3	P	244	PRO	3.5
3	P	274	LYS	3.5
3	O	332	ILE	3.5
2	F	115	VAL	3.5
2	G	212	GLY	3.4
1	I	130	SER	3.4
3	O	394	THR	3.4
2	G	13	ALA	3.4
3	P	295	GLN	3.4
1	E	204	TYR	3.3
2	G	107	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	135	LEU	3.3
3	Y	263	VAL	3.2
2	L	187	GLU	3.2
3	X	444	SER	3.2
3	P	292	ARG	3.2
1	A	152	VAL	3.2
3	P	294	GLN	3.2
3	N	394	THR	3.2
1	H	148	LEU	3.1
3	Y	332	ILE	3.1
1	E	175	THR	3.1
1	I	149	GLY	3.1
2	F	146	VAL	3.1
3	J	240	VAL	3.1
1	A	131	VAL	3.0
2	F	177	SER	3.0
3	Y	238	PRO	3.0
2	F	147	GLN	3.0
3	P	323	VAL	3.0
3	P	259	VAL	3.0
3	O	440	SER	3.0
1	I	147	ALA	3.0
3	O	264	VAL	3.0
1	H	192	VAL	3.0
2	F	144	ALA	3.0
3	Y	289	THR	2.9
2	F	45	LYS	2.9
3	P	332	ILE	2.9
1	I	192	VAL	2.9
2	C	146	VAL	2.9
1	I	200	GLY	2.9
2	G	12	SER	2.9
2	G	116	PHE	2.9
3	O	337	SER	2.9
2	C	144	ALA	2.9
2	G	148	TRP	2.8
3	P	434	ASN	2.8
1	I	208	VAL	2.8
2	G	155	GLN	2.8
2	F	131	SER	2.8
1	D	147	ALA	2.8
2	C	131	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	136	LEU	2.8
2	K	2	VAL	2.8
3	X	263	VAL	2.8
2	C	147	GLN	2.8
1	E	129	PRO	2.8
1	I	203	THR	2.8
3	Y	264	VAL	2.8
2	F	77	GLY	2.8
1	A	160	VAL	2.8
1	H	193	THR	2.8
2	F	145	LYS	2.7
3	O	266	VAL	2.7
3	Y	273	VAL	2.7
3	O	243	PHE	2.7
3	O	350	THR	2.7
3	Y	301	ARG	2.7
3	P	240	VAL	2.7
2	F	120	PRO	2.7
1	E	161	THR	2.7
3	N	338	LYS	2.7
3	J	428	MET	2.7
3	O	260	THR	2.7
2	G	14	SER	2.7
3	P	433	HIS	2.7
3	P	296	TYR	2.7
3	X	240	VAL	2.7
1	D	148	LEU	2.6
1	E	178	ALA	2.6
3	O	273	VAL	2.6
3	P	239	SER	2.6
2	G	153	ALA	2.6
2	G	146	VAL	2.6
2	F	79	GLN	2.6
3	J	378	ALA	2.6
3	O	323	VAL	2.6
1	A	190	SER	2.6
3	J	376	ASP	2.6
3	P	330	ALA	2.6
3	O	329	PRO	2.6
3	P	442	SER	2.6
3	P	297	ASN	2.5
3	O	326	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	194	CYS	2.5
3	P	245	PRO	2.5
2	C	196	VAL	2.5
1	I	148	LEU	2.5
1	D	15	GLY	2.5
2	C	179	LEU	2.5
3	O	333	GLU	2.5
3	O	331	PRO	2.5
3	O	293	GLU	2.5
1	A	161	THR	2.5
1	I	188	LEU	2.5
3	P	238	PRO	2.5
2	F	117	ILE	2.5
3	P	298	SER	2.5
2	G	145	LYS	2.5
1	I	209	ASN	2.5
1	E	219	LYS	2.5
2	G	130	ALA	2.5
2	G	131	SER	2.5
2	F	199	GLN	2.4
1	A	130	SER	2.4
3	X	335	THR	2.4
2	G	206	THR	2.4
3	P	250	THR	2.4
2	G	195	GLU	2.4
3	X	304	SER	2.4
3	P	324	SER	2.4
1	E	192	VAL	2.4
3	P	243	PHE	2.4
3	Y	323	VAL	2.4
3	P	260	THR	2.4
3	P	263	VAL	2.4
1	A	137	SER	2.4
2	B	93	GLY	2.4
3	J	238	PRO	2.4
3	Y	334	LYS	2.4
1	E	221	VAL	2.4
3	X	323	VAL	2.4
2	L	212	GLY	2.3
3	P	289	THR	2.3
2	F	207	LYS	2.3
3	O	241	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	218	ASP	2.3
3	N	329	PRO	2.3
2	G	202	SER	2.3
3	X	385	GLY	2.3
3	Y	241	PHE	2.3
2	F	137	ASN	2.3
3	X	238	PRO	2.3
1	D	193	THR	2.3
1	A	112	ALA	2.3
3	N	239	SER	2.3
3	O	364	SER	2.3
2	G	128	GLY	2.3
3	J	434	ASN	2.3
1	E	145	THR	2.3
1	I	145	THR	2.3
1	M	152	VAL	2.3
1	E	136	PRO	2.3
2	F	133	VAL	2.3
3	O	240	VAL	2.3
3	J	321	CYS	2.3
3	N	301	ARG	2.2
1	E	150	CYS	2.2
2	F	194	CYS	2.2
1	A	178	ALA	2.2
3	Y	265	ASP	2.2
3	P	331	PRO	2.2
1	E	188	LEU	2.2
1	H	204	TYR	2.2
3	O	327	ALA	2.2
2	F	208	SER	2.2
2	G	154	LEU	2.2
3	O	385	GLY	2.2
2	F	18	THR	2.2
3	N	331	PRO	2.2
3	Y	331	PRO	2.2
3	P	287	ALA	2.2
1	E	153	LYS	2.2
1	I	193	THR	2.2
3	O	318	GLU	2.2
3	P	285	HIS	2.2
3	O	321	CYS	2.2
3	X	434	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	Y	274	LYS	2.2
1	I	178	ALA	2.2
3	N	240	VAL	2.2
3	P	257	PRO	2.2
2	F	175	LEU	2.2
1	I	194	VAL	2.2
3	J	377	ILE	2.2
3	P	307	THR	2.2
2	K	192	TYR	2.2
3	X	334	LYS	2.1
3	O	292	ARG	2.1
3	O	302	VAL	2.1
3	X	261	CYS	2.1
3	P	394	THR	2.1
3	N	302	VAL	2.1
1	E	128	GLY	2.1
2	F	155	GLN	2.1
1	I	204	TYR	2.1
3	J	444	SER	2.1
2	G	136	LEU	2.1
1	M	131	VAL	2.1
2	F	156	SER	2.1
3	P	301	ARG	2.1
3	P	276	ASN	2.1
2	F	164	THR	2.1
3	N	281	GLY	2.1
3	P	275	PHE	2.1
3	O	335	THR	2.1
1	I	162	VAL	2.1
3	N	339	ALA	2.1
2	L	211	ARG	2.1
2	F	59	PRO	2.1
3	J	323	VAL	2.1
3	J	263	VAL	2.1
3	X	241	PHE	2.1
2	G	186	TYR	2.1
3	J	339	ALA	2.1
3	J	332	ILE	2.1
3	X	324	SER	2.1
1	E	154	ASP	2.1
3	P	306	LEU	2.1
3	J	375	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	132	VAL	2.1
3	Y	294	GLN	2.1
2	F	88	CYS	2.1
1	E	202	GLN	2.0
3	X	273	VAL	2.0
1	I	146	ALA	2.0
2	B	212	GLY	2.0
2	G	149	LYS	2.0
3	O	280	ASP	2.0
2	G	113	PRO	2.0
2	C	132	VAL	2.0
3	O	250	THR	2.0
2	G	137	ASN	2.0
2	F	113	PRO	2.0
2	G	207	LYS	2.0
3	O	319	TYR	2.0
3	X	287	ALA	2.0
2	B	208	SER	2.0
2	G	114	SER	2.0
3	N	238	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.