



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:31 PM UTC

PDB ID : 1YOV / pdb_00001yov
Title : Insights into the Ubiquitin Transfer Cascade from the refined structure of the activating enzyme for NEDD8
Authors : Walden, H.; Podgorski, M.S.; Schulman, B.A.
Deposited on : 2005-01-28
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

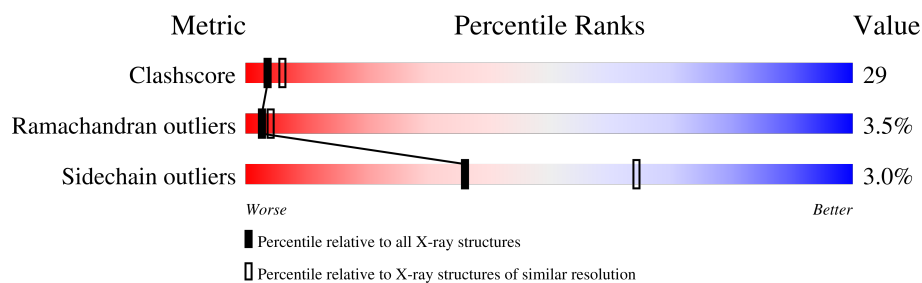
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	537	 62% 32% . .
1	C	537	 47% 45% 6% .
2	B	444	 52% 32% 5% 11%
2	D	444	 40% 40% 6% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14604 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 Amyloid protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4208	2662	718	812	16			
1	C	526	Total	C	N	O	S	0	0	0
			4183	2644	714	809	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	cloning artifact	UNP Q13564
A	-1	LYS	-	cloning artifact	UNP Q13564
A	0	LEU	-	cloning artifact	UNP Q13564
C	-2	MET	-	cloning artifact	UNP Q13564
C	-1	LYS	-	cloning artifact	UNP Q13564
C	0	LEU	-	cloning artifact	UNP Q13564

- Molecule 2 is a protein called Ubiquitin-activating enzyme E1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total	C	N	O	S	0	0	0
			3089	1975	523	573	18			
2	D	382	Total	C	N	O	S	0	0	0
			2972	1901	502	551	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	cloning artifact	UNP Q8TBC4
B	0	SER	-	cloning artifact	UNP Q8TBC4
D	-1	GLY	-	cloning artifact	UNP Q8TBC4
D	0	SER	-	cloning artifact	UNP Q8TBC4

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

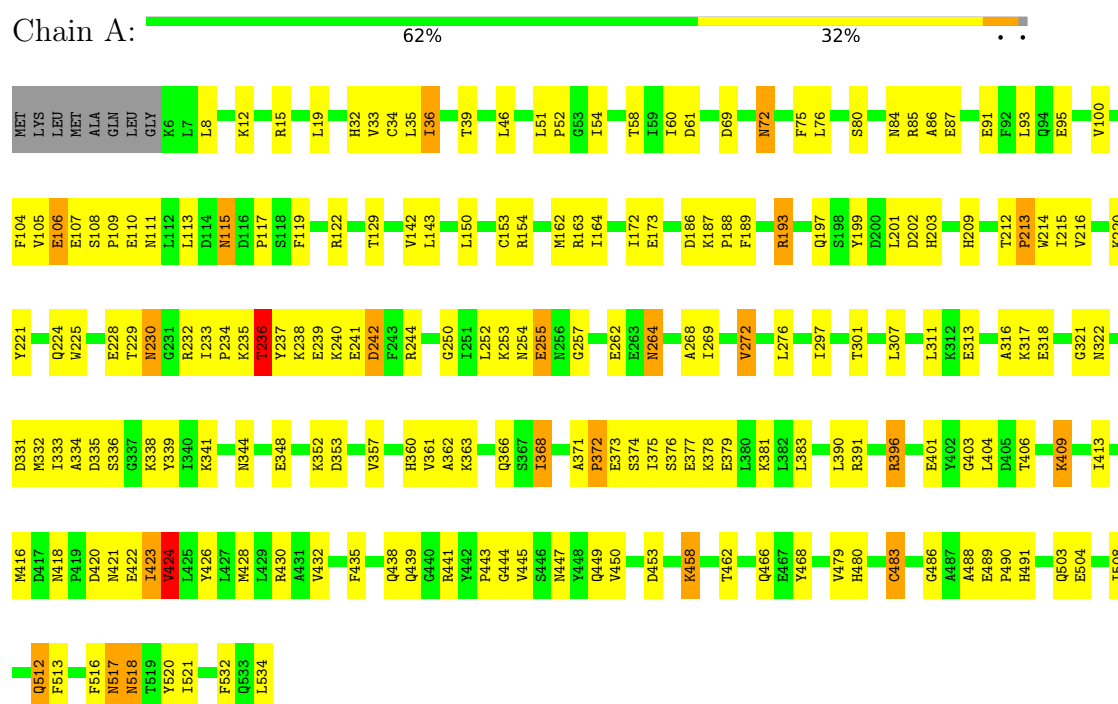
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total 53	O 53	0	0
4	B	62	Total 62	O 62	0	0
4	C	19	Total 19	O 19	0	0
4	D	16	Total 16	O 16	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

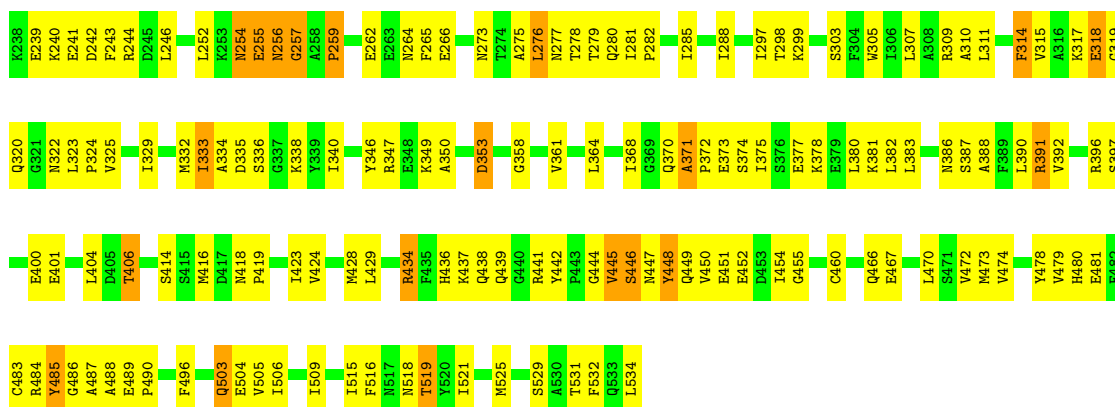
Note EDS was not executed.

• Molecule 1: Amyloid protein-binding protein 1

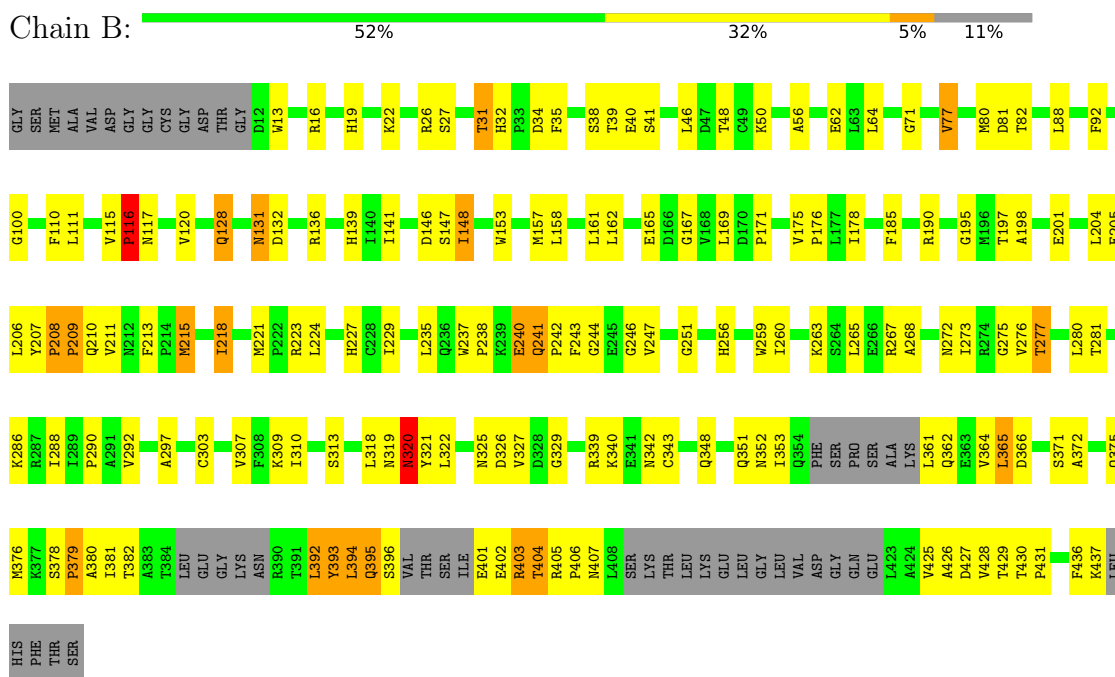


• Molecule 1: Amyloid protein-binding protein 1

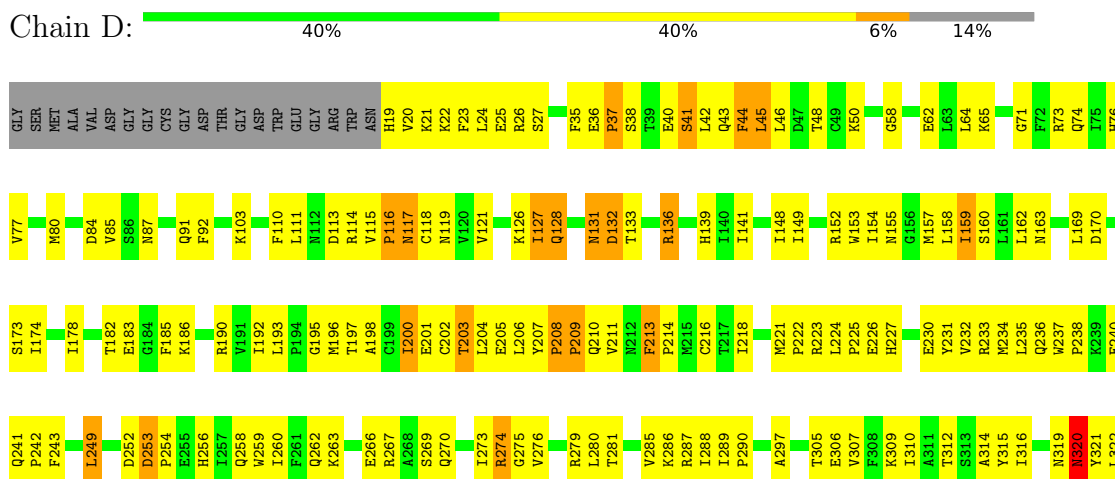




- Molecule 2: Ubiquitin-activating enzyme E1C



- Molecule 2: Ubiquitin-activating enzyme E1C



V323	F324	N325	D326	V327		L330	Y331	T332	Y333	T334	F335	E336	A337	E338	R339	K340		C343	P344	A345		P350	Q351	N352	I353	Q354	PHE	SER	PRO	PRO	SER	ALA	LYS		L361		V364	L365	D366	Y367	L368		S371	A372	S373	L374	Q375	M376	K377	S378	P379	A380	I381	T382	ALA	THR	LEU	GLU	GLY	LYS	N389
R390	T391		S396	VAL	T398	S399	I400	E401	GLU	ARG	THR	ARG	PRO	ASN	LEU	SER	LYS	THR	LEU	LYS	LEU	GLU	LEU	GLY	LEU	VAL	ASP	GLY	GLN	GLU	LEU	ALA	V425	A426	D427	V428	T429	T430	P431	Q432	T433	V434	L435	F436	LYS	LEU	HIS	PHE	THR	SER											

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.40Å 123.60Å 198.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14604	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.49	0/4290	0.94	13/5802 (0.2%)
1	C	0.41	0/4265	0.97	15/5769 (0.3%)
2	B	0.55	1/3158 (0.0%)	1.11	31/4300 (0.7%)
2	D	0.44	0/3036	0.98	16/4130 (0.4%)
All	All	0.47	1/14749 (0.0%)	0.99	75/20001 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	407	ASN	C-O	-6.18	1.15	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	GLN	N-CA-C	-10.88	100.74	114.56
1	C	519	THR	N-CA-C	9.99	124.92	110.24
2	B	320	ASN	N-CA-C	9.87	131.82	110.80
1	A	512	GLN	N-CA-C	8.64	124.17	112.68
2	D	327	VAL	N-CA-C	8.51	118.56	110.30
2	B	56	ALA	N-CA-C	-8.32	102.15	113.30
2	B	319	ASN	CA-C-N	8.25	137.29	121.54
2	B	319	ASN	C-N-CA	8.25	137.29	121.54
2	B	402	GLU	N-CA-C	-8.02	102.75	112.54
2	D	115	VAL	N-CA-C	8.01	114.85	107.56
1	A	439	GLN	N-CA-C	-7.99	100.02	110.33
2	D	37	PRO	N-CA-C	-7.67	96.68	112.47
2	D	45	LEU	N-CA-C	-7.66	101.64	112.13
2	B	404	THR	N-CA-C	-7.63	103.97	113.20
1	C	381	LYS	N-CA-C	-7.43	104.09	113.01
2	D	159	ILE	N-CA-C	-7.28	103.37	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	327	VAL	N-CA-C	7.19	117.29	110.53
2	B	48	THR	N-CA-C	7.05	122.79	114.04
2	B	240	GLU	N-CA-C	-7.02	101.78	110.41
1	C	236	THR	N-CA-C	7.02	121.48	110.32
1	C	276	LEU	N-CA-C	6.70	120.56	112.38
1	A	517	ASN	N-CA-C	6.69	120.42	112.93
2	B	241	GLN	CA-C-N	6.67	128.17	119.84
2	B	241	GLN	C-N-CA	6.67	128.17	119.84
2	B	208	PRO	N-CA-C	6.56	118.70	110.70
2	D	174	ILE	N-CA-C	6.48	117.39	108.84
2	B	88	LEU	N-CA-C	6.37	120.51	112.87
1	C	242	ASP	N-CA-C	-6.36	104.42	111.36
1	C	183	LEU	N-CA-C	-6.31	100.94	110.28
2	B	146	ASP	N-CA-C	6.21	121.08	112.45
1	A	396	ARG	N-CA-C	-6.19	102.55	110.53
2	B	81	ASP	N-CA-C	6.18	118.90	110.55
1	A	236	THR	N-CA-C	6.18	123.96	110.80
2	D	321	TYR	N-CA-C	6.15	118.19	107.49
2	B	430	THR	CA-C-N	6.13	125.69	119.19
2	B	430	THR	C-N-CA	6.13	125.69	119.19
2	B	407	ASN	CA-C-O	6.11	126.88	119.31
1	A	424	VAL	CB-CA-C	-5.95	104.00	112.22
2	D	316	ILE	CA-C-N	5.89	125.91	119.90
2	D	316	ILE	C-N-CA	5.89	125.91	119.90
2	D	320	ASN	N-CA-C	5.84	123.24	110.80
2	B	403	ARG	N-CA-C	-5.82	105.95	113.16
1	A	301	THR	CA-C-N	5.79	125.72	119.76
1	A	301	THR	C-N-CA	5.79	125.72	119.76
2	B	343	CYS	CA-C-N	5.79	125.64	119.28
2	B	343	CYS	C-N-CA	5.79	125.64	119.28
2	D	400	ILE	N-CA-C	5.76	116.41	110.36
1	C	496	PHE	N-CA-C	-5.72	104.74	110.97
1	A	193	ARG	N-CA-C	-5.69	105.00	111.14
1	C	483	CYS	N-CA-C	-5.68	105.84	112.89
2	B	115	VAL	CA-C-N	5.67	126.93	119.84
2	B	115	VAL	C-N-CA	5.67	126.93	119.84
1	C	120	PHE	N-CA-C	5.66	119.29	112.38
2	B	116	PRO	CA-C-N	-5.64	113.70	122.67
2	B	116	PRO	C-N-CA	-5.64	113.70	122.67
2	B	275	GLY	N-CA-C	5.56	122.44	115.21
1	A	242	ASP	N-CA-C	-5.41	105.46	111.36
2	B	329	GLY	N-CA-C	-5.38	102.21	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	41	SER	N-CA-C	-5.38	105.11	110.97
1	A	483	CYS	N-CA-C	-5.29	105.57	112.23
2	D	208	PRO	N-CA-C	5.28	117.14	110.70
2	D	203	THR	N-CA-C	-5.26	105.84	113.21
2	D	253	ASP	CA-C-N	5.21	124.92	119.82
2	D	253	ASP	C-N-CA	5.21	124.92	119.82
1	C	346	TYR	N-CA-C	5.20	116.95	111.28
1	C	275	ALA	N-CA-C	5.20	117.03	111.36
2	B	211	VAL	N-CA-C	5.20	115.97	108.48
2	B	321	TYR	N-CA-C	5.19	116.79	107.80
1	A	69	ASP	N-CA-C	-5.19	105.52	111.07
1	A	491	HIS	N-CA-C	5.16	117.31	111.11
1	C	350	ALA	N-CA-C	-5.09	105.17	111.33
1	C	314	PHE	N-CA-C	5.09	116.91	111.36
2	B	27	SER	N-CA-C	-5.07	103.99	110.53
2	B	147	SER	N-CA-C	5.06	117.97	110.48
1	C	377	GLU	N-CA-C	-5.00	107.12	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4208	0	4157	185	0
1	C	4183	0	4122	299	0
2	B	3089	0	3012	140	0
2	D	2972	0	2914	252	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	53	0	0	7	0
4	B	62	0	0	10	0
4	C	19	0	0	7	0
4	D	16	0	0	2	0
All	All	14604	0	14205	839	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (839) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:ASN:ND2	1:C:519:THR:H	1.49	1.10
2:D:380:ALA:HB3	2:D:426:ALA:HB3	1.34	1.06
1:C:298:THR:HG22	1:C:299:LYS:H	1.20	1.04
2:D:27:SER:HB3	2:D:37:PRO:HG3	1.38	1.01
1:A:489:GLU:H	2:B:19:HIS:HD2	1.10	1.00
1:A:534:LEU:HD22	4:A:535:HOH:O	1.60	0.99
2:D:376:MET:HB3	2:D:427:ASP:OD2	1.65	0.96
2:B:50:LYS:H	2:B:139:HIS:HD2	1.13	0.95
2:B:32:HIS:HD2	2:B:34:ASP:H	1.12	0.95
2:B:207:TYR:C	2:B:209:PRO:HD2	1.92	0.95
1:C:234:PRO:HA	1:C:240:LYS:HZ3	1.30	0.95
2:D:74:GLN:HE22	2:D:119:ASN:HD22	1.00	0.94
2:D:204:LEU:HG	2:D:208:PRO:HG2	1.45	0.94
2:B:32:HIS:CD2	2:B:34:ASP:H	1.85	0.94
2:B:277:THR:HG22	2:B:280:LEU:H	1.33	0.94
1:A:244:ARG:HG2	1:A:272:VAL:HG11	1.50	0.93
1:C:347:ARG:HH12	2:D:274:ARG:HG3	1.31	0.92
2:B:128:GLN:HE21	2:B:128:GLN:H	1.16	0.92
2:B:215:MET:HE1	2:B:235:LEU:HD11	1.49	0.92
2:D:153:TRP:CE2	2:D:431:PRO:HG3	2.05	0.92
2:D:50:LYS:H	2:D:139:HIS:HD2	1.19	0.90
2:D:434:VAL:HG12	2:D:435:LEU:H	1.35	0.90
1:C:518:ASN:ND2	1:C:519:THR:N	2.20	0.90
1:C:518:ASN:HD22	1:C:519:THR:N	1.69	0.90
2:B:204:LEU:O	2:B:208:PRO:HD2	1.72	0.89
2:D:35:PHE:CD1	2:D:314:ALA:HA	2.07	0.89
1:A:215:ILE:HG13	1:A:332:MET:HE1	1.53	0.89
2:D:368:LEU:HB3	2:D:376:MET:HE3	1.55	0.89
1:A:489:GLU:H	2:B:19:HIS:CD2	1.91	0.89
2:B:111:LEU:HD23	2:B:120:VAL:HG21	1.54	0.88
1:A:396:ARG:HH12	1:A:534:LEU:C	1.81	0.88
1:A:269:ILE:O	1:A:272:VAL:HG12	1.73	0.87
2:D:183:GLU:HG2	2:D:289:ILE:HD11	1.57	0.87
1:A:518:ASN:ND2	1:A:534:LEU:H	1.73	0.86
1:A:235:LYS:HB3	1:A:238:LYS:HE3	1.58	0.86
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.75	0.86
1:C:279:THR:HG22	1:C:322:ASN:HD22	1.38	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:TYR:HB2	2:D:208:PRO:HD3	1.58	0.85
1:C:84:ASN:HB3	1:C:87:GLU:HG2	1.59	0.84
1:C:130:GLN:HE22	1:C:155:THR:H	1.24	0.83
1:C:288:ILE:HG23	1:C:305:TRP:HZ3	1.42	0.83
1:C:59:ILE:HG22	1:C:60:ILE:H	1.45	0.82
1:A:201:LEU:HD12	1:A:220:LYS:HG2	1.61	0.82
2:B:50:LYS:H	2:B:139:HIS:CD2	1.98	0.82
2:B:31:THR:CG2	2:B:35:PHE:HB3	2.11	0.81
2:D:224:LEU:H	2:D:227:HIS:CD2	1.97	0.81
2:D:225:PRO:HB3	2:D:276:VAL:HG22	1.60	0.81
1:C:244:ARG:HH22	1:C:273:ASN:HD22	1.25	0.81
2:D:230:GLU:HG3	2:D:234:MET:HE2	1.60	0.81
2:D:35:PHE:CE1	2:D:314:ALA:HA	2.16	0.81
1:A:213:PRO:HB3	1:A:332:MET:HE2	1.62	0.80
2:B:141:ILE:HD12	2:B:158:LEU:HD21	1.63	0.80
2:D:377:LYS:N	2:D:427:ASP:OD2	2.13	0.80
1:C:438:GLN:HG2	1:C:439:GLN:HE22	1.45	0.80
2:D:430:THR:HG21	2:D:432:GLN:HG2	1.64	0.80
1:C:518:ASN:HD22	1:C:519:THR:H	1.27	0.80
1:C:186:ASP:O	1:C:188:PRO:HD3	1.83	0.79
2:D:427:ASP:OD1	2:D:428:VAL:N	2.16	0.79
1:C:232:ARG:C	1:C:234:PRO:HD2	2.07	0.78
2:D:27:SER:CB	2:D:37:PRO:HG3	2.13	0.78
2:B:403:ARG:C	2:B:406:PRO:HD2	2.09	0.78
1:A:396:ARG:HH11	1:A:396:ARG:HG3	1.48	0.78
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.65	0.77
1:A:518:ASN:HD22	1:A:534:LEU:H	1.30	0.77
1:C:298:THR:HG22	1:C:299:LYS:N	1.99	0.77
1:C:438:GLN:HG2	1:C:439:GLN:NE2	1.98	0.77
2:D:224:LEU:H	2:D:227:HIS:HD2	1.32	0.76
2:D:430:THR:CG2	2:D:432:GLN:HG2	2.15	0.76
2:B:403:ARG:O	2:B:406:PRO:HG2	1.84	0.76
2:D:190:ARG:HB2	2:D:320:ASN:O	1.86	0.76
1:A:517:ASN:O	1:A:517:ASN:ND2	2.18	0.76
1:A:238:LYS:HG3	1:A:239:GLU:H	1.50	0.76
1:C:234:PRO:HA	1:C:240:LYS:NZ	2.01	0.75
2:D:241:GLN:N	2:D:242:PRO:HD3	2.01	0.75
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.21	0.75
1:A:396:ARG:NH1	1:A:534:LEU:C	2.45	0.75
2:D:74:GLN:NE2	2:D:119:ASN:HD22	1.83	0.75
1:C:285:ILE:HD11	1:C:388:ALA:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:HB3	2:B:111:LEU:HD22	1.67	0.74
1:A:143:LEU:HD12	1:A:150:LEU:HD22	1.69	0.74
1:A:46:LEU:HD23	1:A:93:LEU:HD13	1.69	0.74
1:A:215:ILE:H	1:A:332:MET:HE1	1.53	0.74
1:C:225:TRP:NE1	1:C:233:ILE:HG12	2.02	0.74
1:C:518:ASN:OD1	1:C:534:LEU:N	2.21	0.74
2:B:32:HIS:HD2	2:B:34:ASP:N	1.86	0.74
1:C:113:LEU:O	1:C:117:PRO:HG3	1.87	0.74
2:D:236:GLN:HE22	2:D:263:LYS:HG2	1.53	0.74
2:D:186:LYS:NZ	2:D:325:ASN:HD21	1.86	0.74
1:A:357:VAL:O	1:A:361:VAL:HG23	1.88	0.73
1:C:59:ILE:HG22	1:C:60:ILE:N	2.03	0.73
1:C:233:ILE:N	1:C:234:PRO:HD2	2.04	0.73
1:C:36:ILE:HG23	1:C:37:ASN:ND2	2.04	0.73
1:A:534:LEU:HD13	4:A:535:HOH:O	1.88	0.72
2:D:202:CYS:HB3	2:D:343:CYS:SG	2.28	0.72
2:B:128:GLN:H	2:B:128:GLN:NE2	1.86	0.72
2:B:427:ASP:OD1	2:B:428:VAL:N	2.23	0.71
2:D:365:LEU:HG	2:D:379:PRO:HG2	1.72	0.71
1:A:215:ILE:H	1:A:332:MET:CE	2.04	0.71
2:D:44:PHE:O	2:D:48:THR:HB	1.90	0.71
1:C:347:ARG:NH1	2:D:274:ARG:HG3	2.04	0.71
1:A:409:LYS:O	1:A:413:ILE:HG12	1.91	0.71
1:A:173:GLU:O	1:A:512:GLN:O	2.09	0.71
1:A:236:THR:HA	1:A:240:LYS:HD2	1.73	0.70
2:D:43:GLN:NE2	2:D:46:LEU:HD12	2.06	0.70
2:D:131:ASN:HD22	2:D:133:THR:H	1.39	0.70
2:B:167:GLY:HA2	2:B:348:GLN:HE22	1.55	0.70
2:B:376:MET:HB3	2:B:427:ASP:OD2	1.91	0.70
2:D:344:PRO:HG3	2:D:373:SER:O	1.91	0.70
2:D:377:LYS:O	2:D:379:PRO:HD3	1.90	0.70
1:A:503:GLN:HA	1:A:503:GLN:HE21	1.55	0.70
1:A:518:ASN:HB3	1:A:532:PHE:O	1.91	0.70
1:A:517:ASN:O	1:A:518:ASN:HB2	1.91	0.69
2:D:204:LEU:O	2:D:208:PRO:HD2	1.91	0.69
2:D:186:LYS:HZ2	2:D:325:ASN:HD21	1.39	0.69
2:D:223:ARG:H	2:D:227:HIS:HD2	1.38	0.69
2:D:376:MET:HE1	2:D:425:VAL:HG11	1.73	0.69
1:A:84:ASN:ND2	1:A:87:GLU:H	1.90	0.69
2:B:237:TRP:O	2:B:240:GLU:O	2.09	0.69
2:D:73:ARG:HG2	2:D:117:ASN:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLU:HG2	1:C:10:GLU:O	1.92	0.69
1:C:282:PRO:HD2	1:C:285:ILE:HD12	1.73	0.69
1:C:36:ILE:CG2	1:C:128:ALA:HA	2.23	0.69
1:C:138:ARG:O	1:C:142:VAL:HG23	1.91	0.69
2:D:221:MET:N	2:D:222:PRO:HD3	2.06	0.69
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.75	0.69
2:B:405:ARG:N	2:B:406:PRO:HD2	2.08	0.69
2:D:351:GLN:NE2	2:D:436:PHE:HE2	1.91	0.68
1:A:421:ASN:O	1:A:424:VAL:HG22	1.93	0.68
1:A:518:ASN:ND2	1:A:534:LEU:N	2.42	0.68
2:B:148:ILE:N	2:B:148:ILE:HD12	2.08	0.68
1:C:61:ASP:OD2	1:C:85:ARG:HD2	1.93	0.68
2:B:223:ARG:H	2:B:227:HIS:HD2	1.40	0.68
1:A:503:GLN:HA	1:A:503:GLN:NE2	2.08	0.68
2:D:35:PHE:HD1	2:D:314:ALA:HA	1.58	0.68
1:A:241:GLU:HA	1:A:244:ARG:HH11	1.56	0.68
1:C:218:ILE:O	1:C:222:LEU:HB2	1.93	0.68
2:B:50:LYS:N	2:B:139:HIS:HD2	1.91	0.68
2:B:31:THR:HG23	2:B:35:PHE:HB3	1.73	0.67
2:D:152:ARG:CZ	2:D:429:THR:HG21	2.24	0.67
2:D:41:SER:HA	2:D:44:PHE:CE2	2.29	0.67
2:D:74:GLN:HE22	2:D:119:ASN:ND2	1.84	0.67
1:C:311:LEU:HD21	1:C:387:SER:HB2	1.75	0.67
1:A:235:LYS:CB	1:A:238:LYS:HE3	2.24	0.67
1:A:396:ARG:NH1	1:A:534:LEU:O	2.28	0.67
1:C:134:SER:HB3	1:C:437:LYS:HE2	1.77	0.67
2:D:43:GLN:C	2:D:45:LEU:H	2.03	0.67
2:B:425:VAL:HG12	2:B:426:ALA:N	2.10	0.67
1:C:38:ALA:HB1	1:C:89:ALA:HB3	1.76	0.67
1:C:336:SER:O	1:C:340:ILE:HG12	1.95	0.66
2:D:434:VAL:HG12	2:D:435:LEU:N	2.10	0.66
1:A:109:PRO:O	1:A:113:LEU:HD23	1.96	0.66
1:C:226:TYR:CE1	1:C:231:GLY:O	2.49	0.66
1:C:438:GLN:HE21	1:C:439:GLN:HE22	1.41	0.66
2:B:40:GLU:HB2	4:B:483:HOH:O	1.94	0.66
1:A:458:LYS:O	1:A:458:LYS:HD3	1.95	0.66
2:D:376:MET:CB	2:D:427:ASP:OD2	2.44	0.66
4:B:485:HOH:O	2:D:126:LYS:HD2	1.95	0.65
1:A:236:THR:HG22	1:A:237:TYR:CD1	2.31	0.65
1:A:84:ASN:HD22	1:A:87:GLU:H	1.45	0.64
1:C:236:THR:HB	1:C:239:GLU:CD	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD2	1:A:360:HIS:HE1	1.61	0.64
1:C:368:ILE:HG22	1:C:370:GLN:HB2	1.78	0.64
2:D:425:VAL:HG12	2:D:426:ALA:N	2.12	0.64
1:C:516:PHE:CD1	1:C:518:ASN:O	2.51	0.64
2:D:153:TRP:CZ2	2:D:431:PRO:HG3	2.32	0.64
1:A:119:PHE:O	1:A:122:ARG:HG2	1.98	0.64
1:C:244:ARG:NH2	1:C:273:ASN:HD22	1.95	0.64
1:C:442:TYR:HB2	1:C:445:VAL:CG2	2.28	0.63
2:D:202:CYS:HB2	2:D:340:LYS:HB3	1.81	0.63
1:C:255:GLU:O	1:C:256:ASN:C	2.40	0.63
1:C:280:GLN:O	1:C:282:PRO:HD3	1.99	0.63
2:D:320:ASN:HB2	4:D:451:HOH:O	1.97	0.63
1:C:143:LEU:HD22	1:C:148:ILE:HG21	1.80	0.63
2:D:210:GLN:HG2	2:D:211:VAL:N	2.14	0.63
1:A:458:LYS:HD3	1:A:458:LYS:C	2.23	0.63
2:B:213:PHE:HB3	2:B:218:ILE:HD13	1.81	0.63
2:B:31:THR:HG23	2:B:35:PHE:CB	2.29	0.63
1:C:349:LYS:HB2	4:C:541:HOH:O	1.99	0.63
2:B:405:ARG:H	2:B:406:PRO:HD2	1.62	0.63
2:B:197:THR:HG22	2:B:198:ALA:N	2.13	0.62
2:D:240:GLU:HB2	2:D:242:PRO:HD3	1.79	0.62
2:D:374:LEU:HD21	2:D:436:PHE:CZ	2.34	0.62
1:A:416:MET:HE1	1:A:424:VAL:HG13	1.81	0.62
1:C:516:PHE:CE1	1:C:518:ASN:O	2.53	0.62
2:D:131:ASN:HD22	2:D:131:ASN:C	2.07	0.62
1:A:12:LYS:HE2	4:B:491:HOH:O	1.98	0.62
1:A:435:PHE:CD2	1:A:443:PRO:HD3	2.35	0.62
1:C:37:ASN:HB2	1:C:129:THR:OG1	1.99	0.62
1:A:254:ASN:HB2	1:A:255:GLU:OE2	2.00	0.62
2:B:148:ILE:HD12	2:B:148:ILE:H	1.63	0.62
1:C:262:GLU:HB3	1:C:264:ASN:OD1	2.00	0.62
2:D:236:GLN:NE2	2:D:263:LYS:HE2	2.14	0.62
1:A:33:VAL:HG12	1:A:54:ILE:HD13	1.80	0.62
1:C:364:LEU:O	1:C:368:ILE:HD13	2.00	0.62
1:C:416:MET:HG3	1:C:472:VAL:HG11	1.82	0.62
1:A:111:ASN:ND2	1:A:115:ASN:HD21	1.96	0.61
1:C:201:LEU:HD22	1:C:209:HIS:ND1	2.15	0.61
1:C:449:GLN:HG2	4:C:548:HOH:O	2.00	0.61
1:C:371:ALA:HB1	1:C:372:PRO:HD2	1.81	0.61
2:D:24:LEU:O	2:D:37:PRO:HA	2.00	0.61
1:C:36:ILE:HG23	1:C:37:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:HG3	1:C:88:ALA:N	2.15	0.61
2:B:62:GLU:HG2	2:B:297:ALA:HA	1.82	0.61
1:C:298:THR:CG2	1:C:299:LYS:H	2.03	0.61
1:A:362:ALA:O	1:A:366:GLN:HG3	2.00	0.61
1:A:421:ASN:HD22	1:A:423:ILE:HB	1.64	0.61
1:A:534:LEU:CD2	4:A:535:HOH:O	2.32	0.61
1:A:72:ASN:C	1:A:72:ASN:ND2	2.59	0.61
1:A:115:ASN:O	1:A:117:PRO:HD3	2.01	0.61
1:A:272:VAL:HG23	1:A:276:LEU:HD11	1.81	0.61
1:A:371:ALA:HB1	1:A:372:PRO:HD2	1.81	0.61
2:B:162:LEU:HD22	2:B:169:LEU:HD11	1.83	0.61
1:C:233:ILE:HD13	1:C:243:PHE:CG	2.36	0.61
1:C:442:TYR:HB2	1:C:445:VAL:HG21	1.82	0.61
1:A:215:ILE:CG1	1:A:332:MET:HE1	2.30	0.61
1:A:317:LYS:HB2	1:A:318:GLU:OE2	2.01	0.60
2:D:243:PHE:HD1	2:D:256:HIS:HD1	1.47	0.60
1:A:449:GLN:HB3	1:A:453:ASP:OD2	2.00	0.60
2:D:203:THR:HG22	2:D:203:THR:O	2.00	0.60
1:A:111:ASN:HD21	1:A:115:ASN:HD21	1.49	0.60
1:A:331:ASP:HB2	2:B:224:LEU:HD11	1.84	0.60
2:B:128:GLN:HE21	2:B:128:GLN:N	1.95	0.60
2:B:365:LEU:O	2:B:365:LEU:HD23	2.01	0.60
1:C:184:ARG:NE	1:C:325:VAL:HG12	2.17	0.60
1:C:225:TRP:CD1	1:C:233:ILE:HG12	2.37	0.60
1:A:235:LYS:HD2	1:A:239:GLU:OE2	2.02	0.60
2:D:365:LEU:O	2:D:365:LEU:HD23	2.01	0.60
1:C:38:ALA:HB1	1:C:89:ALA:CB	2.31	0.60
2:D:236:GLN:HE22	2:D:263:LYS:CG	2.14	0.60
2:D:380:ALA:CB	2:D:426:ALA:HB3	2.21	0.60
2:B:39:THR:HG23	4:B:483:HOH:O	2.00	0.60
2:B:224:LEU:H	2:B:227:HIS:CD2	2.20	0.60
2:D:243:PHE:HD1	2:D:256:HIS:ND1	2.00	0.60
2:B:204:LEU:C	2:B:206:LEU:H	2.10	0.60
1:C:189:PHE:CE1	1:C:192:LEU:HB2	2.37	0.60
2:B:229:ILE:HD13	2:B:281:THR:HA	1.84	0.59
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.82	0.59
1:A:240:LYS:O	1:A:244:ARG:HG3	2.02	0.59
1:A:162:MET:HE3	1:A:516:PHE:CZ	2.37	0.59
2:D:197:THR:HG22	2:D:198:ALA:N	2.17	0.59
1:C:254:ASN:O	1:C:255:GLU:C	2.45	0.59
1:A:423:ILE:HD13	1:A:423:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:HG22	1:C:128:ALA:HA	1.83	0.59
2:B:38:SER:HB3	2:B:41:SER:OG	2.02	0.59
1:A:430:ARG:NH2	4:A:577:HOH:O	2.34	0.59
1:C:12:LYS:HA	2:D:85:VAL:HG12	1.84	0.59
1:C:78:ARG:HG3	1:C:78:ARG:HH11	1.68	0.59
1:C:281:ILE:HD11	1:C:315:VAL:HG11	1.83	0.59
1:C:224:GLN:OE1	1:C:246:LEU:HD11	2.03	0.58
2:D:152:ARG:NE	2:D:429:THR:HG21	2.17	0.58
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.02	0.58
2:B:195:GLY:O	2:B:339:ARG:NH1	2.36	0.58
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.86	0.58
2:D:353:ILE:HG21	2:D:367:TYR:CE2	2.38	0.58
1:C:110:GLU:CD	1:C:110:GLU:H	2.11	0.58
2:D:430:THR:HG22	2:D:432:GLN:H	1.69	0.58
1:A:46:LEU:HD23	1:A:93:LEU:CD1	2.32	0.58
1:C:59:ILE:O	1:C:60:ILE:HG13	2.04	0.58
1:C:240:LYS:O	1:C:244:ARG:HG3	2.04	0.58
2:D:249:LEU:HD11	2:D:253:ASP:HB3	1.84	0.58
1:A:163:ARG:NH1	1:A:401:GLU:OE2	2.36	0.58
1:A:235:LYS:HB3	1:A:238:LYS:CE	2.32	0.58
2:D:224:LEU:HD12	2:D:227:HIS:CE1	2.38	0.58
1:A:373:GLU:C	1:A:375:ILE:H	2.10	0.57
1:C:128:ALA:HB1	1:C:131:LEU:HD11	1.86	0.57
2:B:318:LEU:C	2:B:320:ASN:H	2.12	0.57
1:C:39:THR:HG23	1:C:42:GLY:H	1.69	0.57
1:A:193:ARG:O	1:A:197:GLN:HG3	2.04	0.57
1:A:376:SER:OG	1:A:378:LYS:HG2	2.03	0.57
2:B:251:GLY:O	2:B:286:LYS:HE2	2.04	0.57
2:D:178:ILE:HD12	2:D:307:VAL:HG22	1.87	0.57
1:A:341:LYS:NZ	4:A:582:HOH:O	2.37	0.57
2:B:208:PRO:N	2:B:209:PRO:HD2	2.19	0.57
1:C:319:GLY:O	1:C:320:GLN:HB2	2.03	0.57
1:C:404:LEU:HD21	1:C:467:GLU:HG2	1.84	0.57
1:C:434:ARG:HG2	1:C:434:ARG:HH11	1.69	0.57
1:C:59:ILE:CG2	1:C:60:ILE:H	2.16	0.57
1:C:505:VAL:O	1:C:509:ILE:HG12	2.03	0.57
2:B:80:MET:HA	2:B:80:MET:HE3	1.86	0.57
1:C:445:VAL:HG22	1:C:486:GLY:O	2.04	0.57
2:D:27:SER:HB3	2:D:37:PRO:CG	2.24	0.57
2:D:131:ASN:HD21	2:D:133:THR:HB	1.69	0.57
1:C:378:LYS:NZ	1:C:378:LYS:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.86	0.56
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.86	0.56
1:A:172:ILE:HA	1:A:390:LEU:HD22	1.86	0.56
1:A:317:LYS:HD2	1:A:360:HIS:CE1	2.41	0.56
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.86	0.56
2:D:42:LEU:O	2:D:46:LEU:HG	2.05	0.56
1:C:279:THR:CG2	1:C:322:ASN:HD22	2.13	0.56
2:D:50:LYS:H	2:D:139:HIS:CD2	2.11	0.56
2:D:236:GLN:HE22	2:D:263:LYS:HE2	1.71	0.56
1:A:297:ILE:HG21	1:A:368:ILE:HD11	1.86	0.56
2:D:232:VAL:HA	2:D:236:GLN:HB3	1.88	0.56
2:B:16:ARG:HH12	2:B:117:ASN:HD22	1.54	0.55
2:B:365:LEU:HD23	2:B:365:LEU:C	2.31	0.55
1:C:374:SER:C	1:C:375:ILE:HD12	2.31	0.55
2:D:186:LYS:HZ2	2:D:325:ASN:ND2	2.04	0.55
1:C:33:VAL:CG2	1:C:34:CYS:N	2.70	0.55
2:D:429:THR:HG22	2:D:429:THR:O	2.05	0.55
2:B:425:VAL:HG12	2:B:426:ALA:H	1.70	0.55
1:C:518:ASN:HB3	1:C:532:PHE:O	2.06	0.55
2:B:169:LEU:O	2:B:171:PRO:HD3	2.05	0.55
2:B:208:PRO:O	2:B:210:GLN:N	2.39	0.55
1:A:396:ARG:HG3	1:A:396:ARG:NH1	2.18	0.55
2:D:434:VAL:O	2:D:435:LEU:HG	2.06	0.55
1:A:418:ASN:ND2	1:A:420:ASP:H	2.05	0.55
1:A:214:TRP:HB2	1:A:268:ALA:HA	1.89	0.55
1:C:277:ASN:C	1:C:277:ASN:HD22	2.14	0.55
1:A:480:HIS:HE1	4:B:471:HOH:O	1.90	0.55
1:A:224:GLN:O	1:A:228:GLU:HG3	2.08	0.54
1:C:262:GLU:O	1:C:266:GLU:HG2	2.07	0.54
1:C:314:PHE:HZ	1:C:353:ASP:OD2	1.90	0.54
2:D:324:PHE:HD1	2:D:332:THR:HG22	1.73	0.54
2:B:403:ARG:O	2:B:406:PRO:CG	2.54	0.54
1:A:221:TYR:OH	1:A:250:GLY:HA3	2.07	0.54
1:C:225:TRP:CE2	1:C:233:ILE:HG12	2.42	0.54
1:A:235:LYS:HB2	1:A:239:GLU:HG3	1.90	0.54
1:C:396:ARG:HB2	4:C:539:HOH:O	2.06	0.54
1:C:518:ASN:CG	1:C:519:THR:H	2.09	0.54
2:B:32:HIS:HB3	2:B:313:SER:O	2.07	0.54
1:A:241:GLU:HA	1:A:244:ARG:NH1	2.22	0.54
1:C:223:ALA:O	1:C:226:TYR:HB2	2.08	0.54
1:C:525:MET:HG3	2:D:315:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:ILE:N	2:D:218:ILE:HD12	2.22	0.54
1:C:126:VAL:O	1:C:150:LEU:HD12	2.08	0.54
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.89	0.54
1:C:38:ALA:HB3	1:C:85:ARG:HG2	1.90	0.54
2:D:286:LYS:HB2	2:D:288:ILE:HG13	1.89	0.54
2:D:425:VAL:HG12	2:D:426:ALA:H	1.71	0.54
1:A:35:LEU:HD22	1:A:46:LEU:HD22	1.90	0.53
2:D:390:ARG:O	2:D:391:THR:CB	2.55	0.53
1:C:438:GLN:HE21	1:C:439:GLN:NE2	2.06	0.53
1:A:162:MET:HE2	1:A:520:TYR:HB3	1.89	0.53
2:D:322:LEU:HD23	2:D:322:LEU:C	2.34	0.53
1:C:297:ILE:CD1	1:C:368:ILE:HD11	2.39	0.53
2:D:287:ARG:HH11	2:D:287:ARG:HG2	1.72	0.53
2:D:351:GLN:NE2	2:D:436:PHE:CE2	2.76	0.53
2:D:373:SER:C	2:D:374:LEU:HD12	2.34	0.53
1:A:353:ASP:O	1:A:357:VAL:HG23	2.09	0.53
1:C:174:SER:HB3	1:C:176:PRO:HD3	1.90	0.53
2:D:430:THR:HG22	2:D:432:GLN:N	2.23	0.53
1:A:108:SER:HB2	1:A:109:PRO:HD2	1.90	0.53
1:C:105:VAL:HG12	1:C:107:GLU:H	1.73	0.53
1:C:244:ARG:NH2	1:C:273:ASN:ND2	2.55	0.53
1:A:72:ASN:C	1:A:72:ASN:HD22	2.16	0.53
1:C:108:SER:HB3	1:C:111:ASN:HD22	1.74	0.53
1:C:235:LYS:HG2	4:C:543:HOH:O	2.08	0.53
2:D:170:ASP:O	2:D:173:SER:HB3	2.09	0.53
2:D:216:CYS:HB2	2:D:221:MET:HE2	1.91	0.53
2:B:64:LEU:HB3	2:B:111:LEU:CD2	2.38	0.53
2:B:352:ASN:HA	2:B:437:LYS:O	2.09	0.53
1:C:470:LEU:C	1:C:472:VAL:H	2.17	0.53
2:B:361:LEU:HD23	2:B:361:LEU:C	2.34	0.53
1:C:233:ILE:HB	1:C:276:LEU:HD13	1.91	0.53
1:C:485:TYR:C	1:C:487:ALA:H	2.17	0.53
1:C:186:ASP:CG	1:C:187:LYS:H	2.16	0.52
2:B:361:LEU:O	2:B:364:VAL:HG22	2.09	0.52
1:C:217:ILE:HD11	1:C:264:ASN:ND2	2.24	0.52
1:A:366:GLN:C	1:A:368:ILE:H	2.16	0.52
1:C:84:ASN:ND2	1:C:86:ALA:HB3	2.24	0.52
2:D:58:GLY:HA2	2:D:91:GLN:HG3	1.90	0.52
1:A:117:PRO:C	1:A:119:PHE:H	2.16	0.52
1:A:253:LYS:HB2	1:A:257:GLY:O	2.10	0.52
1:C:484:ARG:HG2	1:C:484:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:GLY:O	2:B:247:VAL:HG23	2.09	0.52
2:D:204:LEU:CG	2:D:208:PRO:HG2	2.31	0.52
1:A:229:THR:O	1:A:230:ASN:CB	2.57	0.52
1:C:10:GLU:OE2	2:D:279:ARG:NH2	2.43	0.52
1:C:255:GLU:O	1:C:256:ASN:O	2.27	0.52
2:B:353:ILE:HG13	2:B:353:ILE:O	2.09	0.52
2:B:46:LEU:HD23	2:B:71:GLY:O	2.09	0.52
1:C:10:GLU:OE2	2:D:279:ARG:NH1	2.42	0.52
1:A:363:LYS:HA	1:A:366:GLN:OE1	2.09	0.51
1:C:236:THR:HB	1:C:239:GLU:OE1	2.10	0.51
2:D:429:THR:O	2:D:429:THR:CG2	2.58	0.51
1:A:462:THR:O	1:A:466:GLN:HG3	2.11	0.51
1:C:144:TRP:CZ3	1:C:397:SER:HA	2.45	0.51
2:D:131:ASN:ND2	2:D:133:THR:H	2.07	0.51
2:D:214:PRO:O	2:D:218:ILE:HD13	2.11	0.51
1:C:37:ASN:C	1:C:39:THR:H	2.18	0.51
1:A:235:LYS:HD3	1:A:238:LYS:HE3	1.92	0.51
1:C:33:VAL:HG22	1:C:34:CYS:N	2.25	0.51
2:B:197:THR:HG22	2:B:198:ALA:H	1.75	0.51
1:C:158:LEU:HG	2:D:23:PHE:HE2	1.75	0.51
1:C:454:ILE:HG23	1:C:455:GLY:N	2.25	0.51
1:C:489:GLU:H	2:D:19:HIS:CE1	2.28	0.51
2:D:20:VAL:C	2:D:22:LYS:H	2.18	0.51
1:A:60:ILE:HD11	1:A:119:PHE:HE2	1.76	0.51
1:A:344:ASN:O	1:A:348:GLU:HG2	2.10	0.51
2:B:401:GLU:O	2:B:404:THR:CB	2.59	0.51
1:C:310:ALA:CB	1:C:361:VAL:HG22	2.41	0.51
1:C:434:ARG:HG2	1:C:434:ARG:NH1	2.26	0.51
2:D:157:MET:O	2:D:160:SER:HB3	2.10	0.51
2:D:48:THR:HG22	2:D:48:THR:O	2.11	0.51
1:C:244:ARG:NH2	1:C:273:ASN:HB2	2.25	0.51
1:C:317:LYS:C	1:C:319:GLY:H	2.19	0.51
2:B:178:ILE:HD11	2:B:310:ILE:HD12	1.93	0.50
2:B:325:ASN:HD22	2:B:326:ASP:N	2.09	0.50
1:C:378:LYS:HB3	1:C:378:LYS:HZ3	1.75	0.50
1:A:19:LEU:HG	2:B:290:PRO:HB3	1.92	0.50
1:C:54:ILE:O	1:C:100:VAL:HG22	2.12	0.50
1:C:164:ILE:HD13	1:C:515:ILE:HD12	1.93	0.50
2:D:226:GLU:OE2	2:D:280:LEU:HD21	2.10	0.50
2:D:281:THR:O	2:D:285:VAL:HG23	2.10	0.50
1:A:371:ALA:HB3	1:A:374:SER:HB3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LYS:HB2	1:C:318:GLU:OE1	2.11	0.50
1:C:419:PRO:O	1:C:424:VAL:HG21	2.12	0.50
2:D:207:TYR:HB2	2:D:208:PRO:CD	2.36	0.50
1:A:376:SER:OG	1:A:379:GLU:HG3	2.11	0.50
1:C:10:GLU:OE2	2:D:279:ARG:CZ	2.60	0.50
2:D:373:SER:O	2:D:374:LEU:HD12	2.12	0.50
1:A:489:GLU:N	2:B:19:HIS:HD2	1.93	0.50
2:B:110:PHE:C	2:B:110:PHE:CD2	2.89	0.50
2:B:148:ILE:H	2:B:148:ILE:CD1	2.23	0.50
1:C:46:LEU:HD21	1:C:57:PHE:CD1	2.47	0.50
1:A:352:LYS:HG2	4:A:568:HOH:O	2.11	0.50
2:B:351:GLN:HB3	2:B:436:PHE:CD2	2.46	0.50
2:D:38:SER:C	2:D:40:GLU:N	2.68	0.50
2:D:46:LEU:HD23	2:D:71:GLY:O	2.12	0.50
1:C:18:ARG:HB3	2:D:290:PRO:HG3	1.93	0.50
1:C:191:GLU:H	1:C:191:GLU:CD	2.19	0.50
2:D:241:GLN:N	2:D:242:PRO:CD	2.72	0.50
1:A:212:THR:HG22	1:A:216:VAL:HB	1.93	0.50
1:C:51:LEU:HD11	2:D:92:PHE:HB3	1.93	0.50
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.42	0.50
2:D:58:GLY:HA2	2:D:91:GLN:CG	2.42	0.50
2:D:266:GLU:O	2:D:269:SER:HB3	2.11	0.50
1:A:36:ILE:O	1:A:60:ILE:O	2.29	0.50
1:C:370:GLN:O	1:C:371:ALA:HB2	2.11	0.50
1:C:400:GLU:O	1:C:406:THR:HB	2.11	0.50
2:D:197:THR:CG2	2:D:198:ALA:N	2.75	0.50
1:A:105:VAL:C	1:A:107:GLU:H	2.20	0.49
2:D:287:ARG:HG2	2:D:287:ARG:NH1	2.27	0.49
1:C:201:LEU:C	1:C:203:HIS:H	2.20	0.49
2:D:240:GLU:CB	2:D:242:PRO:HD3	2.42	0.49
2:D:434:VAL:CG1	2:D:435:LEU:H	2.18	0.49
1:A:202:ASP:OD1	1:A:203:HIS:N	2.45	0.49
1:C:234:PRO:HD3	1:C:276:LEU:HB3	1.93	0.49
1:C:244:ARG:HH21	1:C:273:ASN:HB2	1.78	0.49
1:A:84:ASN:HD21	1:A:86:ALA:HB3	1.77	0.49
1:C:87:GLU:HG3	1:C:88:ALA:H	1.77	0.49
1:C:150:LEU:HD23	1:C:165:ILE:HD12	1.94	0.49
1:A:534:LEU:CD1	4:A:535:HOH:O	2.51	0.49
1:C:424:VAL:HG13	1:C:474:VAL:HG13	1.95	0.49
1:C:221:TYR:HD2	1:C:246:LEU:HG	1.76	0.49
1:C:481:GLU:OE1	1:C:484:ARG:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:N	1:A:188:PRO:HD3	2.27	0.49
1:A:426:TYR:HB2	1:A:521:ILE:HD11	1.95	0.49
1:C:92:PHE:HD2	2:D:114:ARG:NH2	2.11	0.49
1:A:229:THR:O	1:A:230:ASN:HB2	2.11	0.49
2:D:128:GLN:H	2:D:128:GLN:CD	2.19	0.49
1:C:315:VAL:HG13	1:C:322:ASN:N	2.27	0.49
1:A:428:MET:HE2	1:A:479:VAL:HA	1.93	0.49
2:B:318:LEU:C	2:B:320:ASN:N	2.71	0.49
1:C:189:PHE:HB3	1:C:349:LYS:NZ	2.28	0.49
2:D:43:GLN:C	2:D:45:LEU:N	2.71	0.49
2:D:236:GLN:HE21	2:D:259:TRP:HH2	1.60	0.49
2:B:132:ASP:HB3	2:B:136:ARG:NH1	2.28	0.48
1:C:59:ILE:CG2	1:C:60:ILE:N	2.73	0.48
1:C:65:VAL:HG12	1:C:66:SER:N	2.28	0.48
2:D:236:GLN:NE2	2:D:263:LYS:HG2	2.24	0.48
1:A:264:ASN:HD22	1:A:264:ASN:H	1.59	0.48
2:B:148:ILE:N	2:B:148:ILE:CD1	2.76	0.48
1:C:143:LEU:HD12	1:C:150:LEU:HD22	1.95	0.48
1:C:444:GLY:O	1:C:446:SER:N	2.45	0.48
1:A:264:ASN:HD22	1:A:264:ASN:N	2.11	0.48
1:C:150:LEU:HD21	1:C:152:ILE:HD11	1.95	0.48
2:D:126:LYS:HG3	2:D:128:GLN:HG2	1.94	0.48
1:A:318:GLU:H	1:A:318:GLU:CD	2.19	0.48
2:B:82:THR:HG23	2:B:100:GLY:C	2.38	0.48
1:C:18:ARG:HH21	2:D:288:ILE:HD12	1.78	0.48
1:C:428:MET:HE2	1:C:479:VAL:HA	1.96	0.48
2:D:38:SER:C	2:D:40:GLU:H	2.19	0.48
1:A:32:HIS:HE1	1:A:58:THR:OG1	1.97	0.48
1:A:396:ARG:NH1	1:A:534:LEU:OXT	2.40	0.48
1:A:447:ASN:ND2	2:B:26:ARG:HH21	2.12	0.48
1:A:504:GLU:HG3	1:A:516:PHE:CE2	2.48	0.48
2:B:394:LEU:O	2:B:396:SER:N	2.46	0.48
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.44	0.48
1:C:174:SER:O	1:C:175:HIS:HB2	2.13	0.48
1:C:254:ASN:O	1:C:255:GLU:O	2.31	0.48
2:B:242:PRO:HG3	2:B:259:TRP:CZ2	2.49	0.48
2:D:44:PHE:C	2:D:48:THR:HB	2.38	0.48
1:C:175:HIS:N	1:C:176:PRO:CD	2.77	0.48
1:C:371:ALA:HB3	1:C:374:SER:OG	2.13	0.48
2:D:36:GLU:O	2:D:38:SER:N	2.47	0.48
2:B:208:PRO:N	2:B:209:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ILE:HG23	1:C:455:GLY:H	1.79	0.48
1:A:517:ASN:C	1:A:517:ASN:HD22	2.18	0.48
2:B:136:ARG:HG2	2:B:161:LEU:HD22	1.96	0.48
1:C:236:THR:HB	1:C:239:GLU:CG	2.44	0.48
1:C:368:ILE:HD12	1:C:368:ILE:N	2.29	0.48
1:C:484:ARG:O	1:C:486:GLY:N	2.47	0.48
1:A:54:ILE:O	1:A:100:VAL:HG22	2.14	0.47
1:A:117:PRO:C	1:A:119:PHE:N	2.72	0.47
1:A:318:GLU:OE2	1:A:318:GLU:N	2.38	0.47
1:C:236:THR:HB	1:C:239:GLU:HG3	1.96	0.47
1:C:277:ASN:HD22	1:C:278:THR:N	2.12	0.47
1:C:297:ILE:HD11	1:C:368:ILE:HD11	1.94	0.47
2:D:225:PRO:HG3	2:D:273:ILE:HG22	1.96	0.47
1:A:199:TYR:OH	1:A:338:LYS:HD3	2.15	0.47
1:A:213:PRO:CB	1:A:332:MET:HE2	2.37	0.47
1:A:164:ILE:HD11	1:A:508:ILE:HD11	1.96	0.47
1:A:172:ILE:HA	1:A:390:LEU:CD2	2.43	0.47
1:A:334:ALA:O	2:B:221:MET:HE2	2.14	0.47
1:A:339:TYR:CD2	2:B:223:ARG:HB3	2.49	0.47
2:B:309:LYS:NZ	4:B:489:HOH:O	2.47	0.47
1:C:416:MET:C	1:C:418:ASN:N	2.70	0.47
2:D:221:MET:N	2:D:222:PRO:CD	2.77	0.47
1:A:331:ASP:OD1	2:B:223:ARG:HD2	2.15	0.47
2:B:235:LEU:C	2:B:238:PRO:HD2	2.40	0.47
2:B:393:TYR:O	2:B:395:GLN:N	2.43	0.47
2:B:425:VAL:CG1	2:B:426:ALA:N	2.76	0.47
1:C:78:ARG:HD3	1:C:81:ILE:HD12	1.96	0.47
2:D:85:VAL:C	2:D:87:ASN:H	2.23	0.47
2:D:204:LEU:C	2:D:206:LEU:H	2.22	0.47
2:D:233:ARG:HD2	2:D:285:VAL:HA	1.96	0.47
2:D:368:LEU:HD22	2:D:374:LEU:HD23	1.96	0.47
1:C:525:MET:HG3	2:D:315:TYR:CD2	2.50	0.47
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.44	0.47
2:D:208:PRO:O	2:D:210:GLN:N	2.48	0.47
2:D:343:CYS:C	2:D:345:ALA:H	2.22	0.47
1:C:47:LYS:HE3	2:D:65:LYS:NZ	2.30	0.47
1:C:80:SER:O	1:C:81:ILE:C	2.58	0.47
1:C:163:ARG:NH1	1:C:401:GLU:OE2	2.48	0.47
2:D:27:SER:CB	2:D:37:PRO:CG	2.89	0.47
2:D:193:LEU:H	2:D:197:THR:HB	1.78	0.47
2:D:207:TYR:C	2:D:209:PRO:HD2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:ASN:HD22	2:D:336:GLU:HB2	1.79	0.47
1:A:229:THR:O	1:A:230:ASN:ND2	2.47	0.47
1:A:488:ALA:C	1:A:490:PRO:HD3	2.39	0.47
2:B:213:PHE:HB3	2:B:218:ILE:CD1	2.45	0.47
1:C:49:LEU:O	1:C:52:PRO:HG2	2.15	0.47
1:C:164:ILE:CD1	1:C:515:ILE:HD12	2.44	0.47
1:C:428:MET:CE	1:C:479:VAL:HA	2.45	0.47
1:C:503:GLN:HA	1:C:503:GLN:OE1	2.13	0.47
2:D:148:ILE:HD13	2:D:208:PRO:HA	1.97	0.47
1:C:130:GLN:HE22	1:C:155:THR:N	2.04	0.47
1:C:488:ALA:C	1:C:490:PRO:HD3	2.40	0.47
2:D:131:ASN:ND2	2:D:133:THR:HB	2.29	0.47
2:D:163:ASN:N	2:D:173:SER:OG	2.48	0.47
1:A:186:ASP:C	1:A:188:PRO:HD3	2.40	0.47
1:C:436:HIS:ND1	1:C:441:ARG:O	2.45	0.47
1:C:213:PRO:O	1:C:217:ILE:HG13	2.14	0.46
2:D:40:GLU:O	2:D:43:GLN:HB3	2.15	0.46
2:D:224:LEU:HD12	2:D:227:HIS:NE2	2.30	0.46
2:D:258:GLN:C	2:D:258:GLN:CD	2.83	0.46
1:A:91:GLU:O	1:A:95:GLU:HG2	2.15	0.46
1:C:75:PHE:CE2	1:C:93:LEU:HD23	2.50	0.46
1:C:189:PHE:HB3	1:C:349:LYS:HZ2	1.81	0.46
2:D:353:ILE:O	2:D:354:GLN:HB3	2.15	0.46
2:B:153:TRP:CZ2	2:B:431:PRO:HG3	2.50	0.46
1:C:224:GLN:OE1	1:C:246:LEU:HD21	2.15	0.46
1:C:358:GLY:HA2	1:C:380:LEU:HD21	1.97	0.46
1:C:472:VAL:HG12	1:C:473:MET:N	2.31	0.46
2:D:21:LYS:HA	2:D:25:GLU:HG2	1.97	0.46
1:C:33:VAL:CG1	1:C:54:ILE:HD12	2.46	0.46
1:C:285:ILE:HD13	1:C:323:LEU:HD11	1.98	0.46
1:C:442:TYR:HB2	1:C:445:VAL:HG23	1.97	0.46
2:D:213:PHE:HB3	2:D:218:ILE:HD11	1.96	0.46
2:D:232:VAL:HG11	2:D:260:ILE:HG23	1.97	0.46
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.42	0.46
2:B:392:LEU:O	2:B:393:TYR:CB	2.63	0.46
1:C:35:LEU:HG	1:C:37:ASN:H	1.81	0.46
1:C:201:LEU:HD13	1:C:209:HIS:HE1	1.80	0.46
1:C:214:TRP:O	1:C:218:ILE:HG12	2.15	0.46
2:D:216:CYS:SG	2:D:221:MET:HE2	2.56	0.46
1:A:189:PHE:O	1:A:193:ARG:HG3	2.16	0.46
1:C:234:PRO:O	1:C:235:LYS:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ILE:CG2	1:C:370:GLN:HB2	2.45	0.46
1:C:404:LEU:HD22	1:C:467:GLU:O	2.16	0.46
2:D:46:LEU:O	2:D:73:ARG:HB2	2.15	0.46
1:C:158:LEU:HG	2:D:23:PHE:CE2	2.50	0.46
1:C:189:PHE:HB2	1:C:190:PRO:HD2	1.97	0.46
1:C:217:ILE:HD13	1:C:265:PHE:CD1	2.50	0.46
1:C:233:ILE:O	1:C:234:PRO:C	2.59	0.46
1:C:416:MET:SD	1:C:423:ILE:HG23	2.56	0.46
2:D:226:GLU:CD	2:D:226:GLU:H	2.24	0.46
2:D:425:VAL:CG1	2:D:426:ALA:N	2.78	0.46
2:B:82:THR:HG23	2:B:100:GLY:O	2.16	0.46
2:B:224:LEU:H	2:B:227:HIS:HD2	1.63	0.46
1:C:199:TYR:O	1:C:220:LYS:HE2	2.15	0.46
1:A:321:GLY:O	1:A:322:ASN:ND2	2.49	0.46
2:B:322:LEU:C	2:B:322:LEU:HD23	2.41	0.46
1:C:428:MET:HE2	1:C:478:TYR:O	2.15	0.46
2:D:41:SER:C	2:D:43:GLN:N	2.73	0.46
2:D:152:ARG:HB3	2:D:429:THR:HG23	1.98	0.46
1:A:113:LEU:CD1	1:A:142:VAL:HG21	2.46	0.45
1:A:209:HIS:HD2	1:A:262:GLU:OE2	1.99	0.45
1:A:447:ASN:HD22	2:B:26:ARG:NH2	2.13	0.45
2:D:152:ARG:NH2	2:D:201:GLU:OE1	2.42	0.45
2:D:152:ARG:CB	2:D:429:THR:HG23	2.46	0.45
2:D:43:GLN:HE21	2:D:43:GLN:HA	1.81	0.45
2:D:76:HIS:CD2	2:D:121:VAL:HB	2.51	0.45
1:A:416:MET:CE	1:A:424:VAL:HG13	2.46	0.45
2:D:149:ILE:HD11	2:D:377:LYS:NZ	2.31	0.45
1:A:235:LYS:CD	1:A:238:LYS:HE3	2.47	0.45
2:D:324:PHE:CZ	2:D:330:LEU:HD11	2.52	0.45
1:A:163:ARG:NH2	1:A:396:ARG:O	2.49	0.45
1:A:513:PHE:N	1:A:513:PHE:CD1	2.84	0.45
2:B:243:PHE:O	2:B:247:VAL:HG21	2.17	0.45
2:B:256:HIS:O	2:B:260:ILE:HG12	2.16	0.45
1:C:78:ARG:C	1:C:80:SER:H	2.24	0.45
1:C:189:PHE:CZ	1:C:192:LEU:HB2	2.52	0.45
2:D:382:THR:HG23	2:D:390:ARG:C	2.42	0.45
2:B:378:SER:N	2:B:379:PRO:HD3	2.31	0.45
1:C:486:GLY:O	1:C:487:ALA:HB3	2.17	0.45
1:A:373:GLU:C	1:A:375:ILE:N	2.75	0.45
1:C:18:ARG:CB	2:D:290:PRO:HG3	2.47	0.45
1:C:108:SER:HB3	1:C:111:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ARG:HH12	2:D:274:ARG:CG	2.16	0.45
1:A:75:PHE:O	1:A:76:LEU:HD23	2.17	0.45
1:C:386:ASN:O	1:C:390:LEU:HD23	2.16	0.45
1:C:445:VAL:O	1:C:446:SER:HB3	2.16	0.45
1:A:213:PRO:HG3	1:A:334:ALA:CB	2.47	0.45
1:A:215:ILE:N	1:A:332:MET:HE1	2.27	0.45
1:C:14:ASP:O	1:C:18:ARG:HG2	2.17	0.45
1:C:186:ASP:C	1:C:188:PRO:HD3	2.41	0.45
1:C:211:HIS:HD2	2:D:221:MET:SD	2.40	0.45
2:D:374:LEU:HD21	2:D:436:PHE:HZ	1.79	0.45
1:A:401:GLU:OE1	1:A:426:TYR:OH	2.24	0.44
1:C:200:ASP:OD1	1:C:203:HIS:HB2	2.17	0.44
1:C:309:ARG:HB3	1:C:364:LEU:HD21	1.99	0.44
1:C:436:HIS:C	1:C:438:GLN:H	2.23	0.44
2:D:84:ASP:CG	2:D:85:VAL:N	2.75	0.44
2:D:87:ASN:OD1	2:D:103:LYS:HE2	2.17	0.44
2:D:236:GLN:O	2:D:237:TRP:C	2.59	0.44
1:A:421:ASN:ND2	1:A:423:ILE:HB	2.29	0.44
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.47	0.44
2:B:197:THR:CG2	2:B:198:ALA:N	2.80	0.44
1:C:19:LEU:HD13	2:D:185:PHE:CE1	2.52	0.44
1:C:36:ILE:HG21	1:C:128:ALA:HA	1.98	0.44
1:C:303:SER:O	1:C:307:LEU:HG	2.17	0.44
1:C:390:LEU:C	1:C:391:ARG:HG2	2.42	0.44
2:D:23:PHE:CD1	2:D:23:PHE:N	2.85	0.44
2:B:405:ARG:N	2:B:406:PRO:CD	2.73	0.44
1:C:484:ARG:HG2	1:C:484:ARG:NH1	2.32	0.44
2:D:353:ILE:HD13	2:D:367:TYR:HE2	1.82	0.44
1:A:209:HIS:CD2	1:A:252:LEU:HG	2.51	0.44
1:C:329:ILE:HD12	1:C:332:MET:HE3	2.00	0.44
1:C:521:ILE:O	1:C:529:SER:HA	2.18	0.44
2:D:43:GLN:NE2	2:D:43:GLN:HA	2.32	0.44
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.46	0.44
2:B:131:ASN:OD1	2:B:132:ASP:OD1	2.35	0.44
2:B:185:PHE:HB3	2:B:326:ASP:HB3	1.99	0.44
2:B:272:ASN:ND2	4:B:475:HOH:O	2.48	0.44
1:C:143:LEU:HD22	1:C:148:ILE:CG2	2.47	0.44
1:C:314:PHE:CE2	1:C:324:PRO:HG3	2.52	0.44
2:D:213:PHE:HB3	2:D:218:ILE:CD1	2.48	0.44
2:B:139:HIS:O	2:B:176:PRO:HD2	2.17	0.44
2:B:340:LYS:HD2	4:B:502:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ILE:HD12	1:C:480:HIS:CG	2.53	0.44
2:D:243:PHE:N	2:D:243:PHE:CD2	2.85	0.44
2:D:353:ILE:HD13	2:D:367:TYR:CE2	2.52	0.44
2:D:364:VAL:O	2:D:367:TYR:HB3	2.17	0.44
1:A:214:TRP:CD1	1:A:332:MET:HE3	2.53	0.44
1:A:428:MET:CE	1:A:479:VAL:HA	2.48	0.44
1:C:201:LEU:HD22	1:C:209:HIS:CE1	2.53	0.44
2:B:241:GLN:CD	2:B:246:GLY:H	2.26	0.44
2:D:237:TRP:CZ2	2:D:249:LEU:HB2	2.52	0.44
2:D:338:GLU:O	2:D:340:LYS:N	2.47	0.44
1:C:96:LEU:HD22	2:D:92:PHE:HB2	1.99	0.44
2:D:26:ARG:HH11	2:D:26:ARG:HG2	1.82	0.44
2:D:430:THR:HG22	2:D:432:GLN:HG2	1.95	0.44
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.53	0.43
1:C:190:PRO:HB2	1:C:191:GLU:OE2	2.17	0.43
1:C:233:ILE:O	1:C:234:PRO:O	2.36	0.43
1:C:335:ASP:HB3	1:C:338:LYS:CG	2.48	0.43
2:D:202:CYS:HB3	2:D:343:CYS:HB2	1.99	0.43
2:D:305:THR:HG22	2:D:309:LYS:HE3	2.00	0.43
1:C:125:VAL:HG12	1:C:126:VAL:N	2.33	0.43
2:D:136:ARG:HH11	2:D:136:ARG:HG3	1.83	0.43
2:D:208:PRO:O	2:D:209:PRO:C	2.61	0.43
2:D:230:GLU:HG3	2:D:234:MET:CE	2.42	0.43
1:A:313:GLU:O	1:A:316:ALA:HB3	2.18	0.43
1:C:66:SER:H	1:C:69:ASP:HB2	1.84	0.43
1:C:503:GLN:OE1	1:C:506:ILE:HB	2.18	0.43
2:D:132:ASP:C	4:D:444:HOH:O	2.61	0.43
2:D:178:ILE:HD12	2:D:307:VAL:CG2	2.47	0.43
2:D:267:ARG:O	2:D:270:GLN:HB3	2.17	0.43
2:D:306:GLU:O	2:D:310:ILE:HG13	2.19	0.43
1:A:105:VAL:HG12	1:A:107:GLU:HB2	2.00	0.43
2:B:128:GLN:NE2	2:B:128:GLN:N	2.60	0.43
1:C:173:GLU:HG2	4:C:540:HOH:O	2.18	0.43
1:C:380:LEU:C	1:C:382:LEU:N	2.76	0.43
2:D:43:GLN:HE22	2:D:46:LEU:HD12	1.82	0.43
2:D:216:CYS:CB	2:D:221:MET:HE2	2.48	0.43
2:B:425:VAL:CG1	2:B:426:ALA:H	2.30	0.43
1:C:236:THR:CG2	1:C:237:TYR:N	2.82	0.43
2:D:154:ILE:HG23	2:D:155:ASN:N	2.33	0.43
2:D:434:VAL:O	2:D:435:LEU:CG	2.67	0.43
2:B:340:LYS:HE2	2:B:342:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:H	1:C:233:ILE:HG13	1.52	0.43
1:C:450:VAL:O	1:C:452:GLU:N	2.52	0.43
1:C:503:GLN:NE2	2:D:185:PHE:CE2	2.86	0.43
2:D:35:PHE:CE1	2:D:314:ALA:CA	2.97	0.43
2:B:267:ARG:NH1	4:B:457:HOH:O	2.52	0.43
1:C:534:LEU:C	4:C:539:HOH:O	2.61	0.43
1:C:232:ARG:C	1:C:234:PRO:CD	2.88	0.43
1:C:333:ILE:N	1:C:333:ILE:HD12	2.32	0.43
1:C:531:THR:HG22	1:C:532:PHE:N	2.34	0.43
2:D:192:ILE:CD1	2:D:200:ILE:HG13	2.49	0.43
2:D:231:TYR:HD1	2:D:235:LEU:HD12	1.84	0.43
2:D:236:GLN:HE22	2:D:263:LYS:CE	2.30	0.43
2:D:252:ASP:O	2:D:254:PRO:HD3	2.19	0.43
2:B:268:ALA:HB1	2:B:273:ILE:O	2.18	0.43
1:C:143:LEU:CD1	1:C:150:LEU:HD13	2.48	0.43
1:C:397:SER:OG	1:C:400:GLU:HG3	2.19	0.43
1:C:438:GLN:NE2	1:C:439:GLN:HE22	2.11	0.43
2:D:157:MET:O	2:D:157:MET:HE3	2.19	0.43
2:D:365:LEU:HD23	2:D:365:LEU:C	2.44	0.43
2:B:190:ARG:HB2	2:B:320:ASN:O	2.19	0.43
1:C:139:LEU:O	1:C:143:LEU:HG	2.19	0.43
1:C:225:TRP:CD1	1:C:233:ILE:CG1	3.02	0.43
1:A:213:PRO:HB2	1:A:216:VAL:HG23	2.00	0.42
1:C:33:VAL:O	1:C:57:PHE:HA	2.19	0.42
1:C:213:PRO:HG3	1:C:334:ALA:HB1	2.01	0.42
1:C:226:TYR:CD1	1:C:231:GLY:O	2.72	0.42
2:D:335:PHE:CD1	2:D:335:PHE:C	2.96	0.42
1:A:33:VAL:CG1	1:A:54:ILE:HD13	2.48	0.42
1:A:423:ILE:HD13	1:A:426:TYR:HB3	2.01	0.42
1:C:163:ARG:NH2	1:C:396:ARG:O	2.52	0.42
1:C:448:TYR:HD1	2:D:26:ARG:NH1	2.17	0.42
1:A:8:LEU:HD23	1:A:8:LEU:C	2.44	0.42
2:B:303:CYS:O	2:B:307:VAL:HG23	2.18	0.42
1:C:10:GLU:CG	2:D:279:ARG:HH12	2.32	0.42
1:C:277:ASN:C	1:C:277:ASN:ND2	2.77	0.42
1:A:33:VAL:HG22	1:A:34:CYS:N	2.34	0.42
1:A:335:ASP:OD1	1:A:336:SER:N	2.53	0.42
1:A:403:GLY:HA3	1:A:406:THR:OG1	2.20	0.42
1:C:75:PHE:CZ	1:C:96:LEU:HD11	2.55	0.42
1:C:227:SER:O	1:C:229:THR:N	2.52	0.42
1:C:383:LEU:HD12	1:C:383:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:GLU:HG2	1:C:467:GLU:O	2.18	0.42
1:C:380:LEU:C	1:C:382:LEU:H	2.28	0.42
1:C:450:VAL:C	1:C:452:GLU:H	2.28	0.42
2:D:35:PHE:HE1	2:D:314:ALA:HA	1.77	0.42
2:B:207:TYR:C	2:B:209:PRO:CD	2.80	0.42
1:C:217:ILE:HD11	1:C:264:ASN:HD22	1.84	0.42
2:D:169:LEU:HD22	2:D:195:GLY:O	2.20	0.42
2:D:210:GLN:HG2	2:D:211:VAL:H	1.81	0.42
2:D:224:LEU:HB2	2:D:227:HIS:CD2	2.55	0.42
2:D:279:ARG:HG3	2:D:279:ARG:HH11	1.83	0.42
1:A:225:TRP:HH2	1:A:242:ASP:HB3	1.85	0.42
2:D:64:LEU:HB3	2:D:111:LEU:HD13	2.02	0.42
2:D:159:ILE:HG23	2:D:162:LEU:HD12	2.00	0.42
1:A:212:THR:CG2	1:A:216:VAL:HB	2.49	0.42
1:C:182:ASP:OD1	1:C:182:ASP:O	2.38	0.42
1:A:404:LEU:HD23	1:A:468:TYR:CE2	2.55	0.42
2:B:158:LEU:HD22	2:B:175:VAL:HB	2.01	0.42
2:D:262:GLN:O	2:D:266:GLU:HG3	2.20	0.42
1:A:238:LYS:HG3	1:A:239:GLU:N	2.28	0.42
1:A:444:GLY:O	1:A:445:VAL:C	2.63	0.42
2:B:428:VAL:O	2:B:428:VAL:HG12	2.19	0.42
1:C:185:LEU:HD13	1:C:218:ILE:HG21	2.01	0.42
1:C:288:ILE:HD11	1:C:392:VAL:HG23	2.02	0.42
1:C:234:PRO:CA	1:C:240:LYS:HZ3	2.17	0.41
1:C:428:MET:O	1:C:429:LEU:C	2.63	0.41
2:D:35:PHE:HE1	2:D:314:ALA:CB	2.33	0.41
2:D:127:ILE:HD13	2:D:127:ILE:HA	1.79	0.41
2:B:381:ILE:HG22	2:B:382:THR:N	2.35	0.41
1:C:112:LEU:O	1:C:116:ASP:C	2.63	0.41
1:C:206:LYS:HG3	1:C:207:LYS:N	2.35	0.41
1:C:460:CYS:HB3	4:C:536:HOH:O	2.19	0.41
2:D:80:MET:HE3	2:D:80:MET:HA	2.02	0.41
1:A:87:GLU:HG3	1:A:104:PHE:CZ	2.55	0.41
1:A:334:ALA:C	2:B:221:MET:HE2	2.45	0.41
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.55	0.41
2:B:204:LEU:O	2:B:206:LEU:N	2.53	0.41
2:B:401:GLU:C	2:B:404:THR:H	2.28	0.41
1:C:113:LEU:HD21	1:C:120:PHE:HE1	1.85	0.41
1:A:225:TRP:NE1	1:A:233:ILE:HG12	2.35	0.41
1:A:486:GLY:O	2:B:22:LYS:NZ	2.53	0.41
1:C:504:GLU:OE1	1:C:516:PHE:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:MET:HG3	2:D:80:MET:O	2.20	0.41
2:D:334:THR:HG22	2:D:335:PHE:N	2.34	0.41
2:B:157:MET:HE3	2:B:157:MET:O	2.21	0.41
2:D:233:ARG:CD	2:D:285:VAL:HA	2.51	0.41
1:A:51:LEU:N	1:A:52:PRO:HD2	2.35	0.41
1:A:84:ASN:ND2	1:A:106:GLU:HG2	2.36	0.41
2:B:427:ASP:CG	2:B:429:THR:HG22	2.46	0.41
1:C:78:ARG:HD3	1:C:81:ILE:CD1	2.51	0.41
1:C:163:ARG:CD	1:C:518:ASN:ND2	2.83	0.41
1:C:189:PHE:CB	1:C:349:LYS:NZ	2.83	0.41
1:C:241:GLU:OE2	1:C:244:ARG:HD2	2.20	0.41
1:A:39:THR:HB	1:A:489:GLU:OE1	2.21	0.41
1:A:377:GLU:C	1:A:381:LYS:HZ3	2.28	0.41
1:C:210:SER:HA	1:C:262:GLU:OE1	2.20	0.41
1:C:485:TYR:OH	1:C:525:MET:HE3	2.21	0.41
1:A:444:GLY:HA3	1:A:483:CYS:O	2.21	0.41
1:C:36:ILE:HG23	1:C:36:ILE:O	2.20	0.41
1:C:36:ILE:O	1:C:37:ASN:CG	2.63	0.41
1:C:67:GLY:O	1:C:68:GLU:C	2.63	0.41
1:C:373:GLU:O	1:C:373:GLU:HG2	2.21	0.41
2:D:110:PHE:C	2:D:110:PHE:CD2	2.99	0.41
1:A:232:ARG:C	1:A:233:ILE:HG13	2.45	0.41
1:A:311:LEU:HD11	1:A:383:LEU:HD11	2.03	0.41
2:B:62:GLU:HG3	4:B:446:HOH:O	2.19	0.41
2:B:362:GLN:O	2:B:366:ASP:OD1	2.39	0.41
1:C:12:LYS:C	1:C:14:ASP:H	2.29	0.41
1:C:49:LEU:HB3	1:C:54:ILE:HD13	2.02	0.41
1:C:56:SER:HB3	1:C:101:SER:HB2	2.02	0.41
1:C:84:ASN:O	1:C:87:GLU:HG2	2.21	0.41
1:C:184:ARG:NH2	1:C:323:LEU:O	2.41	0.41
1:C:189:PHE:CB	1:C:349:LYS:HZ2	2.33	0.41
1:C:218:ILE:O	1:C:222:LEU:CB	2.67	0.41
1:C:236:THR:O	1:C:240:LYS:HG3	2.20	0.41
2:D:110:PHE:O	2:D:110:PHE:HD2	2.04	0.41
2:D:162:LEU:HA	2:D:173:SER:OG	2.21	0.41
2:D:425:VAL:CG2	2:D:436:PHE:HD1	2.33	0.41
1:A:447:ASN:HD22	2:B:26:ARG:HH21	1.69	0.41
1:C:234:PRO:O	1:C:236:THR:N	2.53	0.41
2:D:43:GLN:O	2:D:45:LEU:N	2.54	0.41
2:D:44:PHE:O	2:D:44:PHE:CD1	2.73	0.41
2:D:249:LEU:HD13	2:D:256:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:LEU:CD1	2:D:256:HIS:HB2	2.51	0.41
2:B:31:THR:HG21	2:B:35:PHE:HB3	2.00	0.40
1:C:124:THR:HG22	1:C:125:VAL:HG23	2.03	0.40
2:D:132:ASP:HA	2:D:157:MET:HE1	2.03	0.40
1:A:390:LEU:O	1:A:391:ARG:HG2	2.22	0.40
2:B:286:LYS:HB2	2:B:288:ILE:HG13	2.02	0.40
1:C:65:VAL:HB	1:C:81:ILE:HA	2.03	0.40
2:D:242:PRO:O	2:D:243:PHE:C	2.64	0.40
1:A:240:LYS:C	1:A:244:ARG:NH1	2.80	0.40
2:B:241:GLN:NE2	2:B:246:GLY:H	2.19	0.40
2:B:263:LYS:HD3	2:B:263:LYS:HA	1.92	0.40
2:D:36:GLU:HB3	2:D:38:SER:OG	2.21	0.40
2:D:430:THR:HA	2:D:431:PRO:HD3	1.87	0.40
1:A:129:THR:HA	1:A:153:CYS:O	2.21	0.40
2:B:364:VAL:HG23	2:B:381:ILE:CD1	2.51	0.40
1:C:257:GLY:O	1:C:259:PRO:HD3	2.22	0.40
2:D:116:PRO:O	2:D:118:CYS:N	2.52	0.40
2:B:265:LEU:HD23	2:B:276:VAL:HB	2.03	0.40
2:B:372:ALA:O	2:B:375:GLN:HG3	2.21	0.40
1:C:28:LEU:HA	1:C:509:ILE:HG21	2.03	0.40
1:C:46:LEU:HD23	1:C:93:LEU:HD13	2.03	0.40
2:D:24:LEU:HD21	2:D:312:THR:HG21	2.04	0.40
2:D:425:VAL:CG1	2:D:426:ALA:H	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/537 (98%)	477 (90%)	39 (7%)	11 (2%)	5	11
1	C	524/537 (98%)	438 (84%)	65 (12%)	21 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	387/444 (87%)	351 (91%)	24 (6%)	12 (3%)	3	5
2	D	372/444 (84%)	298 (80%)	54 (14%)	20 (5%)	1	1
All	All	1810/1962 (92%)	1564 (86%)	182 (10%)	64 (4%)	3	4

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
2	B	320	ASN
2	B	395	GLN
1	C	229	THR
1	C	234	PRO
1	C	235	LYS
1	C	255	GLU
1	C	256	ASN
1	C	446	SER
2	D	116	PRO
2	D	340	LYS
2	D	391	THR
1	A	230	ASN
1	A	438	GLN
1	A	450	VAL
2	B	205	GLU
2	B	379	PRO
2	B	392	LEU
2	B	393	TYR
1	C	83	LYS
1	C	333	ILE
1	C	448	TYR
1	C	451	GLU
2	D	117	ASN
2	D	274	ARG
2	D	275	GLY
1	A	236	THR
1	A	333	ILE
2	B	371	SER
2	B	394	LEU
1	C	186	ASP
1	C	318	GLU
1	C	445	VAL
1	C	447	ASN

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Mol	Chain	Res	Type
1	C	485	TYR
2	D	132	ASP
2	D	196	MET
2	D	209	PRO
2	D	320	ASN
2	D	371	SER
2	D	376	MET
1	A	36	ILE
2	B	92	PHE
2	B	380	ALA
1	C	254	ASN
1	C	257	GLY
2	D	44	PHE
1	A	106	GLU
1	A	368	ILE
1	A	372	PRO
1	C	38	ALA
1	C	252	LEU
2	D	205	GLU
2	D	345	ALA
2	D	390	ARG
2	B	209	PRO
1	C	190	PRO
2	D	249	LEU
2	D	434	VAL
2	B	116	PRO
2	D	350	PRO
1	A	234	PRO
2	D	379	PRO
1	C	371	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	461/467 (99%)	445 (96%)	16 (4%)	32 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	458/467 (98%)	448 (98%)	10 (2%)	45	72
2	B	335/387 (87%)	322 (96%)	13 (4%)	28	55
2	D	325/387 (84%)	317 (98%)	8 (2%)	42	69
All	All	1579/1708 (92%)	1532 (97%)	47 (3%)	36	64

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	72	ASN
1	A	80	SER
1	A	115	ASN
1	A	154	ARG
1	A	213	PRO
1	A	255	GLU
1	A	264	ASN
1	A	272	VAL
1	A	409	LYS
1	A	422	GLU
1	A	423	ILE
1	A	424	VAL
1	A	432	VAL
1	A	441	ARG
1	A	458	LYS
2	B	31	THR
2	B	77	VAL
2	B	116	PRO
2	B	128	GLN
2	B	131	ASN
2	B	148	ILE
2	B	165	GLU
2	B	201	GLU
2	B	215	MET
2	B	218	ILE
2	B	277	THR
2	B	292	VAL
2	B	365	LEU
1	C	33	VAL
1	C	34	CYS
1	C	259	PRO
1	C	353	ASP

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Mol	Chain	Res	Type
1	C	391	ARG
1	C	406	THR
1	C	414	SER
1	C	434	ARG
1	C	466	GLN
1	C	503	GLN
2	D	113	ASP
2	D	127	ILE
2	D	128	GLN
2	D	131	ASN
2	D	136	ARG
2	D	182	THR
2	D	200	ILE
2	D	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	32	HIS
1	A	48	ASN
1	A	64	GLN
1	A	72	ASN
1	A	77	GLN
1	A	84	ASN
1	A	111	ASN
1	A	195	HIS
1	A	211	HIS
1	A	224	GLN
1	A	230	ASN
1	A	249	GLN
1	A	264	ASN
1	A	296	ASN
1	A	320	GLN
1	A	344	ASN
1	A	359	ASN
1	A	360	HIS
1	A	370	GLN
1	A	418	ASN
1	A	421	ASN
1	A	447	ASN
1	A	503	GLN

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Mol	Chain	Res	Type
1	A	517	ASN
1	A	518	ASN
2	B	19	HIS
2	B	32	HIS
2	B	87	ASN
2	B	117	ASN
2	B	125	ASN
2	B	128	GLN
2	B	131	ASN
2	B	139	HIS
2	B	188	ASN
2	B	227	HIS
2	B	236	GLN
2	B	262	GLN
2	B	325	ASN
2	B	348	GLN
2	B	351	GLN
1	C	37	ASN
1	C	72	ASN
1	C	84	ASN
1	C	94	GLN
1	C	97	ASN
1	C	111	ASN
1	C	130	GLN
1	C	145	ASN
1	C	147	GLN
1	C	169	HIS
1	C	273	ASN
1	C	277	ASN
1	C	322	ASN
1	C	359	ASN
1	C	360	HIS
1	C	438	GLN
1	C	439	GLN
1	C	518	ASN
1	C	527	GLN
2	D	19	HIS
2	D	43	GLN
2	D	74	GLN
2	D	76	HIS
2	D	131	ASN
2	D	137	GLN

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Mol	Chain	Res	Type
2	D	139	HIS
2	D	227	HIS
2	D	236	GLN
2	D	282	GLN
2	D	296	ASN
2	D	319	ASN
2	D	325	ASN
2	D	342	ASN
2	D	351	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.