



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:21 PM UTC

PDB ID : 1M3I / pdb_00001m3i
Title : Perfringolysin O, new crystal form
Authors : Rossjohn, J.; Parker, M.; Polekhina, G.; Feil, S.; Tweten, R.
Deposited on : 2002-06-28
Resolution : 2.90 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

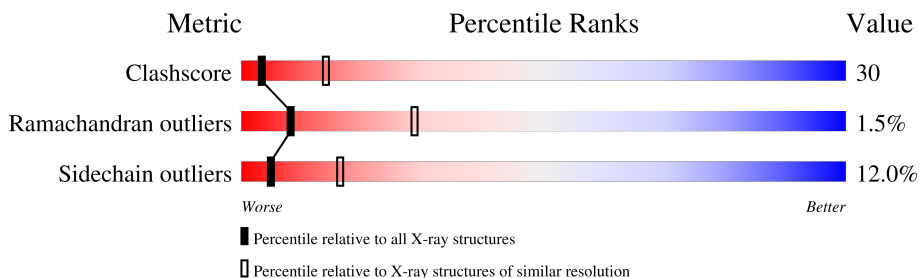
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	471	
1	B	471	
1	C	471	
1	D	471	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14920 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 perfringolysin O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			
1	B	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			
1	C	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			
1	D	465	Total	C	N	O	S	0	0	0
			3657	2304	614	734	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	PHE	see remark 999	UNP P19995
B	114	LEU	PHE	see remark 999	UNP P19995
C	114	LEU	PHE	see remark 999	UNP P19995
D	114	LEU	PHE	see remark 999	UNP P19995

- Molecule 2 is water.

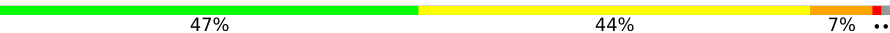
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	88	Total	O	0	0
			88	88		
2	C	58	Total	O	0	0
			58	58		
2	D	76	Total	O	0	0
			76	76		

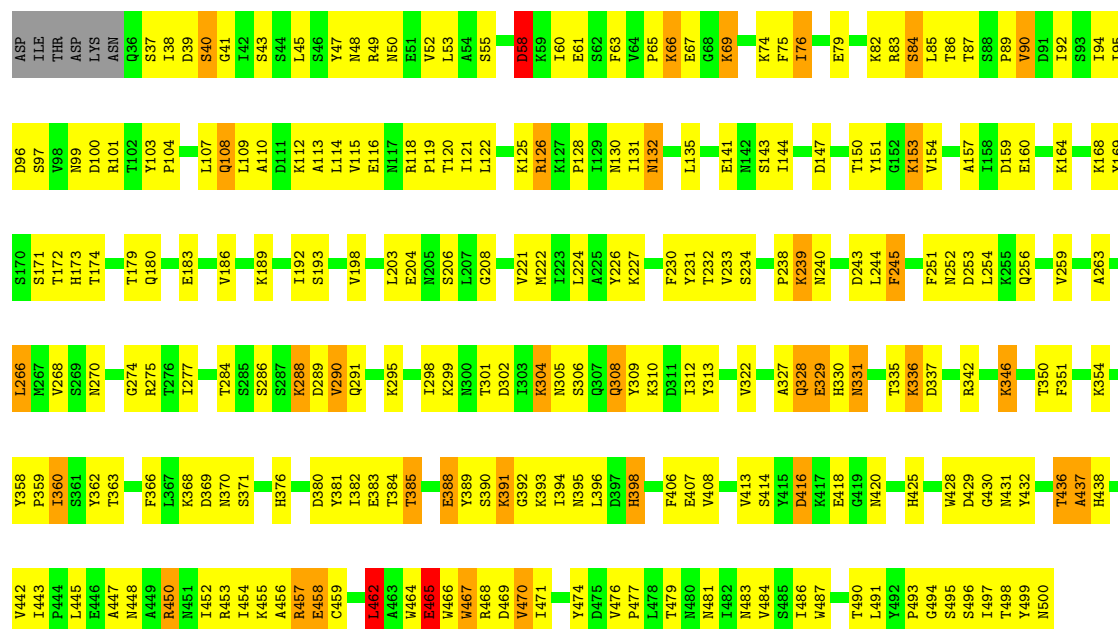
3 Residue-property plots

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.

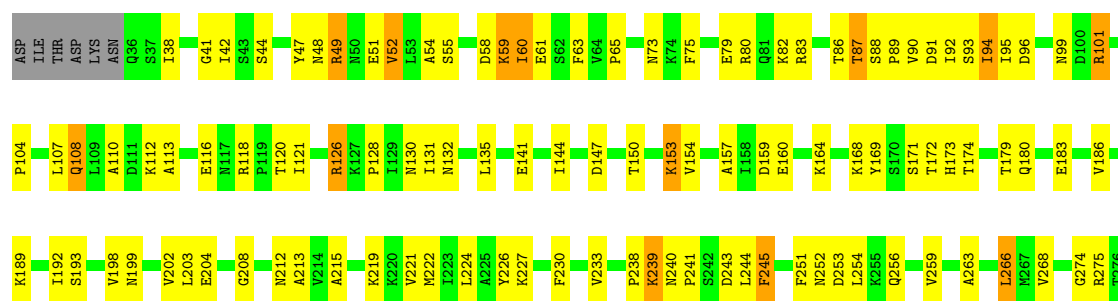
• Molecule 1: perfringolysin O

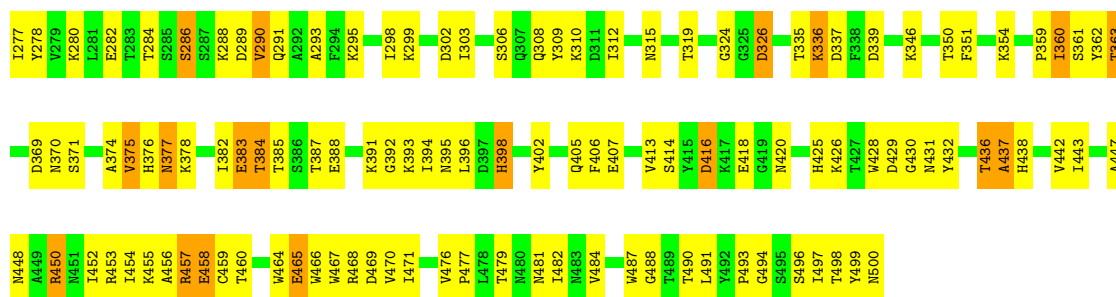
Chain A: 



• Molecule 1: perfringolysin O

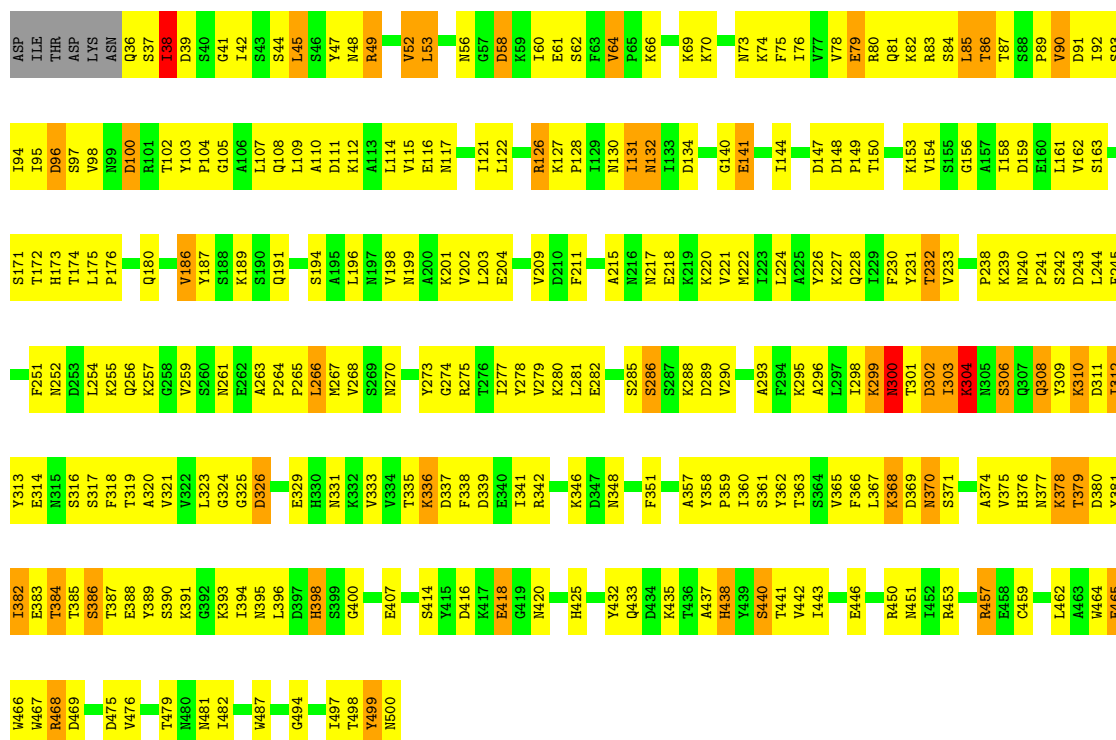
Chain B: 





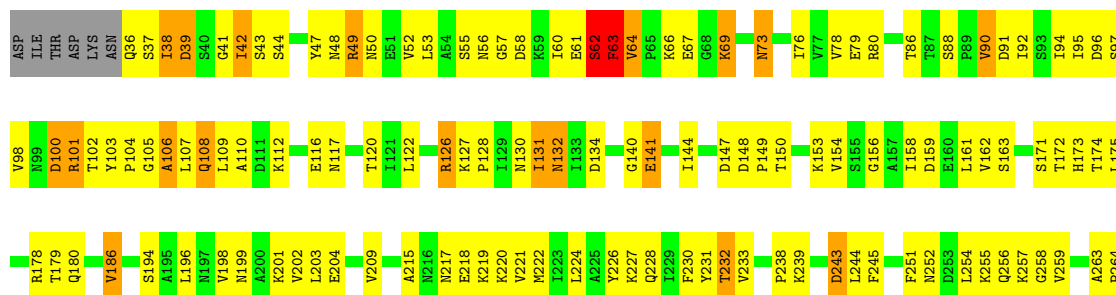
• Molecule 1: perfringolysin O

Chain C: 40% 48% 9% ..



• Molecule 1: perfringolysin O

Chain D: 43% 47% 8% .



S495	S496	T497	T498	Y499	M500	S414	Y415	D416	K417	E418	G419	M420	E421	H425	D429	Q433	D434	K435	T436	A437	H438	Y439	S440	T441	V442	I443	P444	L445	E446	A449	R450	M451	I452	R453	R457	E458	C459	W464	E465	W466	W467	R468	D469	V470	Y474	D475	W476	F477	L478	T479	N480	N481	I482	W487	G494	P265	L266	M267	V268	S269	N270	Y273	G274	R275	T276	I277	Y278	V279	E282	T283	S286	S287	K288	D289	K295	A296	L297	I298	K299	N300	T301	D302	I303	K304	N305	S306	Q307	Q308	Y309	K310	D311	I312	Y313	E314	N315	S316	S317	F318	T319	A320	V321	V322	L323	D326	A327	Q328	E329	H330	N331	K332	Y333	V334	T335	K336	D337	F338	D339	E340	I341	R342	K346	D347	N348	F351	S352	T353	A357	Y358	P359	I360	S361	Y362	T363	F366	L367	K368	D369	N370	S371	V372	A373	A374	V375	H376	N377	K378	E383	T384	T385	S386	K391	G392	K393	I394	N395	L396	D397	H398	S399	G400	E407	D411
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	130.41Å 130.41Å 129.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	95.2 (20.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14920	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

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	0.40	0/3728	0.88	13/5062 (0.3%)
1	B	0.42	0/3728	0.87	9/5062 (0.2%)
1	C	0.44	0/3728	0.88	8/5062 (0.2%)
1	D	0.41	0/3728	0.88	10/5062 (0.2%)
All	All	0.42	0/14912	0.88	40/20248 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	ASN	N-CA-C	12.48	128.45	113.23
1	A	95	ILE	N-CA-C	8.08	118.09	110.74
1	D	63	PHE	N-CA-C	-6.76	98.80	109.07
1	A	383	GLU	N-CA-C	-6.73	101.64	110.53
1	B	336	LYS	N-CA-C	-6.69	104.33	113.30
1	B	126	ARG	N-CA-C	6.62	118.19	108.86
1	A	336	LYS	N-CA-C	-6.60	104.46	113.30
1	C	336	LYS	N-CA-C	-6.56	105.31	113.38
1	D	336	LYS	N-CA-C	-6.52	105.36	113.38
1	D	90	VAL	N-CA-C	-6.51	106.62	111.90
1	A	126	ARG	N-CA-C	6.28	118.09	109.18
1	D	102	THR	N-CA-C	-6.21	98.95	108.76
1	C	301	THR	N-CA-C	-6.04	101.05	110.42
1	A	470	VAL	N-CA-C	-6.01	106.94	112.96
1	C	304	LYS	N-CA-C	5.85	120.96	111.37
1	A	113	ALA	N-CA-C	-5.84	104.82	111.07
1	B	95	ILE	N-CA-C	5.77	117.29	111.00
1	B	135	LEU	N-CA-C	-5.76	102.13	110.08
1	B	221	VAL	N-CA-C	5.72	116.99	108.46
1	B	63	PHE	N-CA-C	5.68	118.69	110.28
1	A	135	LEU	N-CA-C	-5.63	102.31	110.08
1	B	113	ALA	N-CA-C	-5.62	105.06	111.07
1	A	221	VAL	N-CA-C	5.56	116.74	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	THR	N-CA-C	5.55	117.06	109.18
1	D	42	ILE	N-CA-C	5.55	116.94	110.62
1	C	306	SER	N-CA-C	5.54	118.83	111.75
1	A	90	VAL	N-CA-C	-5.44	107.05	113.42
1	D	101	ARG	N-CA-C	5.39	118.19	109.40
1	D	459	CYS	N-CA-C	5.37	117.91	108.56
1	A	436	THR	N-CA-C	5.37	116.80	109.18
1	D	100	ASP	N-CA-C	5.34	117.43	110.43
1	C	459	CYS	N-CA-C	5.32	117.82	108.56
1	D	97	SER	N-CA-C	-5.31	107.46	114.31
1	C	303	ILE	N-CA-C	5.30	117.41	109.20
1	C	499	TYR	N-CA-C	5.27	117.68	109.52
1	D	499	TYR	N-CA-C	5.25	117.66	109.52
1	B	253	ASP	N-CA-C	-5.17	105.56	111.14
1	A	253	ASP	N-CA-C	-5.13	105.60	111.14
1	A	467	TRP	N-CA-C	5.12	118.01	110.59
1	A	58	ASP	N-CA-C	5.05	117.84	109.46

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	3657	0	3611	210	0
1	B	3657	0	3611	185	0
1	C	3657	0	3611	282	0
1	D	3657	0	3611	219	0
2	A	70	0	0	14	0
2	B	88	0	0	6	0
2	C	58	0	0	4	0
2	D	76	0	0	9	0
All	All	14920	0	14444	882	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 30.

All (882) 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:A:335:THR:HG22	1:A:337:ASP:H	1.27	0.99
1:B:335:THR:HG22	1:B:337:ASP:H	1.28	0.98
1:A:87:THR:HG22	1:A:89:PRO:HD3	1.45	0.97
1:C:289:ASP:HB3	1:C:309:TYR:HE1	1.25	0.94
1:A:301:THR:O	1:A:304:LYS:HG3	1.68	0.94
1:C:296:ALA:HB2	1:C:303:ILE:HD13	1.52	0.91
1:C:82:LYS:HA	1:C:382:ILE:HA	1.50	0.91
1:D:457:ARG:HD2	1:D:469:ASP:OD2	1.71	0.90
1:A:222:MET:HE3	1:A:224:LEU:HD21	1.50	0.90
1:B:222:MET:HE3	1:B:224:LEU:HD21	1.52	0.90
1:A:109:LEU:HD21	1:A:122:LEU:HD21	1.53	0.89
1:A:222:MET:HE1	1:A:298:ILE:HD11	1.56	0.88
1:A:104:PRO:HG2	1:A:131:ILE:HD11	1.54	0.88
1:C:481:ASN:HB2	1:C:500:ASN:HB2	1.56	0.88
1:D:481:ASN:HB2	1:D:500:ASN:HB2	1.56	0.87
1:C:457:ARG:HD2	1:C:469:ASP:OD2	1.75	0.87
1:B:222:MET:HE1	1:B:298:ILE:HD11	1.56	0.86
1:C:90:VAL:HG12	1:C:374:ALA:HB2	1.58	0.86
1:A:481:ASN:HB2	1:A:500:ASN:HB2	1.58	0.85
1:C:66:LYS:HG3	1:C:79:GLU:HG3	1.59	0.85
1:D:457:ARG:HG3	1:D:468:ARG:O	1.78	0.84
1:A:75:PHE:HB2	1:A:447:ALA:HB3	1.60	0.83
1:A:131:ILE:HG22	1:A:144:ILE:HG22	1.59	0.83
1:B:481:ASN:HB2	1:B:500:ASN:HB2	1.61	0.82
1:A:464:TRP:HA	1:A:467:TRP:CE3	2.14	0.82
1:B:456:ALA:HB3	1:B:471:ILE:HG22	1.61	0.82
1:B:465:GLU:OE2	1:D:91:ASP:HB2	1.79	0.82
1:C:259:VAL:HG13	1:C:265:PRO:HD3	1.61	0.82
1:D:259:VAL:HG13	1:D:265:PRO:HD3	1.62	0.82
1:B:131:ILE:HG22	1:B:144:ILE:HG22	1.59	0.81
1:A:456:ALA:HB3	1:A:471:ILE:HG22	1.60	0.81
1:D:110:ALA:HB2	1:D:266:LEU:HD21	1.63	0.81
1:A:37:SER:HB3	1:A:40:SER:OG	1.80	0.80
1:A:288:LYS:HB2	2:A:542:HOH:O	1.81	0.80
1:D:429:ASP:HB3	2:D:553:HOH:O	1.81	0.80
1:C:457:ARG:HG3	1:C:468:ARG:O	1.80	0.79
1:C:110:ALA:HB2	1:C:266:LEU:HD21	1.65	0.79
1:B:73:ASN:HA	1:B:391:LYS:HE2	1.64	0.78
1:B:457:ARG:HD2	1:B:469:ASP:OD2	1.84	0.78
1:D:69:LYS:HG3	1:D:76:ILE:HB	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLU:OE2	1:A:490:THR:HG23	1.85	0.77
1:A:75:PHE:CE1	1:A:448:ASN:HB3	2.20	0.77
1:C:289:ASP:HB2	1:C:308:GLN:NE2	2.00	0.76
1:C:275:ARG:HB3	1:C:325:GLY:H	1.50	0.76
1:B:458:GLU:OE2	1:B:490:THR:HG23	1.86	0.76
1:D:335:THR:HG22	1:D:337:ASP:H	1.49	0.76
1:D:61:GLU:HG3	1:D:62:SER:H	1.50	0.75
1:C:39:ASP:OD1	1:C:240:ASN:HB3	1.86	0.75
1:C:37:SER:O	1:C:251:PHE:HB2	1.86	0.75
1:D:80:ARG:HG2	1:D:384:THR:HG22	1.69	0.74
1:D:37:SER:C	1:D:251:PHE:HB2	2.12	0.74
1:A:126:ARG:HB2	1:A:244:LEU:O	1.87	0.74
1:D:37:SER:O	1:D:251:PHE:HB2	1.86	0.74
1:C:335:THR:HG22	1:C:337:ASP:H	1.51	0.74
1:C:108:GLN:HG2	1:C:121:ILE:HD13	1.69	0.73
1:D:61:GLU:CG	1:D:62:SER:H	2.01	0.73
1:B:86:THR:OG1	1:B:378:LYS:HG3	1.88	0.73
1:D:88:SER:HA	1:D:375:VAL:O	1.88	0.73
1:C:89:PRO:C	1:C:91:ASP:H	1.95	0.73
1:A:55:SER:HB3	1:A:115:VAL:HG13	1.69	0.73
1:B:126:ARG:HB2	1:B:244:LEU:O	1.88	0.73
1:C:105:GLY:O	1:C:267:MET:HG3	1.89	0.73
1:C:64:VAL:HB	1:C:80:ARG:NH1	2.03	0.72
1:A:469:ASP:OD2	1:C:180:GLN:HA	1.89	0.72
1:C:36:GLN:O	1:C:251:PHE:HB3	1.89	0.72
1:D:295:LYS:HD2	2:D:539:HOH:O	1.90	0.72
1:D:312:ILE:H	1:D:312:ILE:HD12	1.55	0.71
1:A:252:ASN:O	1:A:256:GLN:HB2	1.90	0.71
1:A:457:ARG:HB2	1:A:464:TRP:CZ3	2.25	0.71
1:C:107:LEU:HD11	1:C:126:ARG:HH21	1.55	0.71
1:C:44:SER:HA	1:C:368:LYS:NZ	2.04	0.71
1:B:464:TRP:HA	1:B:467:TRP:CE3	2.25	0.71
1:A:384:THR:HG22	1:A:385:THR:N	2.06	0.71
1:A:39:ASP:O	1:A:43:SER:HB2	1.90	0.71
1:C:109:LEU:HD21	1:C:122:LEU:HD11	1.72	0.70
1:A:66:LYS:HB2	1:A:66:LYS:NZ	2.05	0.70
1:B:252:ASN:O	1:B:256:GLN:HB2	1.90	0.70
1:D:391:LYS:HE2	1:D:446:GLU:OE1	1.92	0.70
1:C:87:THR:HG22	1:C:89:PRO:HD3	1.73	0.70
1:D:127:LYS:HG3	1:D:245:PHE:O	1.92	0.70
1:C:105:GLY:H	1:C:268:VAL:HB	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:SER:HB2	1:B:388:GLU:HB3	1.73	0.69
1:D:322:VAL:HG21	1:D:327:ALA:HB1	1.73	0.69
1:D:94:ILE:HD13	1:D:359:PRO:HB2	1.74	0.69
1:A:342:ARG:HD3	2:A:503:HOH:O	1.92	0.69
1:C:98:VAL:HG21	1:C:329:GLU:OE2	1.92	0.69
1:D:322:VAL:CG2	1:D:331:ASN:HB3	2.23	0.69
1:A:84:SER:HB2	1:A:380:ASP:OD2	1.93	0.68
1:C:49:ARG:HD3	2:C:505:HOH:O	1.93	0.68
1:A:131:ILE:CG2	1:A:144:ILE:HG22	2.23	0.68
1:D:60:ILE:HG22	1:D:61:GLU:N	2.08	0.68
1:A:310:LYS:HA	1:A:310:LYS:HE2	1.75	0.68
1:B:131:ILE:CG2	1:B:144:ILE:HG22	2.24	0.68
1:A:48:ASN:O	1:A:52:VAL:HG13	1.94	0.68
1:C:127:LYS:HG3	1:C:245:PHE:O	1.93	0.68
1:C:104:PRO:HD2	1:C:154:VAL:HG11	1.75	0.68
1:A:222:MET:HE1	1:A:298:ILE:CD1	2.24	0.68
1:C:289:ASP:HB3	1:C:309:TYR:CE1	2.18	0.68
1:A:131:ILE:HG12	1:A:233:VAL:HG12	1.76	0.67
1:C:289:ASP:HB2	1:C:308:GLN:CD	2.19	0.67
1:C:418:GLU:HB2	1:C:420:ASN:ND2	2.08	0.67
1:C:83:ARG:HB2	1:C:381:TYR:CE1	2.29	0.67
1:D:418:GLU:HB2	1:D:420:ASN:ND2	2.09	0.67
1:C:134:ASP:OD1	1:C:232:THR:HG23	1.95	0.67
1:B:90:VAL:O	1:B:363:THR:HG22	1.94	0.67
1:A:96:ASP:OD2	1:A:99:ASN:HB2	1.95	0.67
1:A:462:LEU:HD11	1:C:232:THR:OG1	1.95	0.67
1:C:53:LEU:HD13	1:C:115:VAL:HG22	1.75	0.67
1:B:198:VAL:HG21	1:B:203:LEU:HD21	1.77	0.66
1:B:460:THR:H	1:B:467:TRP:CD1	2.13	0.66
1:C:45:LEU:H	1:C:368:LYS:HZ2	1.42	0.66
1:D:134:ASP:OD1	1:D:232:THR:HG23	1.96	0.66
1:D:398:HIS:O	1:D:438:HIS:HA	1.96	0.66
1:D:319:THR:HG23	1:D:334:VAL:HG22	1.75	0.66
1:A:55:SER:HB3	1:A:115:VAL:CG1	2.25	0.66
1:A:109:LEU:HD12	2:A:554:HOH:O	1.95	0.66
1:B:90:VAL:HG12	1:B:374:ALA:HB2	1.77	0.66
1:B:295:LYS:HE2	1:B:299:LYS:NZ	2.11	0.66
1:B:222:MET:HE1	1:B:298:ILE:CD1	2.24	0.66
1:C:335:THR:HG22	1:C:336:LYS:H	1.61	0.66
1:B:61:GLU:HG2	1:B:61:GLU:O	1.96	0.66
1:D:52:VAL:HB	2:D:568:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:TYR:HE1	1:C:323:LEU:HD22	1.61	0.65
1:D:94:ILE:HG13	1:D:361:SER:HA	1.77	0.65
1:B:131:ILE:HG12	1:B:233:VAL:HG12	1.79	0.65
1:D:335:THR:HG22	1:D:336:LYS:H	1.60	0.65
1:C:80:ARG:HH11	1:C:80:ARG:HG3	1.61	0.65
1:D:61:GLU:HG3	1:D:62:SER:N	2.12	0.65
1:A:346:LYS:HG3	2:A:527:HOH:O	1.97	0.65
1:B:369:ASP:OD2	1:B:371:SER:HB3	1.96	0.65
1:C:398:HIS:O	1:C:438:HIS:HA	1.96	0.65
1:C:37:SER:C	1:C:251:PHE:HB2	2.23	0.64
1:D:396:LEU:HB2	1:D:441:THR:HG22	1.80	0.64
1:A:37:SER:C	1:A:251:PHE:HB2	2.23	0.64
1:A:66:LYS:HB2	1:A:66:LYS:HZ3	1.62	0.64
1:B:107:LEU:HD11	1:B:126:ARG:HH21	1.61	0.64
1:C:103:TYR:CD1	1:C:154:VAL:HG21	2.32	0.64
1:D:94:ILE:CD1	1:D:359:PRO:HB2	2.26	0.64
1:A:75:PHE:CD1	1:A:448:ASN:HB3	2.32	0.64
1:B:426:LYS:HD2	2:B:548:HOH:O	1.98	0.64
1:C:199:ASN:HB3	1:C:202:VAL:HG23	1.80	0.64
1:A:198:VAL:HG21	1:A:203:LEU:HD21	1.79	0.64
1:A:398:HIS:O	1:A:438:HIS:HA	1.97	0.64
1:C:308:GLN:NE2	1:C:312:ILE:HD11	2.12	0.64
1:A:395:ASN:HD22	1:A:442:VAL:HG22	1.61	0.64
1:D:148:ASP:HB3	1:D:153:LYS:HE2	1.80	0.64
1:D:335:THR:HG22	1:D:336:LYS:N	2.12	0.64
1:C:64:VAL:HB	1:C:80:ARG:HH12	1.63	0.64
1:A:491:LEU:HD22	1:C:176:PRO:HG2	1.80	0.64
1:C:81:GLN:C	1:C:382:ILE:HG13	2.23	0.64
1:C:191:GLN:HA	1:C:379:THR:HG21	1.80	0.64
1:C:61:GLU:HA	1:C:61:GLU:OE1	1.97	0.64
1:A:395:ASN:ND2	1:A:442:VAL:HG22	2.13	0.63
1:B:476:VAL:HG13	1:B:499:TYR:OH	1.98	0.63
1:D:322:VAL:O	1:D:323:LEU:HD23	1.98	0.63
1:B:395:ASN:HD22	1:B:442:VAL:HG22	1.62	0.63
1:C:293:ALA:HB2	1:C:309:TYR:CD1	2.34	0.63
1:D:199:ASN:HB3	1:D:202:VAL:HG23	1.80	0.63
1:B:80:ARG:HD3	1:B:382:ILE:HG21	1.79	0.63
1:A:396:LEU:HD23	1:A:484:VAL:HB	1.81	0.62
1:C:217:ASN:ND2	1:C:384:THR:HB	2.14	0.62
1:B:398:HIS:O	1:B:438:HIS:HA	1.98	0.62
1:A:150:THR:OG1	1:A:153:LYS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASP:OD2	1:A:371:SER:HB3	1.99	0.62
1:A:302:ASP:HA	1:A:304:LYS:HE3	1.80	0.62
1:C:335:THR:HG22	1:C:336:LYS:N	2.14	0.62
1:D:63:PHE:N	1:D:63:PHE:CD2	2.68	0.62
1:C:97:SER:O	1:C:358:TYR:HB3	2.00	0.62
1:A:295:LYS:HE2	1:A:299:LYS:NZ	2.14	0.61
1:A:304:LYS:HD2	1:A:304:LYS:N	2.15	0.61
1:B:395:ASN:ND2	1:B:442:VAL:HG22	2.14	0.61
1:B:173:HIS:HB2	1:B:354:LYS:HG3	1.82	0.61
1:B:458:GLU:CD	1:B:490:THR:HG23	2.25	0.61
1:C:191:GLN:HG3	1:C:381:TYR:CD2	2.35	0.61
1:C:227:LYS:HE3	1:C:360:ILE:HG22	1.81	0.61
1:C:296:ALA:HB2	1:C:303:ILE:CD1	2.27	0.61
1:D:116:GLU:O	1:D:117:ASN:HB2	2.00	0.61
1:D:196:LEU:O	1:D:198:VAL:HG13	2.01	0.61
1:B:315:ASN:HB2	2:B:561:HOH:O	2.01	0.61
1:B:326:ASP:OD1	1:B:326:ASP:N	2.33	0.61
1:D:222:MET:HE1	1:D:298:ILE:HD11	1.81	0.61
1:B:396:LEU:HD23	1:B:484:VAL:HB	1.82	0.61
1:A:335:THR:HG22	1:A:336:LYS:N	2.15	0.61
1:B:222:MET:CE	1:B:298:ILE:HD11	2.31	0.61
1:A:157:ALA:O	1:A:160:GLU:HB2	2.00	0.61
1:A:470:VAL:HG12	1:A:495:SER:HB3	1.83	0.61
1:C:75:PHE:O	1:C:389:TYR:HB2	2.01	0.61
1:A:125:LYS:HE3	2:A:504:HOH:O	1.99	0.60
1:A:335:THR:HG22	1:A:336:LYS:H	1.66	0.60
1:A:254:LEU:HB3	1:A:259:VAL:HG21	1.84	0.60
1:C:148:ASP:HB3	1:C:153:LYS:HE2	1.83	0.60
1:A:173:HIS:HB2	1:A:354:LYS:HG3	1.83	0.60
1:B:324:GLY:HA3	2:B:501:HOH:O	2.01	0.60
1:C:172:THR:HG22	1:C:174:THR:H	1.66	0.60
1:C:196:LEU:O	1:C:198:VAL:HG13	2.01	0.60
1:C:308:GLN:HG3	1:C:309:TYR:N	2.15	0.60
1:C:222:MET:HE1	1:C:298:ILE:HD11	1.83	0.60
1:A:45:LEU:O	1:A:368:LYS:NZ	2.32	0.60
1:B:131:ILE:HG22	1:B:144:ILE:CG2	2.30	0.60
1:C:53:LEU:HD22	1:C:115:VAL:HG23	1.84	0.60
1:D:98:VAL:HG21	1:D:329:GLU:HG2	1.83	0.60
1:A:476:VAL:HG13	1:A:499:TYR:OH	2.01	0.59
1:D:172:THR:HG22	1:D:174:THR:H	1.66	0.59
1:C:80:ARG:HD3	1:C:384:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:HG13	1:C:96:ASP:H	1.66	0.59
1:C:351:PHE:HE2	2:C:535:HOH:O	1.83	0.59
1:D:78:VAL:HG11	1:D:217:ASN:HD21	1.67	0.59
1:A:119:PRO:HD3	2:A:502:HOH:O	2.03	0.59
1:A:131:ILE:HG22	1:A:144:ILE:CG2	2.31	0.59
1:B:457:ARG:HB2	1:B:464:TRP:CZ3	2.36	0.59
1:A:222:MET:CE	1:A:298:ILE:HD11	2.30	0.59
1:A:328:GLN:CG	1:A:329:GLU:H	2.16	0.59
1:B:150:THR:OG1	1:B:153:LYS:HB2	2.03	0.59
1:B:487:TRP:CH2	1:B:496:SER:HB3	2.36	0.59
1:A:487:TRP:CH2	1:A:496:SER:HB3	2.38	0.59
1:A:418:GLU:HB2	1:A:420:ASN:ND2	2.17	0.59
1:A:128:PRO:HB3	1:A:147:ASP:HA	1.85	0.58
1:A:384:THR:CG2	1:A:385:THR:N	2.66	0.58
1:B:335:THR:HG22	1:B:336:LYS:N	2.18	0.58
1:C:47:TYR:CD1	1:C:52:VAL:HG11	2.38	0.58
1:C:82:LYS:HD2	1:C:380:ASP:HB3	1.84	0.58
1:D:337:ASP:OD1	1:D:339:ASP:HB2	2.04	0.58
1:A:458:GLU:CD	1:A:490:THR:HG23	2.27	0.58
1:C:465:GLU:CD	1:C:465:GLU:H	2.12	0.58
1:D:140:GLY:O	1:D:141:GLU:HG3	2.03	0.58
1:A:101:ARG:HG2	2:A:546:HOH:O	2.03	0.58
1:A:391:LYS:HB3	1:A:445:LEU:O	2.04	0.58
1:B:157:ALA:O	1:B:160:GLU:HB2	2.04	0.58
1:C:85:LEU:C	1:C:85:LEU:HD23	2.29	0.58
1:C:186:VAL:HG23	1:C:221:VAL:O	2.04	0.58
1:A:75:PHE:HB2	1:A:447:ALA:CB	2.33	0.58
1:B:108:GLN:HE21	1:B:121:ILE:CD1	2.16	0.58
1:C:100:ASP:C	1:C:102:THR:H	2.12	0.58
1:C:116:GLU:O	1:C:117:ASN:HB2	2.03	0.58
1:D:416:ASP:OD2	1:D:420:ASN:HB2	2.04	0.58
1:D:453:ARG:NH2	2:D:515:HOH:O	2.35	0.58
1:B:477:PRO:O	1:B:479:THR:HG23	2.04	0.58
1:C:286:SER:OG	1:C:386:SER:HB3	2.04	0.58
1:D:275:ARG:HA	1:D:360:ILE:HD11	1.85	0.58
1:A:41:GLY:HA3	1:A:251:PHE:CD1	2.39	0.57
1:B:254:LEU:HB3	1:B:259:VAL:HG21	1.86	0.57
1:C:158:ILE:O	1:C:162:VAL:HG23	2.03	0.57
1:D:61:GLU:CG	1:D:62:SER:N	2.66	0.57
1:D:109:LEU:HD22	1:D:263:ALA:O	2.03	0.57
1:D:147:ASP:O	1:D:149:PRO:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TRP:HA	1:A:467:TRP:CZ3	2.38	0.57
1:C:140:GLY:O	1:C:141:GLU:HG3	2.04	0.57
1:D:275:ARG:NH1	1:D:326:ASP:HB2	2.19	0.57
1:A:60:ILE:HG13	1:A:61:GLU:N	2.20	0.57
1:B:418:GLU:HB2	1:B:420:ASN:ND2	2.19	0.57
1:C:279:VAL:HA	1:C:319:THR:O	2.03	0.57
1:C:337:ASP:OD1	1:C:339:ASP:HB2	2.04	0.57
1:C:498:THR:HG22	1:C:499:TYR:N	2.19	0.57
1:B:295:LYS:HE2	1:B:299:LYS:HZ1	1.68	0.57
1:A:498:THR:HG22	1:A:499:TYR:N	2.19	0.57
1:C:252:ASN:O	1:C:256:GLN:HB2	2.04	0.57
1:C:416:ASP:OD2	1:C:420:ASN:HB2	2.04	0.57
1:C:89:PRO:HD2	1:C:375:VAL:HG13	1.87	0.57
1:C:91:ASP:O	1:C:92:ILE:HG13	2.05	0.57
1:C:128:PRO:HB3	1:C:147:ASP:HA	1.87	0.57
1:C:175:LEU:HB2	1:C:351:PHE:CZ	2.40	0.57
1:D:128:PRO:HB3	1:D:147:ASP:HA	1.87	0.57
1:A:172:THR:HG22	1:A:174:THR:H	1.70	0.57
1:C:45:LEU:HD23	1:C:261:ASN:OD1	2.05	0.57
1:C:147:ASP:O	1:C:149:PRO:HD3	2.04	0.57
1:D:230:PHE:HB3	1:D:351:PHE:CE1	2.40	0.57
1:B:454:ILE:HG21	1:B:484:VAL:HG21	1.86	0.56
1:D:127:LYS:N	1:D:244:LEU:O	2.36	0.56
1:C:323:LEU:HD23	1:C:323:LEU:O	2.05	0.56
1:D:158:ILE:O	1:D:162:VAL:HG23	2.05	0.56
1:D:230:PHE:CE2	1:D:274:GLY:HA2	2.40	0.56
1:A:103:TYR:CD1	1:A:154:VAL:HG21	2.40	0.56
1:A:335:THR:HG22	1:A:337:ASP:N	2.10	0.56
1:B:128:PRO:HB3	1:B:147:ASP:HA	1.88	0.56
1:B:487:TRP:HH2	1:B:496:SER:HB3	1.68	0.56
1:C:396:LEU:HB2	1:C:441:THR:HG22	1.86	0.56
1:D:107:LEU:HD11	1:D:126:ARG:HH21	1.70	0.56
1:D:498:THR:HG22	1:D:499:TYR:N	2.19	0.56
1:A:477:PRO:O	1:A:479:THR:HG23	2.05	0.56
1:C:90:VAL:HA	1:C:374:ALA:HA	1.88	0.56
1:D:175:LEU:HB2	1:D:351:PHE:CE2	2.40	0.56
1:B:454:ILE:HD13	1:B:484:VAL:HG21	1.88	0.56
1:C:382:ILE:O	1:C:382:ILE:HG23	2.06	0.56
1:C:80:ARG:NH1	1:C:80:ARG:HG3	2.20	0.56
1:D:175:LEU:HB2	1:D:351:PHE:CZ	2.40	0.56
1:B:335:THR:HG22	1:B:336:LYS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:HB3	1:C:351:PHE:CE1	2.41	0.56
1:D:252:ASN:O	1:D:256:GLN:HB2	2.06	0.56
1:A:454:ILE:HG21	1:A:484:VAL:HG21	1.88	0.56
1:C:230:PHE:CE2	1:C:274:GLY:HA2	2.41	0.56
1:C:36:GLN:C	1:C:251:PHE:HB3	2.31	0.56
1:A:52:VAL:HG23	1:A:53:LEU:N	2.20	0.55
1:A:416:ASP:OD2	1:A:420:ASN:HB2	2.06	0.55
1:B:263:ALA:HB2	2:B:563:HOH:O	2.06	0.55
1:C:320:ALA:HB3	1:C:333:VAL:HB	1.89	0.55
1:A:92:ILE:HD12	1:A:362:TYR:O	2.06	0.55
1:C:98:VAL:HG12	1:C:358:TYR:CD1	2.41	0.55
1:D:60:ILE:CG2	1:D:61:GLU:N	2.69	0.55
1:B:416:ASP:OD2	1:B:420:ASN:HB2	2.06	0.55
1:C:479:THR:HB	1:C:500:ASN:O	2.07	0.55
1:A:108:GLN:HA	1:A:120:THR:O	2.06	0.55
1:A:322:VAL:H	1:A:331:ASN:ND2	2.03	0.55
1:A:487:TRP:HH2	1:A:496:SER:HB3	1.70	0.55
1:D:321:VAL:HG12	1:D:332:LYS:HA	1.89	0.55
1:C:86:THR:HG23	1:C:378:LYS:HG2	1.88	0.55
1:A:49:ARG:NH2	2:A:517:HOH:O	2.40	0.55
1:B:498:THR:HG22	1:B:499:TYR:N	2.21	0.55
1:C:198:VAL:HG21	1:C:203:LEU:HD21	1.88	0.55
1:A:87:THR:CG2	1:A:89:PRO:HD3	2.29	0.55
1:C:127:LYS:N	1:C:244:LEU:O	2.35	0.55
1:C:39:ASP:OD2	1:C:242:SER:N	2.39	0.55
1:D:186:VAL:HG23	1:D:221:VAL:O	2.06	0.55
1:D:303:ILE:O	1:D:306:SER:HB3	2.07	0.55
1:A:306:SER:HB3	1:A:308:GLN:HG3	1.88	0.54
1:B:204:GLU:O	1:B:208:GLY:HA2	2.07	0.54
1:C:97:SER:O	1:C:359:PRO:HD2	2.06	0.54
1:D:49:ARG:HB3	1:D:366:PHE:CE1	2.43	0.54
1:D:64:VAL:HG12	1:D:417:LYS:O	2.06	0.54
1:D:95:ILE:HG13	1:D:117:ASN:HD22	1.72	0.54
1:A:335:THR:CG2	1:A:337:ASP:H	2.11	0.54
1:C:175:LEU:HB2	1:C:351:PHE:CE2	2.41	0.54
1:D:179:THR:HB	2:D:562:HOH:O	2.06	0.54
1:A:428:TRP:HA	2:A:544:HOH:O	2.07	0.54
1:D:69:LYS:O	1:D:76:ILE:N	2.39	0.54
1:D:103:TYR:HB2	1:D:104:PRO:HD2	1.89	0.54
1:D:433:GLN:O	1:D:435:LYS:HG2	2.07	0.54
1:A:304:LYS:HD2	1:A:304:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASN:HA	1:C:391:LYS:HD2	1.88	0.54
1:C:308:GLN:HE21	1:C:312:ILE:HD11	1.71	0.54
1:D:57:GLY:HA3	1:D:378:LYS:O	2.07	0.54
1:D:309:TYR:HA	1:D:312:ILE:HD13	1.89	0.54
1:B:94:ILE:HD13	1:B:359:PRO:HB2	1.88	0.54
1:C:53:LEU:HG	1:C:114:LEU:HD23	1.88	0.54
1:D:39:ASP:OD2	1:D:39:ASP:N	2.41	0.54
1:D:198:VAL:HG21	1:D:203:LEU:HD21	1.88	0.54
1:A:47:TYR:CD1	1:A:52:VAL:HG11	2.42	0.54
1:C:98:VAL:HG12	1:C:358:TYR:CE1	2.43	0.54
1:A:470:VAL:HG11	1:A:486:ILE:HB	1.89	0.54
1:C:131:ILE:HG22	1:C:144:ILE:HG22	1.90	0.54
1:B:172:THR:HG22	1:B:174:THR:H	1.73	0.54
1:B:289:ASP:HB3	1:B:309:TYR:HE1	1.72	0.54
1:C:227:LYS:HZ1	1:C:361:SER:CB	2.21	0.54
1:D:105:GLY:N	1:D:268:VAL:O	2.36	0.54
1:D:328:GLN:O	1:D:331:ASN:HB2	2.08	0.54
1:D:109:LEU:HD22	1:D:263:ALA:HB1	1.90	0.54
1:A:110:ALA:HB2	1:A:266:LEU:HD21	1.91	0.53
1:D:465:GLU:H	1:D:465:GLU:CD	2.13	0.53
1:A:328:GLN:HG2	1:A:329:GLU:HG2	1.90	0.53
1:A:464:TRP:C	1:A:466:TRP:H	2.16	0.53
1:D:90:VAL:HG12	1:D:374:ALA:HB2	1.89	0.53
1:A:310:LYS:HE2	1:A:313:TYR:HD1	1.72	0.53
1:D:78:VAL:HG11	1:D:217:ASN:ND2	2.24	0.53
1:C:47:TYR:HB2	1:C:52:VAL:CG1	2.38	0.53
1:C:53:LEU:CD2	1:C:115:VAL:HG23	2.39	0.53
1:C:191:GLN:CA	1:C:379:THR:HG21	2.38	0.53
1:D:86:THR:HA	1:D:377:ASN:O	2.07	0.53
1:D:109:LEU:HD12	1:D:120:THR:HG21	1.89	0.53
1:A:396:LEU:HD11	1:A:443:ILE:HD11	1.90	0.53
2:A:541:HOH:O	1:C:462:LEU:HD22	2.08	0.53
1:D:479:THR:HB	1:D:500:ASN:O	2.08	0.53
1:C:83:ARG:N	1:C:381:TYR:O	2.40	0.53
1:A:63:PHE:O	1:A:65:PRO:HD3	2.08	0.53
1:C:110:ALA:HB2	1:C:266:LEU:CD2	2.38	0.53
1:C:217:ASN:HD21	1:C:384:THR:HB	1.74	0.53
1:A:474:TYR:O	1:C:295:LYS:NZ	2.42	0.52
1:D:67:GLU:HG2	1:D:69:LYS:HD3	1.90	0.52
1:B:141:GLU:HB3	1:B:164:LYS:HE2	1.92	0.52
1:D:369:ASP:OD2	1:D:371:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLU:HB2	1:C:385:THR:OG1	2.10	0.52
1:D:304:LYS:O	1:D:313:TYR:HE1	1.91	0.52
1:B:131:ILE:HD12	1:B:154:VAL:HG13	1.92	0.52
1:C:38:ILE:HD12	1:C:242:SER:HB3	1.91	0.52
1:C:148:ASP:H	1:C:153:LYS:HE2	1.75	0.52
1:C:265:PRO:HB2	1:C:367:LEU:HD12	1.91	0.52
1:A:484:VAL:HG22	1:A:497:ILE:HD12	1.92	0.52
1:C:433:GLN:O	1:C:435:LYS:HG2	2.10	0.52
1:B:59:LYS:HD2	1:B:59:LYS:N	2.24	0.52
1:B:89:PRO:HD2	1:B:375:VAL:O	2.10	0.52
1:B:396:LEU:HD11	1:B:443:ILE:HD11	1.91	0.52
1:C:53:LEU:HD22	1:C:115:VAL:CG2	2.40	0.52
1:C:280:LYS:O	1:C:318:PHE:HA	2.10	0.52
1:A:392:GLY:HA3	1:A:479:THR:O	2.10	0.52
1:B:60:ILE:HG23	1:B:60:ILE:O	2.09	0.52
1:B:335:THR:HG22	1:B:337:ASP:N	2.11	0.52
1:B:459:CYS:HA	1:B:467:TRP:CE2	2.45	0.52
1:B:179:THR:HA	1:B:227:LYS:O	2.10	0.52
1:C:89:PRO:C	1:C:91:ASP:N	2.62	0.52
1:A:350:THR:CG2	1:A:351:PHE:N	2.72	0.52
1:B:392:GLY:HA3	1:B:479:THR:O	2.10	0.52
1:C:53:LEU:HD21	1:C:111:ASP:O	2.10	0.52
1:A:38:ILE:HG12	1:A:254:LEU:HD11	1.90	0.51
1:C:95:ILE:HG23	1:C:117:ASN:HD22	1.75	0.51
1:C:369:ASP:OD2	1:C:371:SER:HB3	2.09	0.51
1:D:131:ILE:HG22	1:D:144:ILE:HG22	1.92	0.51
1:A:457:ARG:HD2	1:A:469:ASP:OD1	2.11	0.51
1:C:61:GLU:HG3	1:C:62:SER:N	2.26	0.51
1:C:310:LYS:NZ	1:C:314:GLU:HG3	2.25	0.51
1:B:107:LEU:CD1	1:B:126:ARG:HH21	2.22	0.51
1:B:464:TRP:HA	1:B:467:TRP:CZ3	2.45	0.51
1:C:302:ASP:OD1	1:C:302:ASP:N	2.42	0.51
1:D:110:ALA:HB2	1:D:266:LEU:CD2	2.36	0.51
1:D:148:ASP:H	1:D:153:LYS:HE2	1.74	0.51
1:D:265:PRO:HB2	1:D:367:LEU:HD12	1.92	0.51
1:D:308:GLN:CA	1:D:308:GLN:HE21	2.24	0.51
1:C:265:PRO:HG2	1:C:367:LEU:HD12	1.92	0.51
1:A:454:ILE:HD13	1:A:484:VAL:HG21	1.93	0.51
1:B:350:THR:CG2	1:B:351:PHE:N	2.73	0.51
1:D:63:PHE:N	1:D:63:PHE:HD2	2.09	0.51
1:D:358:TYR:HB3	1:D:359:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:HD12	1:A:476:VAL:O	2.11	0.51
1:B:293:ALA:HB2	1:B:309:TYR:CD1	2.46	0.51
1:C:100:ASP:HB3	1:C:102:THR:OG1	2.10	0.51
1:A:239:LYS:HG3	1:A:240:ASN:ND2	2.26	0.51
1:A:458:GLU:HG2	1:A:459:CYS:H	1.75	0.51
1:C:44:SER:HA	1:C:368:LYS:HZ1	1.73	0.51
1:D:148:ASP:CB	1:D:153:LYS:HE2	2.40	0.51
1:B:239:LYS:HG3	1:B:240:ASN:ND2	2.26	0.51
1:B:484:VAL:HG22	1:B:497:ILE:HD12	1.91	0.51
1:D:55:SER:OG	1:D:377:ASN:HA	2.10	0.51
1:A:491:LEU:HD22	1:C:176:PRO:CG	2.40	0.51
1:C:104:PRO:HD2	1:C:154:VAL:CG1	2.40	0.51
1:D:238:PRO:HG3	1:D:244:LEU:HG	1.93	0.51
1:B:458:GLU:O	1:B:467:TRP:HB3	2.11	0.51
1:C:80:ARG:HD3	1:C:384:THR:HG21	1.93	0.51
1:C:89:PRO:O	1:C:91:ASP:N	2.44	0.51
1:D:144:ILE:HB	1:D:161:LEU:HD21	1.93	0.51
1:A:141:GLU:HB3	1:A:164:LYS:HE2	1.92	0.50
1:A:407:GLU:HG3	1:A:432:TYR:CZ	2.46	0.50
1:A:470:VAL:HG22	1:A:493:PRO:CB	2.41	0.50
1:B:107:LEU:CG	1:B:126:ARG:HH21	2.24	0.50
1:C:80:ARG:HG2	1:C:384:THR:HG22	1.93	0.50
1:C:275:ARG:HA	1:C:360:ILE:HD11	1.93	0.50
1:B:55:SER:OG	1:B:377:ASN:HB2	2.11	0.50
1:C:39:ASP:CG	1:C:242:SER:H	2.18	0.50
1:C:41:GLY:O	1:C:45:LEU:HD12	2.11	0.50
1:B:83:ARG:HH22	1:D:421:GLU:CD	2.19	0.50
1:C:108:GLN:HB2	1:C:266:LEU:HD12	1.93	0.50
1:A:350:THR:HG22	1:A:351:PHE:N	2.25	0.50
1:B:498:THR:HG22	1:B:499:TYR:H	1.76	0.50
1:B:110:ALA:HB2	1:B:266:LEU:HD21	1.94	0.50
1:C:44:SER:HA	1:C:368:LYS:HZ2	1.74	0.50
1:C:47:TYR:HB2	1:C:52:VAL:HG11	1.94	0.50
1:C:321:VAL:HG23	1:C:321:VAL:O	2.11	0.50
1:D:398:HIS:CE1	1:D:400:GLY:H	2.30	0.50
1:D:230:PHE:HZ	1:D:275:ARG:NH1	2.10	0.50
1:D:270:ASN:O	1:D:362:TYR:HB2	2.12	0.50
1:A:37:SER:O	1:A:251:PHE:HB2	2.12	0.50
1:B:350:THR:HG22	1:B:351:PHE:N	2.26	0.50
1:B:452:ILE:HD12	1:B:476:VAL:O	2.12	0.50
1:C:95:ILE:HG23	1:C:117:ASN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LYS:NZ	1:C:361:SER:CB	2.75	0.50
1:D:150:THR:O	1:D:154:VAL:HG23	2.11	0.50
1:A:498:THR:HG22	1:A:499:TYR:H	1.76	0.50
1:A:85:LEU:HD23	1:A:86:THR:N	2.27	0.50
1:A:131:ILE:HD12	1:A:154:VAL:HG13	1.94	0.50
1:C:238:PRO:HG3	1:C:244:LEU:HG	1.93	0.50
1:C:295:LYS:HE2	1:C:299:LYS:NZ	2.27	0.50
1:D:50:ASN:HA	1:D:376:HIS:NE2	2.26	0.50
1:A:204:GLU:O	1:A:208:GLY:HA2	2.11	0.49
1:D:53:LEU:CD1	1:D:373:ALA:HB1	2.42	0.49
1:D:425:HIS:HE1	1:D:453:ARG:NH2	2.10	0.49
1:A:85:LEU:HD23	1:A:85:LEU:C	2.37	0.49
1:A:322:VAL:H	1:A:331:ASN:HD21	1.60	0.49
1:A:394:ILE:HD13	1:A:454:ILE:HD11	1.94	0.49
1:B:309:TYR:O	1:B:312:ILE:N	2.45	0.49
1:D:98:VAL:HG11	1:D:329:GLU:CG	2.41	0.49
1:D:107:LEU:CD2	1:D:267:MET:HB2	2.42	0.49
1:A:66:LYS:NZ	1:A:79:GLU:HG3	2.26	0.49
1:B:407:GLU:HG3	1:B:432:TYR:CZ	2.48	0.49
1:B:464:TRP:O	1:B:466:TRP:N	2.46	0.49
1:C:109:LEU:CD2	1:C:122:LEU:HD11	2.40	0.49
1:C:126:ARG:HG3	1:C:149:PRO:HD2	1.93	0.49
1:A:132:ASN:ND2	1:A:143:SER:OG	2.35	0.49
1:A:291:GLN:O	1:A:295:LYS:HG3	2.13	0.49
1:C:78:VAL:HG12	1:C:386:SER:OG	2.13	0.49
1:B:309:TYR:O	1:B:310:LYS:C	2.55	0.49
1:D:395:ASN:HD22	1:D:442:VAL:HG22	1.77	0.49
1:A:245:PHE:N	1:A:245:PHE:CD1	2.80	0.49
1:A:328:GLN:CG	1:A:329:GLU:HG2	2.42	0.49
1:A:407:GLU:HG3	1:A:432:TYR:OH	2.12	0.49
1:B:104:PRO:HG2	1:B:131:ILE:HD11	1.94	0.49
1:B:245:PHE:CD1	1:B:245:PHE:N	2.80	0.49
1:D:58:ASP:HB3	2:D:524:HOH:O	2.12	0.49
1:C:295:LYS:HE2	1:C:299:LYS:HZ3	1.78	0.49
1:C:377:ASN:ND2	1:C:378:LYS:H	2.10	0.49
1:C:497:ILE:HG23	1:C:497:ILE:O	2.12	0.49
1:D:66:LYS:HG3	1:D:79:GLU:HG2	1.94	0.49
1:A:131:ILE:HG12	1:A:233:VAL:CG1	2.42	0.49
1:C:38:ILE:HG13	1:C:39:ASP:H	1.77	0.49
1:C:98:VAL:HG21	1:C:329:GLU:CD	2.36	0.49
1:D:47:TYR:CE2	1:D:264:PRO:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:OD2	1:B:99:ASN:HB2	2.13	0.49
1:C:270:ASN:O	1:C:362:TYR:HB2	2.13	0.49
1:C:300:ASN:O	1:C:300:ASN:ND2	2.39	0.49
1:B:468:ARG:HB3	1:D:178:ARG:HA	1.94	0.49
1:C:255:LYS:HA	1:C:259:VAL:O	2.12	0.49
1:D:96:ASP:OD2	1:D:100:ASP:HB2	2.13	0.49
2:B:528:HOH:O	1:C:440:SER:HB3	2.12	0.48
1:C:91:ASP:HA	1:C:363:THR:HG22	1.95	0.48
1:C:144:ILE:HB	1:C:161:LEU:HD21	1.95	0.48
1:D:37:SER:O	1:D:38:ILE:C	2.56	0.48
1:D:303:ILE:HG22	1:D:309:TYR:CE2	2.48	0.48
1:D:446:GLU:OE1	1:D:446:GLU:HA	2.12	0.48
1:D:41:GLY:HA3	1:D:251:PHE:CZ	2.49	0.48
1:A:76:ILE:HD13	1:A:76:ILE:N	2.27	0.48
1:A:384:THR:CG2	1:A:385:THR:H	2.26	0.48
1:A:470:VAL:HG22	1:A:493:PRO:HB3	1.96	0.48
1:B:402:TYR:CD1	1:B:458:GLU:HG3	2.48	0.48
1:B:405:GLN:HG3	1:B:459:CYS:SG	2.54	0.48
1:C:91:ASP:C	1:C:92:ILE:HG13	2.39	0.48
1:C:288:LYS:HG3	1:C:289:ASP:OD2	2.14	0.48
1:D:265:PRO:HG2	1:D:367:LEU:HD12	1.95	0.48
1:A:82:LYS:HA	1:A:382:ILE:HG12	1.95	0.48
1:C:451:ASN:O	1:C:453:ARG:NH1	2.47	0.48
1:D:222:MET:HE3	1:D:224:LEU:HD21	1.96	0.48
1:C:105:GLY:N	1:C:268:VAL:O	2.46	0.48
1:C:150:THR:O	1:C:154:VAL:HG23	2.13	0.48
1:D:295:LYS:HE2	1:D:299:LYS:NZ	2.29	0.48
1:A:413:VAL:HG12	1:A:448:ASN:HB2	1.95	0.48
1:B:226:TYR:HB2	1:B:277:ILE:HB	1.96	0.48
1:D:308:GLN:HG3	1:D:309:TYR:N	2.29	0.48
1:D:201:LYS:N	1:D:201:LYS:HE2	2.28	0.48
1:A:226:TYR:HB2	1:A:277:ILE:HB	1.95	0.47
1:B:48:ASN:CG	1:B:51:GLU:HG2	2.39	0.47
1:B:275:ARG:HA	1:B:360:ILE:HD11	1.96	0.47
1:D:498:THR:CG2	1:D:499:TYR:N	2.77	0.47
1:A:418:GLU:HB2	1:A:420:ASN:HD21	1.79	0.47
1:B:108:GLN:HE21	1:B:121:ILE:HD13	1.79	0.47
1:B:335:THR:CG2	1:B:337:ASP:H	2.12	0.47
1:C:61:GLU:HG3	1:C:62:SER:H	1.80	0.47
1:C:148:ASP:CB	1:C:153:LYS:HE2	2.44	0.47
1:C:217:ASN:ND2	1:C:384:THR:CB	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:GLU:HG2	1:D:466:TRP:CZ3	2.49	0.47
1:A:275:ARG:HA	1:A:360:ILE:HD11	1.97	0.47
1:D:476:VAL:HG11	1:D:482:ILE:HD13	1.95	0.47
1:A:305:ASN:O	1:A:306:SER:C	2.58	0.47
1:C:60:ILE:O	1:C:82:LYS:NZ	2.36	0.47
1:C:76:ILE:CD1	1:C:388:GLU:HG3	2.45	0.47
1:C:300:ASN:HD22	1:C:300:ASN:C	2.20	0.47
1:C:300:ASN:ND2	1:C:300:ASN:C	2.73	0.47
1:C:394:ILE:HB	1:C:443:ILE:HB	1.97	0.47
1:A:179:THR:HA	1:A:227:LYS:O	2.15	0.47
1:A:491:LEU:CD2	1:C:176:PRO:HG2	2.44	0.47
1:B:54:ALA:HA	1:B:376:HIS:O	2.15	0.47
1:B:88:SER:N	1:B:89:PRO:HD3	2.30	0.47
1:B:116:GLU:O	1:B:118:ARG:HG2	2.15	0.47
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.80	0.47
1:C:98:VAL:HG13	1:C:324:GLY:O	2.15	0.47
1:C:222:MET:HE3	1:C:224:LEU:HD21	1.97	0.47
1:D:106:ALA:O	1:D:267:MET:HG3	2.15	0.47
1:D:283:THR:HB	1:D:316:SER:OG	2.14	0.47
1:D:487:TRP:NE1	1:D:494:GLY:HA3	2.29	0.47
1:C:267:MET:HG2	1:C:268:VAL:N	2.30	0.47
1:C:358:TYR:HB3	1:C:359:PRO:HD2	1.96	0.47
1:A:268:VAL:HG13	1:A:362:TYR:CD1	2.50	0.47
1:C:285:SER:HB3	1:C:312:ILE:HG23	1.96	0.47
1:C:375:VAL:HG22	1:C:376:HIS:N	2.30	0.47
1:D:451:ASN:O	1:D:453:ARG:NH1	2.48	0.47
1:B:295:LYS:NZ	1:D:474:TYR:O	2.48	0.47
1:C:86:THR:HG23	1:C:378:LYS:CG	2.45	0.47
1:C:498:THR:CG2	1:C:499:TYR:N	2.78	0.47
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.80	0.46
1:B:407:GLU:HG3	1:B:432:TYR:OH	2.13	0.46
1:D:48:ASN:O	1:D:52:VAL:HG22	2.15	0.46
1:D:224:LEU:HB2	1:D:279:VAL:HB	1.97	0.46
1:A:109:LEU:HB3	1:A:263:ALA:HB1	1.97	0.46
1:B:94:ILE:HD12	1:B:361:SER:HA	1.97	0.46
1:D:126:ARG:HG3	1:D:149:PRO:HD2	1.96	0.46
1:A:436:THR:O	1:A:437:ALA:C	2.57	0.46
1:B:413:VAL:HG12	1:B:448:ASN:HB2	1.98	0.46
1:C:95:ILE:CG2	1:C:117:ASN:HB3	2.45	0.46
1:C:227:LYS:NZ	1:C:361:SER:HB3	2.30	0.46
1:C:425:HIS:HE1	1:C:453:ARG:NH2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLU:O	1:A:118:ARG:HG2	2.16	0.46
1:A:429:ASP:C	1:A:431:ASN:H	2.24	0.46
1:B:75:PHE:HB2	1:B:447:ALA:HB3	1.96	0.46
1:C:60:ILE:HG13	1:C:61:GLU:N	2.31	0.46
1:B:487:TRP:N	1:B:494:GLY:O	2.48	0.46
1:C:48:ASN:O	1:C:52:VAL:HG22	2.16	0.46
1:C:108:GLN:HE21	1:C:121:ILE:HD11	1.80	0.46
1:C:446:GLU:OE1	1:C:446:GLU:HA	2.14	0.46
1:A:101:ARG:HB3	1:A:151:TYR:CG	2.50	0.46
1:D:92:ILE:O	1:D:361:SER:HA	2.16	0.46
1:D:339:ASP:O	1:D:342:ARG:HB2	2.16	0.46
1:A:186:VAL:HG13	1:A:192:ILE:HB	1.98	0.46
1:A:491:LEU:C	1:A:493:PRO:HD3	2.41	0.46
1:C:94:ILE:HG22	1:C:360:ILE:O	2.15	0.46
1:C:187:TYR:CE2	1:C:383:GLU:HG2	2.50	0.46
1:C:321:VAL:HA	1:C:331:ASN:O	2.16	0.46
1:C:476:VAL:HG11	1:C:482:ILE:HD13	1.96	0.46
1:B:418:GLU:HB2	1:B:420:ASN:HD21	1.80	0.46
1:C:201:LYS:HE2	1:C:201:LYS:N	2.31	0.46
1:D:64:VAL:O	1:D:80:ARG:HD2	2.16	0.46
1:D:270:ASN:HB2	1:D:363:THR:OG1	2.15	0.46
1:D:301:THR:O	1:D:304:LYS:HG3	2.16	0.46
1:B:101:ARG:NH1	1:B:101:ARG:HG2	2.31	0.45
1:B:168:LYS:HE2	1:B:169:TYR:OH	2.16	0.45
1:C:76:ILE:HD13	1:C:388:GLU:HA	1.97	0.45
1:C:290:VAL:HG22	1:C:312:ILE:HD13	1.98	0.45
1:A:306:SER:O	1:A:309:TYR:N	2.49	0.45
1:C:220:LYS:O	1:C:282:GLU:HA	2.16	0.45
1:C:224:LEU:HB2	1:C:279:VAL:HB	1.97	0.45
1:C:254:LEU:C	1:C:256:GLN:H	2.25	0.45
1:D:60:ILE:CG2	1:D:61:GLU:H	2.29	0.45
1:D:288:LYS:HG3	1:D:289:ASP:OD2	2.16	0.45
1:B:41:GLY:HA3	1:B:251:PHE:CD1	2.52	0.45
1:C:42:ILE:HD12	1:C:241:PRO:CB	2.46	0.45
1:C:78:VAL:HA	1:C:385:THR:O	2.16	0.45
1:C:398:HIS:CE1	1:C:400:GLY:H	2.34	0.45
1:D:38:ILE:O	1:D:42:ILE:HG13	2.17	0.45
1:B:436:THR:O	1:B:437:ALA:C	2.59	0.45
1:D:320:ALA:HB2	1:D:341:ILE:HD12	1.98	0.45
1:A:96:ASP:O	1:A:100:ASP:N	2.48	0.45
1:A:168:LYS:HE2	1:A:169:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:GLU:HG2	1:C:466:TRP:CZ3	2.52	0.45
1:D:148:ASP:H	1:D:153:LYS:CE	2.30	0.45
1:C:96:ASP:O	1:C:100:ASP:N	2.49	0.45
1:C:270:ASN:HB2	1:C:363:THR:OG1	2.17	0.45
1:D:306:SER:O	1:D:307:GLN:C	2.58	0.45
1:A:38:ILE:HG22	1:A:39:ASP:N	2.32	0.45
1:A:60:ILE:CG1	1:A:61:GLU:N	2.80	0.45
1:A:295:LYS:HE2	1:A:299:LYS:HZ1	1.78	0.45
1:B:42:ILE:CD1	1:B:241:PRO:HB3	2.47	0.45
1:B:94:ILE:HD12	1:B:361:SER:CA	2.46	0.45
1:C:395:ASN:HD22	1:C:442:VAL:HG22	1.80	0.45
1:A:85:LEU:HD21	1:A:87:THR:OG1	2.16	0.45
1:A:406:PHE:HB2	1:A:428:TRP:HZ3	1.80	0.45
1:B:429:ASP:C	1:B:431:ASN:H	2.25	0.45
1:D:320:ALA:HB2	1:D:341:ILE:HG23	1.99	0.45
1:A:108:GLN:O	1:A:266:LEU:HD12	2.17	0.45
1:B:47:TYR:O	1:B:47:TYR:CD1	2.69	0.45
1:B:186:VAL:HG13	1:B:192:ILE:HB	1.98	0.45
1:B:280:LYS:HB3	1:B:319:THR:HB	1.98	0.45
1:B:306:SER:C	1:B:308:GLN:N	2.73	0.45
1:C:47:TYR:HD1	1:C:52:VAL:HG11	1.81	0.45
1:C:227:LYS:HE3	1:C:360:ILE:CG2	2.47	0.45
1:A:110:ALA:HB2	1:A:266:LEU:CD2	2.47	0.45
1:B:384:THR:O	1:B:384:THR:HG22	2.17	0.45
1:C:312:ILE:O	1:C:316:SER:HB2	2.17	0.45
1:D:47:TYR:HB2	1:D:52:VAL:HG11	1.99	0.45
1:D:231:TYR:OH	1:D:357:ALA:HB3	2.17	0.45
1:D:91:ASP:OD2	1:D:361:SER:HB2	2.17	0.44
1:C:180:GLN:HB2	1:C:227:LYS:HB3	1.97	0.44
1:A:47:TYR:HD1	1:A:52:VAL:HG11	1.82	0.44
1:A:94:ILE:CD1	1:A:359:PRO:HB2	2.48	0.44
1:A:97:SER:HB3	1:A:358:TYR:HB3	1.99	0.44
1:A:109:LEU:CD2	1:A:122:LEU:HD21	2.37	0.44
1:A:416:ASP:OD1	1:A:418:GLU:N	2.51	0.44
1:D:156:GLY:O	1:D:159:ASP:HB2	2.16	0.44
1:D:255:LYS:HA	1:D:259:VAL:O	2.17	0.44
1:A:114:LEU:HD12	2:A:502:HOH:O	2.17	0.44
1:B:73:ASN:ND2	1:B:391:LYS:HE3	2.32	0.44
1:B:335:THR:HG21	1:B:337:ASP:HB3	2.00	0.44
1:B:394:ILE:HD13	1:B:454:ILE:HD11	1.99	0.44
1:C:49:ARG:NH2	1:C:369:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:TYR:CE1	1:C:323:LEU:HD22	2.47	0.44
1:C:457:ARG:HG2	1:C:467:TRP:HB2	2.00	0.44
1:A:69:LYS:HE3	1:A:69:LYS:HB3	1.85	0.44
1:A:295:LYS:HE2	1:A:299:LYS:HZ2	1.80	0.44
1:A:329:GLU:H	1:A:329:GLU:HG2	1.45	0.44
1:A:487:TRP:N	1:A:494:GLY:O	2.47	0.44
1:B:75:PHE:CB	1:B:447:ALA:HB3	2.48	0.44
1:B:406:PHE:HB2	1:B:428:TRP:HZ3	1.83	0.44
1:B:458:GLU:OE1	1:B:490:THR:HG23	2.17	0.44
1:C:339:ASP:O	1:C:342:ARG:HB2	2.17	0.44
1:D:393:LYS:HD2	2:D:512:HOH:O	2.18	0.44
1:B:83:ARG:NH2	1:D:421:GLU:OE1	2.48	0.44
1:B:268:VAL:HG13	1:B:362:TYR:CD1	2.53	0.44
1:D:254:LEU:C	1:D:256:GLN:H	2.24	0.44
1:D:425:HIS:CE1	1:D:453:ARG:NH2	2.85	0.44
1:A:232:THR:HG21	1:C:466:TRP:CD1	2.53	0.44
1:A:234:SER:HB3	1:A:270:ASN:OD1	2.18	0.44
1:A:327:ALA:HA	2:A:543:HOH:O	2.18	0.44
1:A:406:PHE:O	1:A:431:ASN:HA	2.17	0.44
1:A:465:GLU:HG3	1:A:466:TRP:CZ3	2.53	0.44
1:B:48:ASN:O	1:B:49:ARG:C	2.61	0.44
1:B:73:ASN:ND2	1:B:391:LYS:CE	2.80	0.44
1:B:416:ASP:OD1	1:B:418:GLU:N	2.50	0.44
1:C:303:ILE:CG1	1:C:304:LYS:N	2.80	0.44
1:D:267:MET:HG2	1:D:268:VAL:N	2.32	0.44
1:C:156:GLY:O	1:C:159:ASP:HB2	2.17	0.44
1:C:275:ARG:NH1	1:C:326:ASP:HB2	2.33	0.44
1:D:407:GLU:HB2	1:D:464:TRP:CH2	2.53	0.44
1:A:66:LYS:HZ1	1:A:79:GLU:HG3	1.83	0.44
1:A:244:LEU:HA	2:A:550:HOH:O	2.18	0.44
1:C:36:GLN:N	2:C:518:HOH:O	2.50	0.44
1:C:58:ASP:O	1:C:380:ASP:HB2	2.18	0.44
1:C:231:TYR:OH	1:C:357:ALA:HB3	2.18	0.44
1:D:126:ARG:HB2	1:D:244:LEU:O	2.18	0.44
1:B:303:ILE:HD13	1:B:303:ILE:N	2.33	0.43
1:B:457:ARG:HG3	1:B:468:ARG:O	2.18	0.43
1:C:254:LEU:C	1:C:256:GLN:N	2.76	0.43
1:A:101:ARG:O	1:A:151:TYR:CD1	2.71	0.43
1:A:425:HIS:CE1	1:A:453:ARG:NH2	2.86	0.43
1:B:49:ARG:O	1:B:52:VAL:HG22	2.17	0.43
1:B:87:THR:C	1:B:89:PRO:HD3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:GLY:HA3	1:C:251:PHE:CD1	2.54	0.43
1:D:96:ASP:HB2	1:D:100:ASP:HB3	2.00	0.43
1:D:180:GLN:HB2	1:D:227:LYS:HB3	1.99	0.43
1:D:254:LEU:C	1:D:256:GLN:N	2.76	0.43
1:D:310:LYS:O	1:D:314:GLU:HB2	2.19	0.43
1:D:335:THR:CG2	1:D:336:LYS:H	2.30	0.43
1:A:192:ILE:HG23	1:A:193:SER:N	2.34	0.43
1:D:36:GLN:C	1:D:251:PHE:HB3	2.43	0.43
1:D:98:VAL:HG11	1:D:329:GLU:HG3	2.00	0.43
1:D:226:TYR:HB2	1:D:277:ILE:HB	1.99	0.43
1:D:497:ILE:HG23	1:D:497:ILE:O	2.18	0.43
1:A:172:THR:CG2	1:A:174:THR:H	2.31	0.43
1:B:189:LYS:O	1:B:193:SER:HB3	2.19	0.43
1:C:90:VAL:HA	1:C:374:ALA:CB	2.48	0.43
1:D:96:ASP:CB	1:D:100:ASP:CB	2.97	0.43
1:A:238:PRO:HB2	1:A:243:ASP:HB2	2.01	0.43
1:B:101:ARG:HG2	1:B:101:ARG:HH11	1.83	0.43
1:B:131:ILE:HG12	1:B:233:VAL:CG1	2.46	0.43
1:B:491:LEU:C	1:B:493:PRO:HD3	2.42	0.43
1:C:66:LYS:HG3	1:C:79:GLU:CG	2.38	0.43
1:C:90:VAL:HA	1:C:374:ALA:CA	2.48	0.43
1:C:148:ASP:H	1:C:153:LYS:CE	2.32	0.43
1:C:187:TYR:CZ	1:C:383:GLU:HG2	2.53	0.43
1:D:263:ALA:N	1:D:264:PRO:HD3	2.34	0.43
1:A:180:GLN:HB2	1:A:227:LYS:HB3	1.99	0.43
1:B:94:ILE:HD12	1:B:361:SER:N	2.33	0.43
1:B:172:THR:CG2	1:B:174:THR:H	2.32	0.43
1:C:108:GLN:HE21	1:C:121:ILE:CD1	2.32	0.43
1:C:265:PRO:HB2	1:C:367:LEU:CD1	2.48	0.43
1:B:275:ARG:NH2	1:B:350:THR:O	2.52	0.43
1:B:457:ARG:CZ	1:D:180:GLN:NE2	2.82	0.43
1:C:122:LEU:HD22	1:C:257:LYS:CB	2.49	0.43
1:C:275:ARG:HH11	1:C:326:ASP:HB2	1.84	0.43
1:C:310:LYS:HZ3	1:C:314:GLU:HG3	1.84	0.43
1:C:407:GLU:HB2	1:C:464:TRP:CH2	2.54	0.43
1:B:407:GLU:HB3	1:B:455:LYS:HB3	2.01	0.43
1:B:456:ALA:O	1:B:470:VAL:N	2.47	0.43
1:B:457:ARG:HG3	1:B:468:ARG:C	2.44	0.43
1:C:263:ALA:N	1:C:264:PRO:HD3	2.34	0.43
1:D:73:ASN:O	1:D:73:ASN:CG	2.60	0.43
1:D:95:ILE:HG13	1:D:117:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LYS:O	1:D:282:GLU:HA	2.19	0.43
1:D:312:ILE:HD12	1:D:312:ILE:N	2.28	0.43
1:A:75:PHE:O	1:A:389:TYR:HB2	2.19	0.43
1:B:47:TYR:CD1	1:B:47:TYR:C	2.97	0.43
1:B:406:PHE:O	1:B:431:ASN:HA	2.19	0.43
1:D:109:LEU:HD12	1:D:120:THR:CG2	2.49	0.43
1:B:199:ASN:HB3	1:B:202:VAL:HG23	2.01	0.42
1:B:425:HIS:CE1	1:B:453:ARG:NH2	2.87	0.42
1:B:488:GLY:N	2:B:525:HOH:O	2.45	0.42
1:C:425:HIS:CE1	1:C:453:ARG:NH2	2.87	0.42
1:C:487:TRP:NE1	1:C:494:GLY:HA3	2.34	0.42
1:A:408:VAL:N	1:A:431:ASN:HD21	2.17	0.42
1:B:83:ARG:NH1	1:D:421:GLU:OE1	2.51	0.42
1:B:108:GLN:HA	1:B:120:THR:O	2.19	0.42
1:C:122:LEU:HD22	1:C:257:LYS:HB2	2.00	0.42
1:D:215:ALA:C	1:D:217:ASN:H	2.26	0.42
1:D:487:TRP:HH2	1:D:496:SER:HB3	1.83	0.42
1:D:56:ASN:HD22	1:D:57:GLY:N	2.18	0.42
1:A:483:ASN:O	1:A:497:ILE:HA	2.19	0.42
1:B:360:ILE:HD13	1:B:360:ILE:HA	1.80	0.42
1:D:61:GLU:CD	1:D:62:SER:H	2.27	0.42
1:D:172:THR:HG22	1:D:173:HIS:N	2.34	0.42
1:A:58:ASP:OD2	1:A:58:ASP:N	2.50	0.42
1:A:407:GLU:HB3	1:A:455:LYS:HB3	2.01	0.42
1:B:302:ASP:C	1:B:303:ILE:HD13	2.45	0.42
1:C:107:LEU:CD1	1:C:126:ARG:HH21	2.25	0.42
1:C:204:GLU:HA	1:C:209:VAL:H	1.85	0.42
1:D:273:TYR:HA	1:D:358:TYR:O	2.19	0.42
1:B:180:GLN:HB2	1:B:227:LYS:HB3	2.01	0.42
1:B:289:ASP:O	1:B:290:VAL:C	2.62	0.42
1:A:144:ILE:HG21	1:A:157:ALA:HB1	2.02	0.42
1:B:212:ASN:O	1:B:213:ALA:C	2.62	0.42
1:B:230:PHE:CE2	1:B:274:GLY:HA2	2.54	0.42
1:B:291:GLN:O	1:B:295:LYS:HG3	2.20	0.42
1:C:303:ILE:CG1	1:C:304:LYS:H	2.33	0.42
1:D:53:LEU:HD11	1:D:373:ALA:HB1	2.01	0.42
1:D:107:LEU:HD23	1:D:267:MET:HB2	2.01	0.42
1:D:478:LEU:HD22	2:D:534:HOH:O	2.20	0.42
1:A:107:LEU:O	1:A:121:ILE:HA	2.19	0.42
1:A:230:PHE:CE2	1:A:274:GLY:HA2	2.55	0.42
1:A:464:TRP:O	1:A:466:TRP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:GLY:HA3	1:C:251:PHE:CE1	2.55	0.42
1:C:273:TYR:HA	1:C:358:TYR:O	2.19	0.42
1:D:173:HIS:HB2	1:D:353:THR:OG1	2.20	0.42
1:A:231:TYR:CD2	1:A:231:TYR:C	2.97	0.42
1:D:199:ASN:OD1	1:D:201:LYS:HG2	2.20	0.42
1:A:407:GLU:HA	1:A:431:ASN:ND2	2.35	0.42
1:B:238:PRO:HB2	1:B:243:ASP:HB2	2.01	0.42
1:C:126:ARG:HB2	1:C:244:LEU:O	2.20	0.42
1:C:407:GLU:HG3	1:C:432:TYR:OH	2.20	0.42
1:D:295:LYS:HA	1:D:298:ILE:HD12	2.02	0.42
1:A:52:VAL:HG21	1:A:366:PHE:CZ	2.54	0.41
1:A:52:VAL:CG2	1:A:53:LEU:N	2.83	0.41
1:B:219:LYS:HE2	1:B:282:GLU:OE2	2.19	0.41
1:C:215:ALA:C	1:C:217:ASN:H	2.27	0.41
1:C:226:TYR:HB2	1:C:277:ILE:HB	2.02	0.41
1:C:259:VAL:HG13	1:C:265:PRO:CD	2.41	0.41
1:C:265:PRO:CG	1:C:367:LEU:HD12	2.50	0.41
1:D:394:ILE:HB	1:D:443:ILE:HB	2.01	0.41
1:B:61:GLU:O	1:B:61:GLU:CG	2.68	0.41
1:C:500:ASN:ND2	2:C:525:HOH:O	2.54	0.41
1:D:258:GLY:O	1:D:263:ALA:HB3	2.20	0.41
1:D:457:ARG:HG2	1:D:467:TRP:HB2	2.01	0.41
1:A:289:ASP:O	1:A:290:VAL:C	2.63	0.41
1:B:110:ALA:HB2	1:B:266:LEU:CD2	2.50	0.41
1:B:192:ILE:HG23	1:B:193:SER:N	2.34	0.41
1:D:122:LEU:HD22	1:D:257:LYS:CB	2.50	0.41
1:D:310:LYS:HE2	1:D:310:LYS:HA	2.02	0.41
1:A:308:GLN:O	1:A:312:ILE:HG13	2.20	0.41
1:A:453:ARG:HH11	1:A:453:ARG:HG2	1.85	0.41
1:C:172:THR:HG22	1:C:173:HIS:N	2.36	0.41
1:C:274:GLY:O	1:C:360:ILE:HD11	2.21	0.41
1:C:295:LYS:HA	1:C:298:ILE:HD12	2.01	0.41
1:D:122:LEU:HD22	1:D:257:LYS:HB2	2.02	0.41
1:D:339:ASP:O	1:D:342:ARG:N	2.54	0.41
1:A:74:LYS:NZ	1:A:388:GLU:HG2	2.36	0.41
1:A:83:ARG:HB3	1:A:381:TYR:CZ	2.55	0.41
1:A:94:ILE:HD12	1:A:359:PRO:HB2	2.03	0.41
1:A:103:TYR:HB2	1:A:104:PRO:HD2	2.01	0.41
1:B:108:GLN:HE21	1:B:121:ILE:HD11	1.86	0.41
1:C:52:VAL:HG21	1:C:366:PHE:CZ	2.55	0.41
1:C:92:ILE:HG21	1:C:362:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HB	1:A:450:ARG:HD3	2.02	0.41
1:B:413:VAL:HB	1:B:450:ARG:HD3	2.02	0.41
1:D:476:VAL:CG1	1:D:482:ILE:HD13	2.50	0.41
1:B:38:ILE:HA	1:B:251:PHE:HB2	2.01	0.41
1:B:290:VAL:O	1:B:291:GLN:C	2.62	0.41
1:C:61:GLU:OE1	1:C:61:GLU:CA	2.66	0.41
1:C:108:GLN:HB2	1:C:266:LEU:CD1	2.50	0.41
1:C:325:GLY:HA2	1:C:358:TYR:HD1	1.86	0.41
1:C:377:ASN:CG	1:C:378:LYS:N	2.78	0.41
1:D:50:ASN:HA	1:D:376:HIS:CE1	2.56	0.41
1:D:108:GLN:HA	1:D:120:THR:O	2.21	0.41
1:D:204:GLU:HA	1:D:209:VAL:H	1.85	0.41
1:A:50:ASN:HA	1:A:376:HIS:NE2	2.35	0.41
1:A:189:LYS:O	1:A:193:SER:HB3	2.20	0.41
1:A:335:THR:HG21	1:A:337:ASP:HB3	2.02	0.41
1:B:198:VAL:HG11	1:B:278:TYR:CE2	2.56	0.41
1:C:407:GLU:HG3	1:C:432:TYR:CE2	2.56	0.41
1:D:78:VAL:HG22	1:D:386:SER:HB2	2.02	0.41
1:D:265:PRO:HB2	1:D:367:LEU:CD1	2.51	0.41
1:D:444:PRO:HD2	2:D:503:HOH:O	2.21	0.41
1:A:309:TYR:HA	1:A:312:ILE:HD12	2.02	0.41
1:C:105:GLY:HA2	1:C:267:MET:CG	2.51	0.41
1:C:222:MET:CE	1:C:281:LEU:HD13	2.51	0.41
1:D:96:ASP:CB	1:D:100:ASP:HB3	2.51	0.41
1:D:132:ASN:O	1:D:233:VAL:HA	2.21	0.41
1:D:274:GLY:O	1:D:360:ILE:HD11	2.21	0.41
1:B:337:ASP:OD1	1:B:339:ASP:HB2	2.20	0.41
1:B:351:PHE:CD1	1:B:351:PHE:C	2.98	0.41
1:C:64:VAL:CB	1:C:80:ARG:NH1	2.80	0.41
1:D:307:GLN:O	1:D:310:LYS:HB2	2.21	0.41
1:D:335:THR:CG2	1:D:336:LYS:N	2.80	0.41
1:B:144:ILE:HG21	1:B:157:ALA:HB1	2.03	0.40
1:B:212:ASN:O	1:B:215:ALA:N	2.54	0.40
1:C:310:LYS:HE2	1:C:313:TYR:HB2	2.03	0.40
1:C:154:VAL:O	1:C:158:ILE:HG13	2.21	0.40
1:C:191:GLN:N	1:C:379:THR:HG21	2.35	0.40
1:D:238:PRO:CB	1:D:243:ASP:HB2	2.52	0.40
1:D:417:LYS:HB2	1:D:417:LYS:NZ	2.36	0.40
1:B:42:ILE:HD12	1:B:241:PRO:CB	2.51	0.40
1:B:42:ILE:C	1:B:44:SER:H	2.30	0.40
1:B:83:ARG:HG3	1:B:383:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:OE1	1:C:348:ASN:O	2.39	0.40
1:C:365:VAL:HG13	1:C:370:ASN:C	2.47	0.40
1:D:53:LEU:HD23	1:D:53:LEU:HA	1.95	0.40
1:D:109:LEU:CD2	1:D:263:ALA:O	2.69	0.40
1:D:465:GLU:HG2	1:D:466:TRP:CE3	2.56	0.40
1:D:470:VAL:HG12	1:D:495:SER:HB3	2.04	0.40
1:B:497:ILE:HG23	1:B:497:ILE:O	2.21	0.40
1:C:132:ASN:O	1:C:233:VAL:HA	2.21	0.40
1:C:189:LYS:HA	1:C:211:PHE:CE2	2.57	0.40
1:C:199:ASN:OD1	1:C:201:LYS:HG2	2.21	0.40
1:C:338:PHE:O	1:C:341:ILE:HB	2.22	0.40
1:A:335:THR:CG2	1:A:336:LYS:N	2.83	0.40
1:A:368:LYS:NZ	2:A:551:HOH:O	2.44	0.40
1:B:91:ASP:C	1:B:92:ILE:HD12	2.46	0.40
1:B:477:PRO:HG2	1:B:499:TYR:CE2	2.57	0.40
1:B:482:ILE:HG23	1:B:497:ILE:HD11	2.04	0.40
1:C:79:GLU:HB2	1:C:385:THR:HG1	1.87	0.40
1:C:335:THR:CG2	1:C:336:LYS:N	2.82	0.40
1:C:476:VAL:CG1	1:C:482:ILE:HD13	2.51	0.40
1:D:228:GLN:OE1	1:D:348:ASN:O	2.40	0.40
1:D:297:LEU:HD21	1:D:318:PHE:CZ	2.56	0.40
1:D:411:ASP:O	1:D:449:ALA:HA	2.22	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	463/471 (98%)	421 (91%)	35 (8%)	7 (2%)	8	28
1	B	463/471 (98%)	417 (90%)	39 (8%)	7 (2%)	8	28
1	C	463/471 (98%)	416 (90%)	41 (9%)	6 (1%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	463/471 (98%)	424 (92%)	31 (7%)	8 (2%)	7	26
All	All	1852/1884 (98%)	1678 (91%)	146 (8%)	28 (2%)	8	28

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	B	58	ASP
1	D	38	ILE
1	D	62	SER
1	A	465	GLU
1	B	465	GLU
1	D	438	HIS
1	A	416	ASP
1	B	416	ASP
1	C	90	VAL
1	C	368	LYS
1	C	437	ALA
1	C	438	HIS
1	D	368	LYS
1	D	437	ALA
1	A	437	ALA
1	B	437	ALA
1	D	307	GLN
1	A	330	HIS
1	B	65	PRO
1	C	141	GLU
1	D	106	ALA
1	D	141	GLU
1	A	430	GLY
1	C	38	ILE
1	A	290	VAL
1	B	290	VAL
1	B	430	GLY

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	412/418 (99%)	367 (89%)	45 (11%)	6	20
1	B	412/418 (99%)	371 (90%)	41 (10%)	7	24
1	C	412/418 (99%)	349 (85%)	63 (15%)	3	9
1	D	412/418 (99%)	363 (88%)	49 (12%)	5	16
All	All	1648/1672 (99%)	1450 (88%)	198 (12%)	5	16

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	58	ASP
1	A	66	LYS
1	A	67	GLU
1	A	69	LYS
1	A	76	ILE
1	A	84	SER
1	A	90	VAL
1	A	108	GLN
1	A	112	LYS
1	A	130	ASN
1	A	132	ASN
1	A	153	LYS
1	A	159	ASP
1	A	171	SER
1	A	183	GLU
1	A	206	SER
1	A	239	LYS
1	A	245	PHE
1	A	266	LEU
1	A	284	THR
1	A	286	SER
1	A	288	LYS
1	A	304	LYS
1	A	308	GLN
1	A	328	GLN
1	A	329	GLU
1	A	331	ASN
1	A	346	LYS
1	A	360	ILE
1	A	363	THR

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Mol	Chain	Res	Type
1	A	370	ASN
1	A	385	THR
1	A	388	GLU
1	A	390	SER
1	A	391	LYS
1	A	393	LYS
1	A	398	HIS
1	A	414	SER
1	A	450	ARG
1	A	457	ARG
1	A	458	GLU
1	A	462	LEU
1	A	465	GLU
1	A	468	ARG
1	B	49	ARG
1	B	52	VAL
1	B	59	LYS
1	B	60	ILE
1	B	79	GLU
1	B	82	LYS
1	B	87	THR
1	B	93	SER
1	B	94	ILE
1	B	101	ARG
1	B	108	GLN
1	B	112	LYS
1	B	130	ASN
1	B	132	ASN
1	B	153	LYS
1	B	159	ASP
1	B	171	SER
1	B	183	GLU
1	B	239	LYS
1	B	245	PHE
1	B	266	LEU
1	B	284	THR
1	B	286	SER
1	B	288	LYS
1	B	326	ASP
1	B	346	LYS
1	B	360	ILE
1	B	363	THR

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Mol	Chain	Res	Type
1	B	370	ASN
1	B	375	VAL
1	B	377	ASN
1	B	383	GLU
1	B	384	THR
1	B	385	THR
1	B	387	THR
1	B	393	LYS
1	B	398	HIS
1	B	414	SER
1	B	450	ARG
1	B	457	ARG
1	B	458	GLU
1	C	38	ILE
1	C	45	LEU
1	C	49	ARG
1	C	52	VAL
1	C	53	LEU
1	C	56	ASN
1	C	58	ASP
1	C	64	VAL
1	C	69	LYS
1	C	70	LYS
1	C	74	LYS
1	C	79	GLU
1	C	84	SER
1	C	85	LEU
1	C	86	THR
1	C	93	SER
1	C	96	ASP
1	C	100	ASP
1	C	112	LYS
1	C	126	ARG
1	C	130	ASN
1	C	131	ILE
1	C	132	ASN
1	C	163	SER
1	C	171	SER
1	C	186	VAL
1	C	194	SER
1	C	218	GLU
1	C	232	THR

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Mol	Chain	Res	Type
1	C	239	LYS
1	C	243	ASP
1	C	266	LEU
1	C	286	SER
1	C	299	LYS
1	C	300	ASN
1	C	302	ASP
1	C	304	LYS
1	C	306	SER
1	C	308	GLN
1	C	310	LYS
1	C	311	ASP
1	C	312	ILE
1	C	317	SER
1	C	326	ASP
1	C	346	LYS
1	C	370	ASN
1	C	378	LYS
1	C	379	THR
1	C	382	ILE
1	C	384	THR
1	C	386	SER
1	C	387	THR
1	C	390	SER
1	C	393	LYS
1	C	398	HIS
1	C	414	SER
1	C	418	GLU
1	C	440	SER
1	C	450	ARG
1	C	457	ARG
1	C	465	GLU
1	C	468	ARG
1	C	475	ASP
1	D	39	ASP
1	D	43	SER
1	D	44	SER
1	D	49	ARG
1	D	62	SER
1	D	63	PHE
1	D	64	VAL
1	D	69	LYS

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Mol	Chain	Res	Type
1	D	73	ASN
1	D	101	ARG
1	D	108	GLN
1	D	112	LYS
1	D	126	ARG
1	D	130	ASN
1	D	131	ILE
1	D	132	ASN
1	D	163	SER
1	D	171	SER
1	D	186	VAL
1	D	194	SER
1	D	218	GLU
1	D	219	LYS
1	D	232	THR
1	D	239	LYS
1	D	243	ASP
1	D	266	LEU
1	D	286	SER
1	D	299	LYS
1	D	305	ASN
1	D	306	SER
1	D	308	GLN
1	D	311	ASP
1	D	328	GLN
1	D	330	HIS
1	D	346	LYS
1	D	370	ASN
1	D	375	VAL
1	D	383	GLU
1	D	393	LYS
1	D	398	HIS
1	D	414	SER
1	D	418	GLU
1	D	440	SER
1	D	446	GLU
1	D	450	ARG
1	D	457	ARG
1	D	465	GLU
1	D	468	ARG
1	D	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	108	GLN
1	A	132	ASN
1	A	197	ASN
1	A	205	ASN
1	A	217	ASN
1	A	240	ASN
1	A	307	GLN
1	A	315	ASN
1	A	328	GLN
1	A	331	ASN
1	A	355	ASN
1	A	370	ASN
1	A	395	ASN
1	A	420	ASN
1	A	433	GLN
1	A	451	ASN
1	A	483	ASN
1	A	500	ASN
1	B	50	ASN
1	B	73	ASN
1	B	81	GLN
1	B	108	GLN
1	B	132	ASN
1	B	166	ASN
1	B	173	HIS
1	B	197	ASN
1	B	240	ASN
1	B	308	GLN
1	B	355	ASN
1	B	370	ASN
1	B	376	HIS
1	B	395	ASN
1	B	420	ASN
1	B	433	GLN
1	B	451	ASN
1	B	483	ASN
1	B	500	ASN
1	C	48	ASN
1	C	99	ASN
1	C	108	GLN
1	C	117	ASN

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Mol	Chain	Res	Type
1	C	197	ASN
1	C	205	ASN
1	C	217	ASN
1	C	240	ASN
1	C	308	GLN
1	C	315	ASN
1	C	370	ASN
1	C	377	ASN
1	C	395	ASN
1	C	420	ASN
1	C	483	ASN
1	C	500	ASN
1	D	56	ASN
1	D	73	ASN
1	D	99	ASN
1	D	108	GLN
1	D	117	ASN
1	D	180	GLN
1	D	197	ASN
1	D	205	ASN
1	D	217	ASN
1	D	240	ASN
1	D	308	GLN
1	D	331	ASN
1	D	348	ASN
1	D	370	ASN
1	D	395	ASN
1	D	420	ASN
1	D	483	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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.