



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:27 PM UTC

PDB ID : 1J0C / pdb_00001j0c
Title : ACC deaminase mutated to catalytic residue
Authors : Ose, T.; Fujino, A.; Yao, M.; Honma, M.; Tanaka, I.
Deposited on : 2002-11-12
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

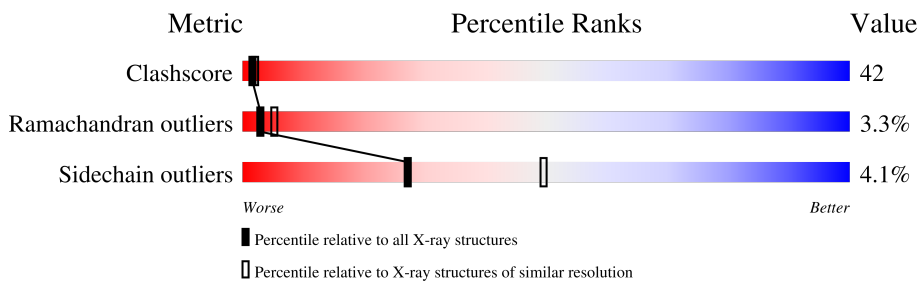
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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	341	37% 55% 8%
1	B	341	32% 60% 8% .
1	C	341	47% 49% .
1	D	341	45% 49% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10853 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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			
1	B	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			
1	C	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			
1	D	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	SER	engineered mutation	UNP Q7M523
A	51	THR	LYS	engineered mutation	UNP Q7M523
B	1	ALA	SER	engineered mutation	UNP Q7M523
B	51	THR	LYS	engineered mutation	UNP Q7M523
C	1	ALA	SER	engineered mutation	UNP Q7M523
C	51	THR	LYS	engineered mutation	UNP Q7M523
D	1	ALA	SER	engineered mutation	UNP Q7M523
D	51	THR	LYS	engineered mutation	UNP Q7M523

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

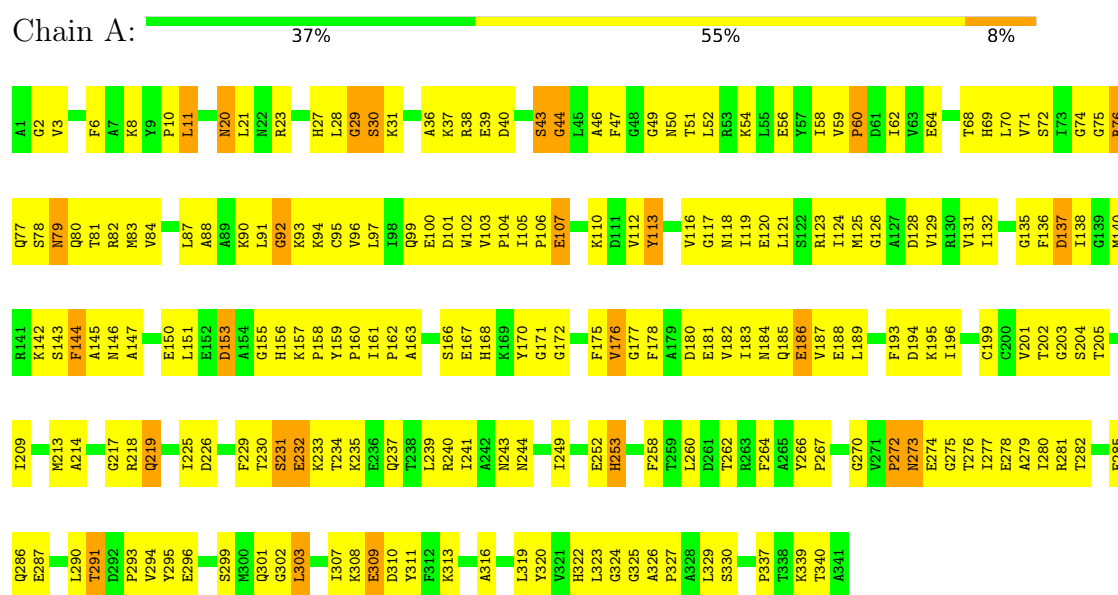
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	44	Total	O	0	0
			44	44		
3	C	132	Total	O	0	0
			132	132		
3	D	150	Total	O	0	0
			150	150		

3 Residue-property plots

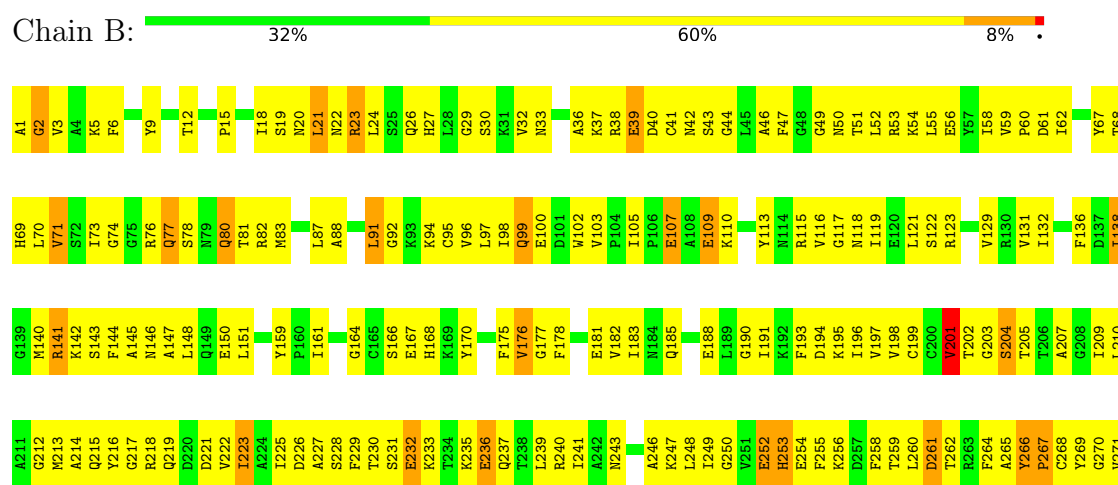
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

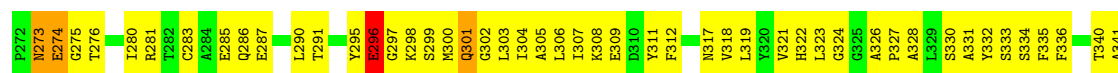
Note EDS was not executed.

• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



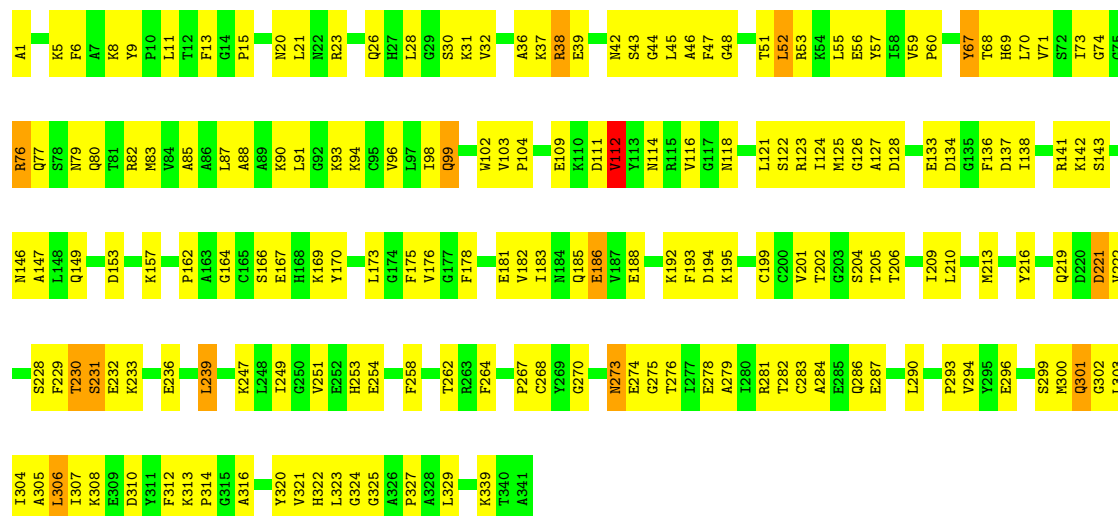
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





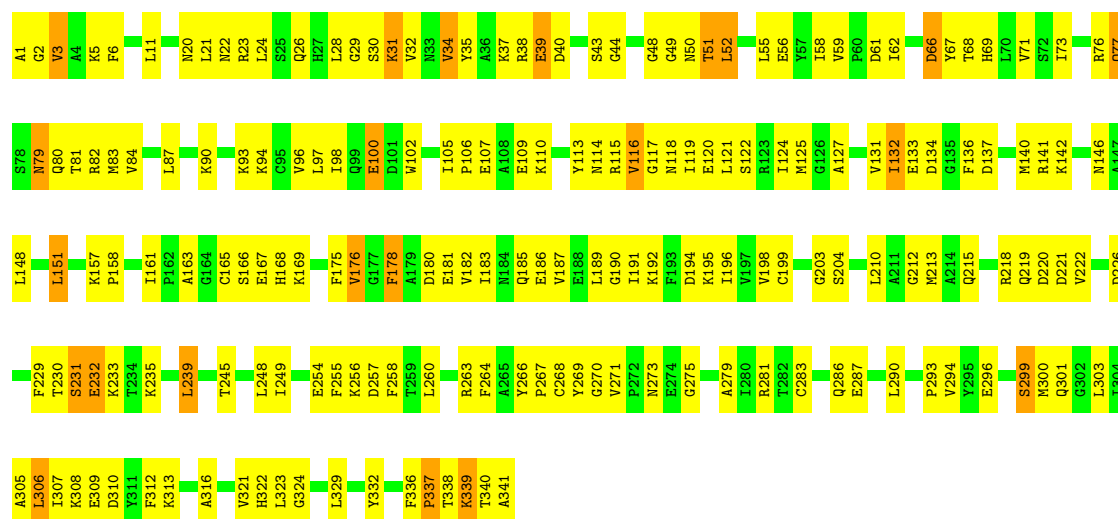
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain C: 47% 49% .



• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain D: 45% 49% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.17Å 268.26Å 186.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.75	Depositor
% Data completeness (in resolution range)	99.9 (10.00-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10853	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: PLP

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	0/2656	0.96	11/3593 (0.3%)
1	B	0.40	0/2656	0.97	9/3593 (0.3%)
1	C	0.49	0/2656	1.03	12/3593 (0.3%)
1	D	0.49	0/2656	1.05	14/3593 (0.4%)
All	All	0.45	0/10624	1.00	46/14372 (0.3%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	VAL	N-CA-C	-8.53	101.92	110.62
1	C	230	THR	N-CA-C	-8.40	100.45	111.71
1	D	176	VAL	N-CA-C	-8.35	100.66	111.09
1	B	3	VAL	N-CA-C	-8.19	100.95	113.16
1	A	176	VAL	N-CA-C	-7.87	101.25	111.09
1	D	161	ILE	CA-C-N	7.73	129.50	119.84
1	D	161	ILE	C-N-CA	7.73	129.50	119.84
1	A	203	GLY	N-CA-C	7.67	124.89	114.92
1	C	133	GLU	N-CA-C	7.63	122.17	113.02
1	C	294	VAL	N-CA-C	7.10	117.91	111.81
1	D	43	SER	N-CA-C	6.98	119.94	108.99
1	D	39	GLU	N-CA-C	-6.65	104.65	112.89
1	D	203	GLY	N-CA-C	6.64	124.54	115.30
1	B	39	GLU	N-CA-C	-6.54	105.12	113.23
1	C	176	VAL	N-CA-C	-6.54	102.68	111.44
1	C	38	ARG	N-CA-C	6.44	119.62	109.39
1	D	3	VAL	N-CA-C	-6.43	107.23	113.53
1	D	263	ARG	N-CA-C	6.41	120.70	113.01
1	C	222	VAL	N-CA-C	6.17	117.68	108.54
1	C	186	GLU	N-CA-C	-6.00	104.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASN	N-CA-C	-5.93	104.20	112.45
1	A	95	CYS	N-CA-C	5.91	118.44	107.99
1	A	153	ASP	N-CA-C	-5.89	105.75	113.12
1	D	307	ILE	N-CA-C	-5.89	105.38	110.74
1	A	39	GLU	N-CA-C	-5.86	105.89	113.16
1	D	79	ASN	N-CA-C	-5.75	106.39	113.41
1	D	299	SER	N-CA-C	-5.74	105.16	111.82
1	A	40	ASP	N-CA-C	-5.63	106.63	112.93
1	D	34	VAL	N-CA-C	5.60	116.80	108.23
1	A	44	GLY	N-CA-C	-5.57	106.11	115.80
1	B	80	GLN	N-CA-C	5.52	116.98	110.97
1	D	178	PHE	N-CA-C	-5.48	104.95	111.69
1	A	186	GLU	N-CA-C	-5.46	105.33	111.28
1	C	44	GLY	N-CA-C	-5.40	106.65	115.46
1	B	177	GLY	N-CA-C	-5.38	107.65	114.16
1	B	266	TYR	N-CA-C	5.36	115.77	109.60
1	C	221	ASP	N-CA-C	-5.33	106.62	113.23
1	D	38	ARG	N-CA-C	5.24	117.86	108.17
1	C	301	GLN	N-CA-C	-5.23	105.49	111.14
1	C	39	GLU	N-CA-C	-5.15	106.83	113.01
1	A	294	VAL	N-CA-C	5.08	116.39	112.12
1	C	67	TYR	N-CA-C	5.07	117.51	109.50
1	B	301	GLN	N-CA-C	-5.06	104.76	112.04
1	A	43	SER	N-CA-C	5.04	115.80	108.14
1	B	27	HIS	N-CA-C	-5.01	106.67	112.89
1	B	91	LEU	N-CA-C	-5.01	107.14	113.20

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	2605	0	2589	249	0
1	B	2605	0	2589	305	0
1	C	2605	0	2589	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2605	0	2589	181	0
2	A	15	0	7	1	0
2	B	15	0	7	2	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
3	A	47	0	0	9	0
3	B	44	0	0	12	0
3	C	132	0	0	24	0
3	D	150	0	0	27	0
All	All	10853	0	10384	874	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 42.

All (874) 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:B:23:ARG:HH11	1:B:23:ARG:HB3	1.20	1.05
1:B:217:GLY:HA2	1:B:219:GLN:HE22	1.19	1.04
1:D:132:ILE:HG22	1:D:133:GLU:H	1.29	0.98
1:B:196:ILE:HG22	1:B:319:LEU:HB3	1.45	0.97
1:B:273:ASN:ND2	1:B:276:THR:H	1.61	0.96
1:B:237:GLN:HG3	1:B:240:ARG:HH12	1.32	0.95
1:D:151:LEU:HD23	1:D:158:PRO:HB3	1.46	0.94
1:C:142:LYS:HG2	1:C:146:ASN:HD21	1.33	0.94
1:A:51:THR:HG21	1:A:80:GLN:HA	1.50	0.94
1:A:11:LEU:HB2	1:A:56:GLU:HG2	1.49	0.92
1:C:37:LYS:HG2	1:C:178:PHE:HE1	1.35	0.91
1:B:42:ASN:HD22	1:B:49:GLY:H	1.18	0.90
1:B:205:THR:O	1:B:209:ILE:HG13	1.72	0.90
1:B:281:ARG:HD3	3:B:527:HOH:O	1.70	0.89
1:B:239:LEU:HD13	1:B:258:PHE:HD2	1.38	0.88
1:D:100:GLU:HG2	1:D:134:ASP:HB2	1.57	0.86
1:A:322:HIS:HD2	1:A:324:GLY:H	1.20	0.86
1:C:37:LYS:HG2	1:C:178:PHE:CE1	2.11	0.85
1:D:226:ASP:HB2	1:D:260:LEU:HD11	1.57	0.85
1:D:21:LEU:HD22	1:D:287:GLU:HG3	1.58	0.85
1:B:201:VAL:HB	1:B:228:SER:HB2	1.59	0.84
1:A:116:VAL:HG13	1:B:330:SER:HB3	1.59	0.83
1:D:271:VAL:HG23	3:D:836:HOH:O	1.77	0.83
1:C:23:ARG:NH1	1:C:23:ARG:HB3	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:HIS:HD1	1:A:94:LYS:HB2	1.44	0.82
1:B:214:ALA:HA	1:B:219:GLN:HE21	1.42	0.82
1:B:268:CYS:HB3	3:B:540:HOH:O	1.78	0.82
1:B:18:ILE:HA	1:B:37:LYS:HA	1.60	0.81
1:A:62:ILE:HD13	1:A:70:LEU:HD21	1.62	0.80
1:A:23:ARG:HH12	1:A:286:GLN:HA	1.45	0.80
1:A:81:THR:HB	1:A:97:LEU:HD13	1.62	0.80
1:A:120:GLU:OE2	1:B:333:SER:HA	1.82	0.79
1:C:185:GLN:HA	1:C:188:GLU:HG2	1.65	0.79
1:D:190:GLY:C	1:D:191:ILE:HD12	2.08	0.79
1:B:281:ARG:O	1:B:285:GLU:HG3	1.83	0.78
1:D:22:ASN:O	1:D:26:GLN:HG3	1.83	0.78
1:B:252:GLU:CD	1:B:252:GLU:H	1.92	0.78
1:B:49:GLY:HA3	1:B:83:MET:HE1	1.66	0.77
1:C:99:GLN:HE21	1:C:99:GLN:HA	1.50	0.77
1:B:76:ARG:NH1	1:B:131:VAL:HG13	1.99	0.77
1:B:217:GLY:HA2	1:B:219:GLN:NE2	1.97	0.77
1:D:293:PRO:HD3	1:D:329:LEU:HD23	1.67	0.77
1:B:217:GLY:CA	1:B:219:GLN:HE22	1.94	0.77
1:A:230:THR:HA	3:A:438:HOH:O	1.84	0.77
1:A:166:SER:HA	1:A:204:SER:HB3	1.67	0.77
1:C:194:ASP:O	1:C:195:LYS:HD3	1.84	0.76
1:B:239:LEU:HD13	1:B:258:PHE:CD2	2.20	0.76
1:B:199:CYS:SG	1:B:299:SER:HB3	2.26	0.76
1:C:51:THR:HG21	1:C:80:GLN:HA	1.68	0.76
1:D:283:CYS:SG	1:D:300:MET:HE3	2.25	0.76
1:D:67:TYR:O	1:D:93:LYS:HE3	1.86	0.76
1:A:322:HIS:CD2	1:A:324:GLY:H	2.03	0.75
1:B:185:GLN:HA	1:B:188:GLU:HG2	1.68	0.75
1:A:232:GLU:N	1:A:232:GLU:OE1	2.20	0.75
1:B:21:LEU:HD22	1:B:287:GLU:HG3	1.69	0.75
1:B:100:GLU:HA	1:B:132:ILE:O	1.87	0.75
1:A:273:ASN:HD22	1:A:275:GLY:H	1.33	0.74
1:C:274:GLU:O	1:C:278:GLU:HG3	1.86	0.74
1:D:313:LYS:HG2	1:D:316:ALA:HB2	1.69	0.74
1:A:116:VAL:HG12	1:A:117:GLY:N	2.03	0.74
1:A:69:HIS:CE1	1:A:94:LYS:HD2	2.23	0.74
1:B:175:PHE:O	1:B:178:PHE:HB3	1.87	0.73
1:A:217:GLY:C	1:A:219:GLN:HE21	1.96	0.73
1:C:170:TYR:HB3	1:C:173:LEU:HD12	1.69	0.73
1:B:32:VAL:HG11	1:B:312:PHE:HD1	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASN:HD22	1:A:275:GLY:N	1.86	0.73
1:B:260:LEU:O	1:B:262:THR:HG23	1.89	0.73
1:B:195:LYS:HD3	1:B:221:ASP:HA	1.69	0.73
1:B:21:LEU:HA	1:B:287:GLU:OE1	1.89	0.72
1:B:107:GLU:O	1:B:110:LYS:HG2	1.89	0.72
1:B:103:VAL:HG22	1:B:269:TYR:O	1.88	0.72
1:C:76:ARG:HD2	1:C:114:ASN:OD1	1.89	0.72
1:D:186:GLU:CD	1:D:218:ARG:HH22	1.97	0.72
1:A:281:ARG:O	1:A:285:GLU:HG3	1.90	0.72
1:B:70:LEU:HD11	1:B:87:LEU:HD12	1.70	0.72
1:D:146:ASN:HB2	3:D:842:HOH:O	1.89	0.72
1:C:77:GLN:HE22	1:C:118:ASN:H	1.37	0.72
1:D:212:GLY:O	1:D:215:GLN:HG3	1.90	0.72
1:A:116:VAL:O	1:A:119:ILE:HG22	1.90	0.71
1:A:59:VAL:HG13	1:A:91:LEU:HD11	1.71	0.71
1:A:70:LEU:HD12	1:A:88:ALA:HA	1.71	0.71
1:A:76:ARG:NE	1:A:131:VAL:HG13	2.06	0.71
1:A:11:LEU:HD21	1:A:87:LEU:HD23	1.70	0.71
1:A:23:ARG:NH1	1:A:286:GLN:HA	2.05	0.71
1:A:119:ILE:HG23	1:A:120:GLU:N	2.05	0.71
1:A:166:SER:HB3	1:A:241:ILE:HD11	1.72	0.71
1:B:70:LEU:CD1	1:B:87:LEU:HD12	2.20	0.70
1:B:273:ASN:HD21	1:B:276:THR:H	1.40	0.70
1:C:339:LYS:HA	3:C:726:HOH:O	1.91	0.70
1:D:82:ARG:HH12	1:D:83:MET:HE2	1.56	0.70
1:A:20:ASN:C	1:A:20:ASN:HD22	1.98	0.70
1:A:37:LYS:HD3	1:A:178:PHE:CZ	2.26	0.70
1:C:80:GLN:HG2	3:C:603:HOH:O	1.91	0.70
1:B:23:ARG:HH11	1:B:23:ARG:CB	1.99	0.70
1:B:210:LEU:HD23	1:B:222:VAL:HG21	1.74	0.69
1:C:9:TYR:CD2	1:C:59:VAL:HG11	2.27	0.69
1:B:15:PRO:HA	1:B:181:GLU:OE1	1.92	0.69
1:C:232:GLU:HB2	3:C:667:HOH:O	1.92	0.69
1:C:273:ASN:ND2	1:C:276:THR:H	1.91	0.69
1:C:321:VAL:HG12	1:C:323:LEU:HD21	1.74	0.69
1:D:308:LYS:HG3	3:D:840:HOH:O	1.91	0.69
1:A:21:LEU:HA	1:A:287:GLU:OE2	1.93	0.69
1:B:32:VAL:HG11	1:B:312:PHE:CD1	2.27	0.69
1:C:121:LEU:HD22	1:D:290:LEU:HD13	1.74	0.69
1:B:42:ASN:HD22	1:B:49:GLY:N	1.88	0.69
1:C:23:ARG:HH11	1:C:23:ARG:CB	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HG11	1:A:249:ILE:HG21	1.74	0.69
1:B:196:ILE:HD13	1:B:213:MET:HE2	1.75	0.69
1:A:29:GLY:O	1:A:31:LYS:N	2.26	0.69
1:B:24:LEU:HD21	1:B:300:MET:HE1	1.74	0.69
1:B:219:GLN:CD	1:B:219:GLN:H	2.01	0.69
1:B:107:GLU:HG2	1:B:110:LYS:HE3	1.72	0.68
1:A:49:GLY:HA3	1:A:83:MET:CE	2.23	0.68
1:D:132:ILE:HG22	1:D:133:GLU:N	2.06	0.68
1:B:301:GLN:HG3	1:B:302:GLY:N	2.09	0.68
1:C:53:ARG:HB2	3:C:720:HOH:O	1.93	0.68
1:A:121:LEU:HD22	1:B:290:LEU:HD13	1.74	0.68
1:C:68:THR:HG23	1:C:157:LYS:HB2	1.76	0.68
1:A:147:ALA:HA	1:A:150:GLU:HB3	1.76	0.68
1:C:134:ASP:HB3	1:C:141:ARG:HH21	1.60	0.67
1:A:77:GLN:NE2	1:A:118:ASN:HB2	2.08	0.67
1:D:308:LYS:HD3	3:D:823:HOH:O	1.93	0.67
1:B:19:SER:N	1:B:36:ALA:O	2.23	0.67
1:A:123:ARG:HG3	1:A:129:VAL:HG21	1.77	0.67
1:C:23:ARG:NH1	1:C:286:GLN:O	2.28	0.66
1:C:290:LEU:HD13	1:D:121:LEU:HD22	1.78	0.66
1:D:293:PRO:HD3	1:D:329:LEU:CD2	2.26	0.66
1:A:214:ALA:HA	1:A:219:GLN:HG3	1.77	0.66
1:A:239:LEU:HD13	1:A:258:PHE:HD2	1.61	0.66
1:B:81:THR:HB	1:B:97:LEU:HD13	1.76	0.66
1:B:199:CYS:HB3	3:B:545:HOH:O	1.95	0.66
1:B:264:PHE:CZ	1:B:302:GLY:HA2	2.32	0.65
1:D:198:VAL:HG23	1:D:321:VAL:HB	1.78	0.65
1:D:77:GLN:HA	1:D:77:GLN:NE2	2.12	0.65
1:B:183:ILE:HD12	1:B:183:ILE:H	1.62	0.64
1:B:144:PHE:HZ	1:B:161:ILE:H	1.46	0.64
1:C:321:VAL:HG12	1:C:323:LEU:CD2	2.28	0.64
1:B:274:GLU:HG3	3:B:515:HOH:O	1.95	0.64
1:C:51:THR:HG22	3:C:732:HOH:O	1.96	0.64
1:A:59:VAL:HG21	1:A:87:LEU:HD21	1.80	0.64
1:A:274:GLU:O	1:A:278:GLU:HB2	1.97	0.64
1:B:140:MET:HG2	1:B:167:GLU:OE1	1.97	0.64
1:C:103:VAL:CG2	1:C:270:GLY:HA3	2.27	0.64
1:B:117:GLY:O	1:B:121:LEU:HG	1.98	0.64
1:B:214:ALA:HB2	1:B:255:PHE:HZ	1.62	0.64
1:C:143:SER:HA	1:C:146:ASN:HD22	1.62	0.64
1:C:76:ARG:HG2	1:C:76:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:HIS:HD2	1:D:324:GLY:H	1.46	0.63
1:B:67:TYR:HE1	1:B:159:TYR:HD1	1.46	0.63
1:B:183:ILE:HG12	1:B:216:TYR:CE2	2.34	0.63
1:A:21:LEU:HD22	1:A:287:GLU:HG3	1.79	0.63
1:B:228:SER:HB3	3:B:526:HOH:O	1.98	0.63
3:C:701:HOH:O	1:D:341:ALA:HB1	1.99	0.63
1:C:15:PRO:HA	1:C:181:GLU:OE1	1.97	0.63
1:D:186:GLU:OE1	1:D:218:ARG:NH2	2.32	0.63
1:B:143:SER:HA	1:B:146:ASN:HD22	1.64	0.63
1:B:239:LEU:HD21	1:B:256:LYS:O	1.99	0.63
1:B:267:PRO:HG2	1:B:271:VAL:HB	1.80	0.63
1:C:23:ARG:HB3	1:C:23:ARG:HH11	1.59	0.63
1:C:175:PHE:O	1:C:178:PHE:HB3	1.99	0.63
1:B:235:LYS:HB2	1:B:260:LEU:HD23	1.78	0.62
1:A:96:VAL:HG21	1:A:151:LEU:HD21	1.80	0.62
1:C:20:ASN:ND2	3:C:675:HOH:O	2.31	0.62
1:D:23:ARG:NH1	1:D:286:GLN:HA	2.14	0.62
1:A:107:GLU:HA	1:A:110:LYS:HD3	1.81	0.62
1:B:196:ILE:HG13	1:B:222:VAL:HA	1.80	0.62
1:A:8:LYS:HE3	1:A:56:GLU:OE1	1.99	0.62
1:A:69:HIS:HD2	1:A:158:PRO:HG3	1.64	0.62
1:A:72:SER:HA	1:A:161:ILE:O	2.00	0.62
1:B:312:PHE:CE1	1:B:318:VAL:HG21	2.35	0.62
1:B:37:LYS:NZ	1:B:185:GLN:OE1	2.30	0.62
1:D:59:VAL:HG22	1:D:87:LEU:HD21	1.80	0.62
1:A:194:ASP:O	1:A:195:LYS:HD3	2.00	0.61
1:A:120:GLU:OE1	1:B:330:SER:HA	1.99	0.61
1:B:216:TYR:HB3	3:B:510:HOH:O	1.99	0.61
1:C:153:ASP:HB2	3:C:691:HOH:O	2.00	0.61
1:C:169:LYS:HA	3:C:650:HOH:O	2.00	0.61
1:B:322:HIS:CD2	1:B:324:GLY:H	2.17	0.61
1:A:119:ILE:HG23	1:A:120:GLU:H	1.66	0.61
1:A:107:GLU:O	1:A:110:LYS:HE2	2.00	0.61
1:A:23:ARG:HE	1:B:92:GLY:HA3	1.66	0.61
1:A:50:ASN:HB3	1:A:323:LEU:HB3	1.83	0.61
1:A:186:GLU:OE1	1:A:218:ARG:NH2	2.29	0.61
1:C:69:HIS:ND1	1:C:94:LYS:HB2	2.16	0.61
1:D:37:LYS:HD3	1:D:178:PHE:CE1	2.35	0.61
1:B:50:ASN:HB3	1:B:323:LEU:HD22	1.82	0.61
1:A:124:ILE:C	1:A:126:GLY:H	2.09	0.60
1:A:80:GLN:O	1:A:84:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HD2	1:A:82:ARG:O	2.02	0.60
1:B:176:VAL:HG11	1:B:249:ILE:HG21	1.82	0.60
1:B:185:GLN:HA	1:B:188:GLU:CG	2.29	0.60
1:A:273:ASN:ND2	1:A:276:THR:H	1.99	0.60
1:C:103:VAL:HG21	1:C:270:GLY:HA3	1.83	0.60
1:D:21:LEU:HD12	1:D:34:VAL:HG12	1.84	0.60
1:A:99:GLN:HE21	1:A:99:GLN:HA	1.67	0.60
1:A:233:LYS:HG3	1:A:234:THR:N	2.16	0.60
1:A:116:VAL:HG12	1:A:117:GLY:H	1.66	0.60
1:B:29:GLY:O	1:B:30:SER:HB2	2.00	0.60
1:A:69:HIS:HD1	1:A:94:LYS:CB	2.13	0.60
1:B:141:ARG:HA	1:B:141:ARG:HH11	1.66	0.60
1:A:195:LYS:HE2	3:A:413:HOH:O	2.00	0.59
1:B:266:TYR:HA	1:B:267:PRO:O	2.02	0.59
1:C:79:ASN:OD1	1:C:325:GLY:HA2	2.01	0.59
1:C:230:THR:CB	1:C:233:LYS:HE2	2.32	0.59
1:A:182:VAL:O	1:A:186:GLU:HG3	2.01	0.59
1:D:191:ILE:HD12	1:D:191:ILE:N	2.17	0.59
1:A:49:GLY:HA3	1:A:83:MET:SD	2.42	0.59
1:B:164:GLY:C	1:B:166:SER:H	2.09	0.59
1:B:303:LEU:O	1:B:307:ILE:HG13	2.02	0.59
1:B:138:ILE:HG21	1:B:201:VAL:O	2.03	0.59
1:C:46:ALA:O	1:C:47:PHE:HB2	2.01	0.59
1:A:138:ILE:H	1:A:233:LYS:HZ2	1.49	0.59
1:B:239:LEU:HD21	1:B:256:LYS:C	2.27	0.59
1:C:278:GLU:HB3	3:C:722:HOH:O	2.03	0.59
1:A:196:ILE:CD1	1:A:213:MET:HE2	2.32	0.59
1:B:273:ASN:HD22	1:B:276:THR:H	1.49	0.59
1:D:68:THR:OG1	1:D:69:HIS:HD2	1.86	0.59
1:B:62:ILE:HG21	1:B:70:LEU:HD21	1.83	0.59
1:B:143:SER:CA	1:B:146:ASN:HD22	2.16	0.58
1:B:193:PHE:CE1	1:B:319:LEU:HD22	2.37	0.58
1:C:142:LYS:HG2	1:C:146:ASN:ND2	2.12	0.58
1:A:193:PHE:CE2	1:A:319:LEU:HD13	2.38	0.58
1:A:232:GLU:HG2	1:A:233:LYS:H	1.69	0.58
1:A:185:GLN:HA	1:A:188:GLU:HG2	1.85	0.58
1:B:296:GLU:HG2	1:B:322:HIS:HD2	1.68	0.58
1:C:231:SER:OG	1:C:262:THR:HG21	2.04	0.58
1:C:310:ASP:HA	3:C:621:HOH:O	2.02	0.58
1:B:18:ILE:HG12	1:B:37:LYS:HG3	1.86	0.58
1:D:77:GLN:CA	1:D:77:GLN:HE21	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:VAL:HG12	1:D:187:VAL:O	2.02	0.58
1:A:49:GLY:HA3	1:A:83:MET:HE1	1.85	0.57
1:A:119:ILE:HD11	1:A:123:ARG:NH2	2.19	0.57
1:B:71:VAL:HG11	1:B:148:LEU:HD23	1.85	0.57
1:C:283:CYS:SG	1:C:300:MET:HE3	2.44	0.57
1:A:100:GLU:HA	1:A:132:ILE:HG23	1.86	0.57
1:A:201:VAL:HG21	1:A:295:TYR:CE2	2.39	0.57
1:B:296:GLU:HG2	1:B:322:HIS:CD2	2.38	0.57
1:A:79:ASN:HA	1:A:118:ASN:ND2	2.20	0.57
1:A:142:LYS:HG2	1:A:146:ASN:ND2	2.19	0.57
1:D:37:LYS:HD3	1:D:178:PHE:CZ	2.39	0.57
1:C:182:VAL:O	1:C:186:GLU:HG3	2.05	0.57
1:C:239:LEU:HD13	1:C:258:PHE:CD2	2.39	0.57
1:B:107:GLU:HG2	1:B:110:LYS:CE	2.34	0.57
1:D:61:ASP:HB2	3:D:788:HOH:O	2.04	0.57
1:B:22:ASN:CG	1:B:23:ARG:N	2.62	0.57
1:B:183:ILE:HG23	1:D:187:VAL:HG11	1.85	0.57
1:A:186:GLU:HG2	1:A:193:PHE:CD1	2.39	0.57
1:D:273:ASN:HD22	1:D:275:GLY:H	1.51	0.57
1:A:105:ILE:HG21	1:A:110:LYS:HA	1.85	0.57
1:C:112:VAL:O	1:C:116:VAL:HG22	2.05	0.57
1:A:116:VAL:CG1	1:A:117:GLY:N	2.67	0.57
1:B:49:GLY:HA3	1:B:83:MET:CE	2.34	0.57
1:C:321:VAL:CG1	1:C:323:LEU:HD21	2.35	0.57
1:A:282:THR:O	1:A:286:GLN:HG2	2.05	0.57
1:C:239:LEU:HD13	1:C:258:PHE:HD2	1.70	0.57
1:D:1:ALA:HB3	3:D:791:HOH:O	2.04	0.57
1:D:21:LEU:HD22	1:D:287:GLU:CG	2.33	0.57
1:A:140:MET:HG2	1:A:167:GLU:OE2	2.04	0.56
1:A:166:SER:HB3	1:A:241:ILE:CD1	2.35	0.56
1:A:291:THR:HG22	1:A:296:GLU:CB	2.35	0.56
1:A:36:ALA:HA	1:A:320:TYR:O	2.05	0.56
1:A:291:THR:HG22	1:A:296:GLU:HB3	1.85	0.56
1:B:98:ILE:HD11	1:B:147:ALA:HB2	1.87	0.56
1:D:50:ASN:HB2	1:D:175:PHE:HZ	1.69	0.56
1:C:70:LEU:HD12	1:C:88:ALA:HB2	1.87	0.56
1:C:111:ASP:O	1:C:112:VAL:HG23	2.06	0.56
1:C:149:GLN:HG3	1:C:153:ASP:OD2	2.04	0.56
1:A:123:ARG:CG	1:A:129:VAL:HG21	2.36	0.56
1:B:216:TYR:HA	3:B:522:HOH:O	2.04	0.56
1:B:235:LYS:HB2	1:B:260:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PRO:HD3	1:A:329:LEU:HD13	1.87	0.56
1:B:96:VAL:HG21	1:B:151:LEU:HD11	1.88	0.56
1:B:302:GLY:O	1:B:306:LEU:HD13	2.06	0.56
1:A:79:ASN:CG	1:A:118:ASN:HD21	2.12	0.56
1:B:237:GLN:HA	1:B:240:ARG:CZ	2.36	0.56
1:B:298:LYS:O	1:B:301:GLN:HG2	2.06	0.56
1:B:237:GLN:HB2	1:B:240:ARG:HH22	1.71	0.56
1:B:76:ARG:C	1:B:78:SER:H	2.14	0.55
1:B:147:ALA:O	1:B:150:GLU:HB3	2.05	0.55
1:A:23:ARG:NH2	1:B:92:GLY:HA2	2.21	0.55
1:B:226:ASP:HB2	1:B:262:THR:HG22	1.88	0.55
1:B:87:LEU:C	1:B:87:LEU:HD13	2.31	0.55
1:B:209:ILE:O	1:B:213:MET:HG2	2.05	0.55
1:B:76:ARG:CZ	1:B:131:VAL:HG13	2.37	0.55
1:B:228:SER:O	1:B:230:THR:HG23	2.05	0.55
1:B:273:ASN:HD22	1:B:273:ASN:C	2.15	0.55
1:A:235:LYS:O	1:A:239:LEU:HB2	2.05	0.55
1:A:290:LEU:O	1:A:322:HIS:HE1	1.89	0.55
1:B:214:ALA:HA	1:B:219:GLN:NE2	2.18	0.55
1:D:50:ASN:HB2	1:D:175:PHE:CZ	2.42	0.55
1:D:339:LYS:NZ	1:D:341:ALA:HB2	2.22	0.55
1:A:46:ALA:O	1:A:47:PHE:HB2	2.07	0.55
1:D:290:LEU:HD12	3:D:720:HOH:O	2.07	0.55
1:C:310:ASP:HB2	3:C:682:HOH:O	2.07	0.55
1:B:198:VAL:CG2	1:B:323:LEU:HD11	2.37	0.55
1:D:192:LYS:HG3	3:D:817:HOH:O	2.06	0.55
1:B:51:THR:O	1:B:55:LEU:HG	2.07	0.55
1:D:6:PHE:CD1	1:D:6:PHE:N	2.73	0.55
1:A:70:LEU:HD12	1:A:88:ALA:CA	2.36	0.54
1:A:266:TYR:CD1	1:A:267:PRO:HA	2.42	0.54
1:C:192:LYS:HD3	1:C:193:PHE:N	2.23	0.54
1:A:119:ILE:CG2	1:A:120:GLU:N	2.70	0.54
1:A:196:ILE:HD12	1:A:213:MET:HE2	1.89	0.54
1:B:107:GLU:C	1:B:109:GLU:H	2.15	0.54
1:D:221:ASP:HA	3:D:834:HOH:O	2.07	0.54
1:D:254:GLU:HG2	1:D:255:PHE:N	2.22	0.54
1:A:150:GLU:OE1	1:A:151:LEU:HD12	2.08	0.54
1:D:20:ASN:ND2	1:D:35:TYR:CE2	2.75	0.54
1:A:186:GLU:HG2	1:A:193:PHE:HD1	1.73	0.54
1:B:46:ALA:O	1:B:47:PHE:HB2	2.07	0.54
1:D:271:VAL:N	3:D:836:HOH:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:CZ	1:A:302:GLY:HA2	2.42	0.54
1:B:76:ARG:NH1	1:B:99:GLN:O	2.41	0.54
1:A:69:HIS:ND1	1:A:94:LYS:HB2	2.20	0.54
1:B:194:ASP:O	1:B:195:LYS:HD3	2.08	0.54
1:C:138:ILE:H	1:C:233:LYS:NZ	2.06	0.54
1:B:24:LEU:HB2	1:B:287:GLU:HG2	1.90	0.54
1:B:40:ASP:HB3	1:B:324:GLY:CA	2.38	0.54
1:B:275:GLY:O	1:B:276:THR:C	2.51	0.54
1:C:37:LYS:HE3	1:C:178:PHE:CE1	2.42	0.54
1:A:325:GLY:C	1:A:327:PRO:HD2	2.34	0.53
1:B:23:ARG:HH22	1:B:286:GLN:HA	1.73	0.53
1:C:28:LEU:HD22	1:C:308:LYS:HE3	1.89	0.53
1:A:38:ARG:NH1	1:B:44:GLY:HA3	2.23	0.53
1:A:101:ASP:O	1:A:135:GLY:HA2	2.09	0.53
1:A:237:GLN:HG3	1:A:240:ARG:NH2	2.24	0.53
1:C:102:TRP:CD1	1:C:136:PHE:HA	2.43	0.53
1:A:119:ILE:CG2	1:A:120:GLU:H	2.22	0.53
1:B:203:GLY:O	1:B:205:THR:N	2.41	0.53
1:B:304:ILE:O	1:B:308:LYS:HG2	2.08	0.53
1:D:51:THR:HG23	3:D:851:HOH:O	2.09	0.53
1:D:137:ASP:HB3	1:D:141:ARG:NH1	2.23	0.53
1:D:210:LEU:HD23	1:D:222:VAL:HG21	1.89	0.53
1:D:230:THR:HB	1:D:233:LYS:HD3	1.90	0.53
1:D:51:THR:OG1	1:D:83:MET:SD	2.64	0.53
1:D:109:GLU:OE2	1:D:332:TYR:HA	2.09	0.53
1:D:189:LEU:HB3	1:D:191:ILE:HD13	1.89	0.53
1:B:33:ASN:HB2	1:B:317:ASN:OD1	2.08	0.53
1:B:51:THR:HG21	1:B:80:GLN:HA	1.88	0.53
1:B:237:GLN:HA	1:B:240:ARG:NH2	2.23	0.53
1:D:166:SER:HA	1:D:204:SER:HB3	1.89	0.53
1:D:283:CYS:HB2	1:D:300:MET:HE3	1.91	0.53
1:A:153:ASP:C	1:A:155:GLY:H	2.16	0.53
1:B:68:THR:C	1:B:69:HIS:HD2	2.17	0.53
1:B:214:ALA:HB2	1:B:255:PHE:CZ	2.44	0.53
1:D:66:ASP:O	1:D:157:LYS:HD3	2.09	0.53
1:D:120:GLU:O	1:D:124:ILE:HG13	2.08	0.53
1:A:100:GLU:HA	1:A:132:ILE:CG2	2.39	0.53
1:A:147:ALA:HA	1:A:150:GLU:CB	2.38	0.53
1:B:185:GLN:HA	1:B:188:GLU:CD	2.34	0.53
1:A:229:PHE:O	1:A:230:THR:HG23	2.09	0.53
1:D:82:ARG:NH1	1:D:83:MET:HE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASP:O	1:D:195:LYS:HD3	2.07	0.53
1:A:27:HIS:C	1:A:29:GLY:H	2.17	0.53
1:C:67:TYR:O	1:C:93:LYS:NZ	2.42	0.53
1:A:132:ILE:CD1	1:A:143:SER:HB3	2.39	0.53
1:B:69:HIS:CD2	1:B:94:LYS:HB2	2.44	0.53
1:B:218:ARG:O	1:B:219:GLN:C	2.51	0.53
1:C:205:THR:O	1:C:209:ILE:HG13	2.09	0.53
1:D:81:THR:HB	1:D:97:LEU:HD13	1.91	0.53
1:D:339:LYS:HZ1	1:D:341:ALA:HB2	1.74	0.53
1:B:217:GLY:CA	1:B:219:GLN:NE2	2.65	0.52
1:A:20:ASN:C	1:A:20:ASN:ND2	2.62	0.52
1:D:23:ARG:HH12	1:D:286:GLN:HA	1.74	0.52
1:D:254:GLU:OE2	1:D:256:LYS:HE3	2.09	0.52
1:D:77:GLN:HA	1:D:77:GLN:HE21	1.71	0.52
1:B:40:ASP:HB3	1:B:324:GLY:HA2	1.90	0.52
1:C:20:ASN:C	1:C:20:ASN:HD22	2.18	0.52
1:C:5:LYS:HG3	1:C:6:PHE:CD1	2.45	0.52
1:A:231:SER:OG	1:A:262:THR:HG21	2.09	0.52
1:B:37:LYS:HD3	1:B:178:PHE:CE1	2.44	0.52
1:B:239:LEU:HB2	1:B:258:PHE:HE2	1.73	0.52
1:B:261:ASP:OD2	1:B:306:LEU:HD11	2.09	0.52
1:B:214:ALA:HA	1:B:219:GLN:HG3	1.92	0.52
1:D:29:GLY:O	1:D:31:LYS:N	2.42	0.52
1:A:124:ILE:HG12	1:B:336:PHE:CD2	2.44	0.52
1:D:305:ALA:O	1:D:309:GLU:HG2	2.10	0.52
1:A:29:GLY:O	1:A:31:LYS:HG2	2.10	0.52
1:A:167:GLU:HG3	3:A:439:HOH:O	2.09	0.52
1:A:226:ASP:HB2	1:A:260:LEU:HD11	1.91	0.52
1:C:273:ASN:HD22	1:C:275:GLY:N	2.08	0.52
1:D:235:LYS:HG3	1:D:258:PHE:CE2	2.45	0.52
1:C:1:ALA:HB3	3:C:687:HOH:O	2.10	0.52
1:C:313:LYS:HD2	1:C:314:PRO:O	2.10	0.52
1:D:116:VAL:HG23	1:D:117:GLY:N	2.25	0.52
1:B:123:ARG:HG3	1:B:129:VAL:HG21	1.91	0.51
1:C:123:ARG:NH1	3:C:626:HOH:O	2.43	0.51
1:A:116:VAL:CG1	1:A:117:GLY:H	2.21	0.51
1:A:138:ILE:HG12	1:A:233:LYS:HD2	1.91	0.51
1:B:21:LEU:HA	1:B:287:GLU:CD	2.35	0.51
1:B:226:ASP:CB	1:B:262:THR:HG22	2.40	0.51
1:B:291:THR:HA	3:B:536:HOH:O	2.09	0.51
1:D:115:ARG:O	1:D:120:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:HA3	1:B:38:ARG:NH1	2.25	0.51
1:A:205:THR:O	1:A:209:ILE:HG13	2.11	0.51
1:A:326:ALA:N	1:A:327:PRO:CD	2.73	0.51
1:B:235:LYS:HA	1:B:258:PHE:HZ	1.75	0.51
1:B:67:TYR:CE1	1:B:159:TYR:HD1	2.27	0.51
1:B:145:ALA:HA	1:B:148:LEU:HD12	1.93	0.51
1:C:300:MET:O	1:C:304:ILE:HG13	2.10	0.51
1:D:218:ARG:HD2	1:D:221:ASP:OD2	2.11	0.51
1:A:103:VAL:HG22	1:A:270:GLY:HA3	1.92	0.51
1:B:193:PHE:CD1	1:B:319:LEU:HD22	2.46	0.51
1:A:79:ASN:HA	1:A:118:ASN:HD22	1.75	0.51
1:D:77:GLN:HE22	1:D:118:ASN:H	1.58	0.51
1:C:230:THR:OG1	1:C:233:LYS:HE2	2.11	0.51
1:B:212:GLY:HA2	1:B:215:GLN:HE21	1.76	0.51
1:B:216:TYR:N	1:B:216:TYR:CD1	2.79	0.51
1:B:326:ALA:N	1:B:327:PRO:CD	2.74	0.51
1:D:219:GLN:HG2	1:D:220:ASP:N	2.26	0.51
1:C:169:LYS:HG2	1:C:170:TYR:CE2	2.46	0.50
1:D:82:ARG:HA	1:D:122:SER:OG	2.12	0.50
1:D:270:GLY:HA2	1:D:294:VAL:HG13	1.93	0.50
1:D:283:CYS:CB	1:D:300:MET:HE3	2.41	0.50
1:B:164:GLY:C	1:B:166:SER:N	2.68	0.50
1:A:58:ILE:HG23	1:A:168:HIS:NE2	2.26	0.50
1:A:69:HIS:CD2	1:A:158:PRO:HG3	2.46	0.50
1:B:1:ALA:HA	1:B:249:ILE:O	2.12	0.50
1:C:138:ILE:H	1:C:233:LYS:HZ1	1.59	0.50
1:A:184:ASN:O	1:A:187:VAL:HB	2.11	0.50
1:B:69:HIS:ND1	1:B:151:LEU:HD13	2.27	0.50
1:C:31:LYS:HD3	1:C:310:ASP:OD1	2.11	0.50
1:C:284:ALA:HB1	1:D:125:MET:HG2	1.94	0.50
1:D:140:MET:SD	1:D:167:GLU:HG3	2.51	0.50
1:C:13:PHE:CE1	1:C:43:SER:C	2.89	0.50
1:D:49:GLY:HA3	1:D:83:MET:HE1	1.93	0.50
1:B:295:TYR:O	1:B:297:GLY:N	2.44	0.50
1:A:59:VAL:N	1:A:60:PRO:CD	2.75	0.50
1:A:225:ILE:HG21	1:A:299:SER:HA	1.94	0.50
1:B:67:TYR:HE1	1:B:159:TYR:CD1	2.27	0.50
1:A:11:LEU:CB	1:A:56:GLU:HG2	2.31	0.49
1:A:82:ARG:O	1:A:125:MET:HE1	2.12	0.49
1:A:243:ASN:O	1:A:244:ASN:C	2.55	0.49
1:B:20:ASN:C	1:B:20:ASN:HD22	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:SER:HA	1:C:204:SER:HB3	1.94	0.49
1:D:66:ASP:HA	3:D:815:HOH:O	2.11	0.49
1:B:76:ARG:HH12	1:B:131:VAL:HG13	1.74	0.49
1:C:249:ILE:HG13	1:C:251:VAL:HG23	1.94	0.49
1:B:2:GLY:O	1:B:5:LYS:HG2	2.12	0.49
1:B:219:GLN:CD	1:B:219:GLN:N	2.70	0.49
1:C:8:LYS:HD3	1:C:57:TYR:CZ	2.47	0.49
1:C:43:SER:HB3	1:C:52:LEU:HD23	1.94	0.49
1:C:73:ILE:HG13	1:C:98:ILE:HB	1.94	0.49
1:A:92:GLY:C	1:A:93:LYS:HG2	2.37	0.49
1:A:231:SER:O	1:A:232:GLU:C	2.55	0.49
1:B:119:ILE:HG22	3:B:529:HOH:O	2.11	0.49
1:B:252:GLU:CD	1:B:252:GLU:N	2.67	0.49
1:B:312:PHE:CD1	1:B:318:VAL:HG21	2.47	0.49
1:B:340:THR:O	1:B:341:ALA:C	2.55	0.49
1:D:79:ASN:HB2	2:D:701:PLP:O3	2.12	0.49
1:B:237:GLN:CB	1:B:240:ARG:HH22	2.26	0.49
1:D:40:ASP:HB3	1:D:324:GLY:HA2	1.95	0.49
1:A:69:HIS:HE1	1:A:94:LYS:HD2	1.75	0.49
1:B:5:LYS:HG3	1:B:6:PHE:CE1	2.47	0.49
1:B:235:LYS:O	1:B:239:LEU:HB2	2.12	0.49
1:C:296:GLU:HG3	1:C:322:HIS:CD2	2.48	0.49
1:D:2:GLY:O	1:D:249:ILE:HA	2.13	0.49
1:A:58:ILE:C	1:A:60:PRO:HD2	2.38	0.49
1:C:15:PRO:CA	1:C:181:GLU:OE1	2.61	0.49
1:B:19:SER:HB2	1:B:38:ARG:HD3	1.95	0.48
1:C:85:ALA:HB3	1:C:125:MET:HE3	1.94	0.48
1:A:151:LEU:C	1:A:153:ASP:H	2.21	0.48
1:B:59:VAL:O	1:B:60:PRO:C	2.55	0.48
1:B:61:ASP:OD2	1:B:159:TYR:CE1	2.66	0.48
1:C:98:ILE:HD11	1:C:147:ALA:HB2	1.94	0.48
1:D:59:VAL:CG2	1:D:87:LEU:HD21	2.42	0.48
1:A:181:GLU:O	1:A:185:GLN:HG3	2.12	0.48
1:B:98:ILE:HD11	1:B:147:ALA:CB	2.43	0.48
1:D:29:GLY:C	1:D:31:LYS:N	2.71	0.48
1:A:123:ARG:O	1:A:126:GLY:N	2.47	0.48
1:B:61:ASP:OD2	1:B:159:TYR:HE1	1.96	0.48
1:C:199:CYS:HB2	1:C:299:SER:HB3	1.93	0.48
1:D:24:LEU:O	1:D:28:LEU:HG	2.14	0.48
1:D:76:ARG:NH2	1:D:132:ILE:O	2.45	0.48
1:B:204:SER:H	1:B:241:ILE:CD1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:NH1	1:C:23:ARG:CB	2.65	0.48
1:D:273:ASN:HD22	1:D:275:GLY:N	2.12	0.48
1:D:55:LEU:HD13	1:D:87:LEU:HD22	1.94	0.48
1:D:71:VAL:HG21	1:D:158:PRO:HB2	1.96	0.48
1:D:245:THR:O	1:D:248:LEU:HB2	2.13	0.48
1:A:103:VAL:CG2	1:A:270:GLY:HA3	2.44	0.48
1:C:46:ALA:C	1:C:48:GLY:H	2.22	0.48
1:A:82:ARG:NH1	1:A:83:MET:HG3	2.29	0.48
1:A:330:SER:HB3	1:B:116:VAL:CG1	2.44	0.48
1:B:74:GLY:O	1:B:99:GLN:HA	2.14	0.48
1:B:215:GLN:HB2	1:B:216:TYR:CD1	2.49	0.48
1:C:279:ALA:HB2	1:C:301:GLN:HB2	1.95	0.48
1:D:229:PHE:CE2	1:D:267:PRO:O	2.66	0.48
1:A:311:TYR:CD2	1:A:311:TYR:O	2.67	0.48
1:B:254:GLU:HG2	1:B:255:PHE:N	2.29	0.48
1:C:232:GLU:OE1	1:C:232:GLU:N	2.47	0.48
1:D:114:ASN:ND2	3:D:828:HOH:O	2.47	0.48
1:A:21:LEU:HD22	1:A:287:GLU:CG	2.44	0.47
1:A:75:GLY:O	1:A:77:GLN:N	2.47	0.47
1:A:80:GLN:HG2	3:A:445:HOH:O	2.14	0.47
1:B:62:ILE:HD13	1:B:70:LEU:HD21	1.96	0.47
1:B:178:PHE:O	1:B:182:VAL:HG23	2.13	0.47
1:B:195:LYS:HD2	1:B:221:ASP:O	2.14	0.47
1:C:51:THR:O	1:C:55:LEU:HG	2.14	0.47
1:D:6:PHE:HD1	1:D:6:PHE:H	1.61	0.47
1:A:87:LEU:HD13	1:A:87:LEU:C	2.39	0.47
1:A:217:GLY:C	1:A:219:GLN:NE2	2.70	0.47
1:C:59:VAL:N	1:C:60:PRO:CD	2.77	0.47
1:D:175:PHE:O	1:D:178:PHE:HB3	2.14	0.47
1:D:235:LYS:HG3	1:D:258:PHE:HE2	1.79	0.47
1:A:29:GLY:O	1:A:30:SER:C	2.57	0.47
1:A:37:LYS:NZ	1:A:185:GLN:OE1	2.48	0.47
1:A:193:PHE:CD2	1:A:319:LEU:HB2	2.49	0.47
1:B:166:SER:HA	1:B:204:SER:HB3	1.96	0.47
1:B:264:PHE:CE1	1:B:302:GLY:HA2	2.50	0.47
1:C:11:LEU:HB2	1:C:56:GLU:HG2	1.95	0.47
1:D:196:ILE:HD11	1:D:213:MET:HE2	1.96	0.47
1:D:235:LYS:NZ	1:D:257:ASP:OD2	2.46	0.47
1:D:269:TYR:CD2	1:D:269:TYR:C	2.93	0.47
1:A:202:THR:N	2:A:401:PLP:O3P	2.45	0.47
1:B:12:THR:HA	1:B:43:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ILE:HD13	1:B:261:ASP:HB3	1.97	0.47
1:A:157:LYS:N	1:A:158:PRO:HD3	2.29	0.47
1:B:5:LYS:HE3	1:B:248:LEU:O	2.15	0.47
1:B:243:ASN:O	1:B:246:ALA:HB3	2.14	0.47
1:C:96:VAL:HA	1:C:128:ASP:HB3	1.96	0.47
1:C:267:PRO:O	1:C:268:CYS:HB3	2.13	0.47
1:A:38:ARG:HH12	1:B:44:GLY:HA3	1.79	0.47
1:A:99:GLN:HA	1:A:99:GLN:NE2	2.29	0.47
1:A:138:ILE:H	1:A:233:LYS:NZ	2.12	0.47
1:A:199:CYS:HB2	1:A:299:SER:HB3	1.96	0.47
1:A:281:ARG:HH21	1:A:337:PRO:HD2	1.80	0.47
1:A:303:LEU:O	1:A:307:ILE:HG13	2.15	0.47
1:B:24:LEU:HD12	1:B:24:LEU:O	2.14	0.47
1:B:102:TRP:CD1	1:B:136:PHE:HA	2.50	0.47
1:C:80:GLN:OE1	1:C:164:GLY:HA2	2.15	0.47
1:C:262:THR:HB	3:C:681:HOH:O	2.14	0.47
1:C:306:LEU:HB3	1:C:312:PHE:CE1	2.50	0.47
1:D:77:GLN:NE2	1:D:77:GLN:CA	2.73	0.47
1:B:58:ILE:HG23	1:B:168:HIS:NE2	2.30	0.47
1:B:118:ASN:ND2	1:B:328:ALA:HB2	2.30	0.47
1:B:175:PHE:C	1:B:178:PHE:H	2.22	0.47
1:B:226:ASP:OD2	1:B:227:ALA:N	2.47	0.47
1:C:21:LEU:HB3	1:C:287:GLU:HG3	1.95	0.47
1:C:281:ARG:HD3	3:C:705:HOH:O	2.14	0.47
1:C:314:PRO:C	1:C:316:ALA:H	2.23	0.47
1:D:308:LYS:HD2	3:D:785:HOH:O	2.14	0.47
1:B:266:TYR:HA	1:B:267:PRO:C	2.40	0.47
1:C:20:ASN:ND2	1:C:20:ASN:C	2.72	0.47
1:B:161:ILE:HG22	1:B:161:ILE:O	2.14	0.47
1:A:153:ASP:C	1:A:155:GLY:N	2.73	0.46
1:B:32:VAL:HG21	1:B:307:ILE:HG12	1.97	0.46
1:B:240:ARG:HG2	1:B:240:ARG:HH11	1.79	0.46
1:B:322:HIS:HD2	1:B:324:GLY:H	1.61	0.46
1:B:334:SER:C	1:B:336:PHE:H	2.23	0.46
1:C:91:LEU:O	1:C:93:LYS:HD3	2.15	0.46
1:D:29:GLY:C	1:D:31:LYS:H	2.23	0.46
1:D:105:ILE:O	1:D:106:PRO:C	2.58	0.46
1:D:199:CYS:HB2	1:D:299:SER:HB3	1.96	0.46
1:A:163:ALA:HA	3:A:445:HOH:O	2.15	0.46
1:C:239:LEU:CD1	1:C:258:PHE:HD2	2.28	0.46
1:A:144:PHE:O	1:A:146:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:O	1:A:178:PHE:HB3	2.14	0.46
1:A:187:VAL:O	1:D:169:LYS:NZ	2.45	0.46
1:B:196:ILE:CD1	1:B:213:MET:HE2	2.45	0.46
1:B:197:VAL:HG13	1:B:223:ILE:O	2.15	0.46
1:B:248:LEU:C	1:B:250:GLY:H	2.23	0.46
1:C:164:GLY:C	1:C:166:SER:H	2.23	0.46
1:A:70:LEU:HD12	1:A:88:ALA:CB	2.45	0.46
1:B:230:THR:O	1:B:232:GLU:N	2.49	0.46
1:C:99:GLN:HA	1:C:99:GLN:NE2	2.25	0.46
1:C:103:VAL:HG22	1:C:270:GLY:HA3	1.97	0.46
1:C:164:GLY:C	1:C:166:SER:N	2.73	0.46
1:D:39:GLU:HB2	1:D:322:HIS:O	2.16	0.46
1:D:192:LYS:HE3	3:D:806:HOH:O	2.14	0.46
1:D:266:TYR:HD2	3:D:716:HOH:O	1.99	0.46
1:B:229:PHE:CA	1:B:265:ALA:HB1	2.45	0.46
1:B:283:CYS:HB2	1:B:300:MET:HE2	1.98	0.46
1:C:124:ILE:C	1:C:126:GLY:H	2.23	0.46
1:A:239:LEU:HD13	1:A:258:PHE:CD2	2.47	0.46
1:B:204:SER:H	1:B:241:ILE:HD13	1.80	0.46
1:D:80:GLN:O	1:D:84:VAL:HG23	2.15	0.46
1:D:127:ALA:HA	3:D:783:HOH:O	2.14	0.46
1:D:168:HIS:ND1	1:D:169:LYS:N	2.63	0.46
1:A:183:ILE:HD12	1:A:183:ILE:N	2.31	0.46
1:B:77:GLN:HE22	1:B:117:GLY:HA3	1.80	0.46
1:B:145:ALA:O	1:B:148:LEU:HB2	2.16	0.46
1:B:201:VAL:HG22	1:B:202:THR:HG23	1.97	0.46
1:B:229:PHE:HD1	1:B:265:ALA:HB3	1.80	0.46
1:B:276:THR:O	1:B:280:ILE:HG13	2.16	0.46
1:C:322:HIS:CD2	1:C:324:GLY:H	2.34	0.46
1:A:132:ILE:HD13	1:A:143:SER:HB3	1.97	0.46
1:A:172:GLY:O	1:A:176:VAL:HG23	2.16	0.46
1:A:264:PHE:CD1	1:A:264:PHE:N	2.84	0.46
1:B:20:ASN:O	1:B:22:ASN:N	2.41	0.46
1:B:115:ARG:NH1	1:B:115:ARG:HB2	2.30	0.46
1:B:280:ILE:HG23	1:B:291:THR:OG1	2.16	0.46
1:C:26:GLN:HA	1:C:30:SER:OG	2.16	0.46
1:A:62:ILE:HG12	1:A:159:TYR:CD2	2.51	0.46
1:A:82:ARG:HD2	1:A:82:ARG:C	2.41	0.46
1:C:253:HIS:ND1	1:C:254:GLU:N	2.64	0.46
1:D:134:ASP:HB3	1:D:141:ARG:HH21	1.80	0.46
1:D:310:ASP:HA	3:D:782:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:O	1:B:23:ARG:HD3	2.16	0.45
1:B:69:HIS:CE1	1:B:151:LEU:HD22	2.51	0.45
1:C:192:LYS:HG3	3:C:694:HOH:O	2.15	0.45
1:C:231:SER:HB3	1:C:232:GLU:OE1	2.14	0.45
1:D:77:GLN:NE2	1:D:118:ASN:HB2	2.32	0.45
1:A:3:VAL:HG22	1:A:3:VAL:O	2.15	0.45
1:B:103:VAL:CG1	1:B:270:GLY:HA3	2.46	0.45
1:B:119:ILE:N	3:B:529:HOH:O	2.49	0.45
1:B:190:GLY:C	1:B:191:ILE:HG13	2.41	0.45
1:A:196:ILE:HD11	1:A:213:MET:HE2	1.99	0.45
1:B:42:ASN:ND2	1:B:49:GLY:C	2.75	0.45
1:A:28:LEU:HD12	1:A:307:ILE:HD12	1.97	0.45
1:B:39:GLU:O	1:B:42:ASN:ND2	2.50	0.45
1:B:103:VAL:CG2	1:B:270:GLY:HA3	2.47	0.45
1:C:51:THR:OG1	1:C:83:MET:HE3	2.16	0.45
1:A:54:LYS:HZ3	1:A:204:SER:HG	1.62	0.45
1:A:71:VAL:HG23	1:A:96:VAL:O	2.16	0.45
1:C:183:ILE:HG12	1:C:216:TYR:CE2	2.51	0.45
1:D:71:VAL:HG21	1:D:148:LEU:HD23	1.99	0.45
1:A:105:ILE:HG12	1:A:113:TYR:CD2	2.52	0.45
1:B:235:LYS:HA	1:B:258:PHE:CZ	2.50	0.45
1:D:81:THR:HB	1:D:97:LEU:HD22	1.99	0.45
1:D:308:LYS:HB3	3:D:823:HOH:O	2.16	0.45
1:A:58:ILE:HG23	1:A:168:HIS:HE2	1.81	0.45
1:A:209:ILE:O	1:A:213:MET:HG2	2.17	0.45
1:B:12:THR:HG23	1:B:56:GLU:OE2	2.17	0.45
1:B:20:ASN:C	1:B:20:ASN:ND2	2.75	0.45
1:B:67:TYR:HD1	1:B:159:TYR:HB2	1.81	0.45
1:C:138:ILE:HG12	1:C:233:LYS:HE3	1.98	0.45
1:A:186:GLU:CD	1:A:218:ARG:HH22	2.22	0.45
1:C:305:ALA:O	1:C:308:LYS:N	2.50	0.45
1:D:82:ARG:NH1	1:D:83:MET:HG3	2.32	0.45
1:D:256:LYS:HD2	1:D:256:LYS:N	2.31	0.45
1:D:313:LYS:NZ	1:D:316:ALA:HA	2.32	0.45
1:B:142:LYS:C	1:B:146:ASN:ND2	2.75	0.45
1:B:303:LEU:HD13	1:B:307:ILE:HD11	1.98	0.45
1:D:239:LEU:HD13	1:D:258:PHE:CD2	2.52	0.45
1:A:75:GLY:C	1:A:77:GLN:H	2.25	0.45
1:A:290:LEU:HD13	1:B:121:LEU:HD22	1.99	0.45
1:C:137:ASP:HA	1:C:233:LYS:NZ	2.32	0.45
1:B:201:VAL:CG2	1:B:202:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:O	1:B:296:GLU:C	2.61	0.44
1:D:20:ASN:ND2	3:D:719:HOH:O	2.49	0.44
1:D:100:GLU:CG	1:D:134:ASP:HB2	2.37	0.44
1:A:23:ARG:NE	1:B:92:GLY:HA3	2.30	0.44
1:A:112:VAL:HG13	1:A:116:VAL:HG21	1.99	0.44
1:B:82:ARG:HE	1:B:82:ARG:HB3	1.64	0.44
1:B:252:GLU:O	1:B:253:HIS:C	2.60	0.44
1:C:230:THR:O	1:C:233:LYS:HG2	2.18	0.44
1:D:76:ARG:CZ	1:D:131:VAL:HG13	2.47	0.44
1:D:77:GLN:HE22	1:D:118:ASN:N	2.14	0.44
1:A:100:GLU:HB2	1:A:102:TRP:NE1	2.32	0.44
1:A:121:LEU:HD13	1:B:290:LEU:HD11	1.99	0.44
1:A:185:GLN:HA	1:A:188:GLU:CG	2.48	0.44
1:A:232:GLU:CD	3:A:438:HOH:O	2.60	0.44
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.78	0.44
1:C:216:TYR:CD1	1:C:216:TYR:N	2.86	0.44
1:D:109:GLU:O	1:D:113:TYR:HB2	2.17	0.44
1:D:142:LYS:HE3	3:D:842:HOH:O	2.18	0.44
1:D:198:VAL:HG22	1:D:323:LEU:HD11	1.99	0.44
1:A:6:PHE:CD1	1:A:6:PHE:N	2.86	0.44
1:B:334:SER:O	1:B:336:PHE:N	2.50	0.44
1:D:32:VAL:HG11	1:D:312:PHE:HB2	1.99	0.44
1:D:48:GLY:HA2	1:D:52:LEU:CD2	2.48	0.44
1:B:18:ILE:HG12	1:B:37:LYS:CG	2.46	0.44
1:C:219:GLN:C	1:C:221:ASP:H	2.25	0.44
1:D:107:GLU:O	1:D:110:LYS:HG2	2.17	0.44
1:D:336:PHE:O	1:D:337:PRO:O	2.34	0.44
1:C:38:ARG:NH1	1:D:44:GLY:HA3	2.33	0.44
1:A:166:SER:CA	1:A:204:SER:HB3	2.45	0.44
1:A:308:LYS:C	1:A:310:ASP:H	2.26	0.44
1:B:87:LEU:HD13	1:B:87:LEU:O	2.18	0.44
1:B:116:VAL:HG12	1:B:117:GLY:N	2.32	0.44
1:B:225:ILE:O	1:B:226:ASP:C	2.59	0.44
1:C:202:THR:N	2:C:601:PLP:O3P	2.48	0.44
1:C:247:LYS:HB3	1:C:247:LYS:HE2	1.75	0.44
1:A:156:HIS:O	1:A:157:LYS:HD2	2.18	0.44
1:A:232:GLU:HB3	3:A:405:HOH:O	2.18	0.44
1:A:339:LYS:HG2	1:A:340:THR:N	2.33	0.44
1:B:9:TYR:HB3	1:B:59:VAL:HB	1.99	0.44
1:B:24:LEU:HD21	1:B:300:MET:CE	2.45	0.44
1:B:59:VAL:HG13	1:B:91:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:O	1:B:132:ILE:HD13	2.18	0.44
1:B:141:ARG:NH1	1:B:141:ARG:HB3	2.33	0.44
1:B:54:LYS:NZ	1:B:164:GLY:O	2.44	0.44
1:B:166:SER:HB3	1:B:241:ILE:HD11	1.99	0.44
1:B:195:LYS:CD	1:B:221:ASP:HA	2.45	0.44
1:C:273:ASN:HD22	1:C:275:GLY:H	1.65	0.44
1:A:102:TRP:CD1	1:A:136:PHE:HA	2.52	0.43
1:A:159:TYR:CD1	1:A:160:PRO:HD2	2.53	0.43
1:B:9:TYR:CG	1:B:59:VAL:HG11	2.53	0.43
1:B:269:TYR:HA	3:B:532:HOH:O	2.18	0.43
1:D:21:LEU:HD12	1:D:34:VAL:CG1	2.48	0.43
1:D:254:GLU:CD	1:D:256:LYS:HE3	2.43	0.43
1:D:290:LEU:O	1:D:322:HIS:HE1	2.01	0.43
1:D:308:LYS:HE3	3:D:840:HOH:O	2.16	0.43
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.91	0.43
1:A:138:ILE:HG23	1:A:233:LYS:HZ1	1.83	0.43
1:A:252:GLU:O	1:A:253:HIS:C	2.59	0.43
1:C:32:VAL:CG2	1:C:307:ILE:HD13	2.48	0.43
3:C:618:HOH:O	1:D:281:ARG:HD2	2.18	0.43
1:D:116:VAL:O	1:D:119:ILE:HG22	2.18	0.43
1:B:40:ASP:CB	1:B:324:GLY:HA2	2.48	0.43
1:B:300:MET:O	1:B:304:ILE:HG13	2.18	0.43
1:D:68:THR:OG1	1:D:69:HIS:CD2	2.67	0.43
1:D:69:HIS:CE1	1:D:94:LYS:HD2	2.53	0.43
1:D:73:ILE:HG13	1:D:98:ILE:HB	1.99	0.43
1:A:324:GLY:HA2	3:A:407:HOH:O	2.19	0.43
1:B:267:PRO:HG2	1:B:268:CYS:H	1.84	0.43
1:C:219:GLN:NE2	1:C:253:HIS:CD2	2.86	0.43
1:A:21:LEU:CA	1:A:287:GLU:OE2	2.65	0.43
1:A:23:ARG:NH1	1:A:23:ARG:HG2	2.34	0.43
1:B:68:THR:C	1:B:69:HIS:CD2	2.96	0.43
1:B:283:CYS:O	1:B:287:GLU:HB2	2.18	0.43
1:C:73:ILE:HG12	1:C:74:GLY:N	2.33	0.43
1:C:143:SER:CA	1:C:146:ASN:HD22	2.31	0.43
1:D:5:LYS:HB2	1:D:6:PHE:CD1	2.53	0.43
1:A:112:VAL:CG1	1:A:116:VAL:HG21	2.48	0.43
1:B:207:ALA:O	1:B:210:LEU:HB2	2.19	0.43
1:C:13:PHE:CD1	1:C:42:ASN:O	2.71	0.43
1:D:340:THR:O	1:D:340:THR:HG22	2.18	0.43
1:A:2:GLY:HA3	1:A:249:ILE:O	2.19	0.43
1:A:313:LYS:O	1:A:316:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:HE1	1:B:332:TYR:CE1	2.37	0.43
1:B:142:LYS:O	1:B:142:LYS:HG2	2.19	0.43
1:B:175:PHE:CZ	1:B:205:THR:HG23	2.53	0.43
1:C:290:LEU:HD11	1:D:121:LEU:HD13	2.01	0.43
1:A:273:ASN:HD22	1:A:273:ASN:C	2.27	0.43
1:B:185:GLN:CA	1:B:188:GLU:HG2	2.44	0.43
1:B:202:THR:N	2:B:501:PLP:O3P	2.49	0.43
1:B:280:ILE:HG12	1:B:291:THR:OG1	2.18	0.43
1:A:43:SER:OG	1:A:44:GLY:N	2.51	0.43
1:B:51:THR:OG1	1:B:83:MET:SD	2.77	0.43
1:B:230:THR:HB	1:B:233:LYS:HE2	2.01	0.43
1:C:279:ALA:CB	1:C:301:GLN:HB2	2.49	0.43
1:A:272:PRO:CG	1:A:277:ILE:HD11	2.48	0.43
1:C:103:VAL:HA	1:C:104:PRO:HD3	1.82	0.43
1:C:149:GLN:HE21	1:C:153:ASP:CG	2.27	0.43
1:A:77:GLN:NE2	1:A:77:GLN:HA	2.34	0.42
1:A:120:GLU:OE2	1:B:333:SER:CA	2.61	0.42
1:B:59:VAL:HB	1:B:60:PRO:HD3	1.99	0.42
1:B:311:TYR:O	1:B:311:TYR:CD2	2.72	0.42
1:C:15:PRO:HB3	1:C:181:GLU:OE1	2.19	0.42
1:D:255:PHE:N	1:D:255:PHE:CD1	2.86	0.42
1:D:191:ILE:N	1:D:191:ILE:CD1	2.82	0.42
1:A:187:VAL:O	1:D:169:LYS:CE	2.67	0.42
1:B:175:PHE:HA	1:B:178:PHE:HB2	2.00	0.42
1:C:36:ALA:HA	1:C:320:TYR:O	2.20	0.42
1:D:59:VAL:HA	1:D:62:ILE:HD12	2.01	0.42
1:D:268:CYS:HB2	3:D:727:HOH:O	2.19	0.42
1:A:116:VAL:CG1	1:B:330:SER:HB3	2.42	0.42
1:A:151:LEU:C	1:A:153:ASP:N	2.77	0.42
1:A:199:CYS:HB2	1:A:295:TYR:O	2.19	0.42
1:A:279:ALA:HB2	1:A:301:GLN:HB3	2.02	0.42
1:B:109:GLU:HG2	1:B:331:ALA:O	2.19	0.42
1:B:195:LYS:HA	1:B:221:ASP:O	2.20	0.42
1:D:73:ILE:HD11	1:D:100:GLU:OE2	2.19	0.42
1:D:182:VAL:O	1:D:183:ILE:C	2.62	0.42
1:A:119:ILE:O	1:A:120:GLU:C	2.63	0.42
1:A:287:GLU:HA	1:A:287:GLU:OE1	2.19	0.42
1:B:22:ASN:CG	1:B:23:ARG:H	2.26	0.42
1:B:197:VAL:HA	1:B:223:ILE:O	2.18	0.42
1:D:11:LEU:HB2	1:D:56:GLU:HG2	2.00	0.42
1:D:232:GLU:HB2	3:D:847:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:O	1:A:117:GLY:C	2.60	0.42
1:B:18:ILE:HG23	1:B:319:LEU:HD11	2.02	0.42
1:B:235:LYS:CE	1:B:260:LEU:HB3	2.49	0.42
1:C:28:LEU:HD22	1:C:308:LYS:CE	2.50	0.42
1:C:32:VAL:HG21	1:C:307:ILE:CD1	2.49	0.42
1:D:102:TRP:CD1	1:D:136:PHE:HA	2.54	0.42
1:B:102:TRP:HB3	1:B:269:TYR:CE2	2.54	0.42
1:B:217:GLY:C	1:B:219:GLN:NE2	2.77	0.42
1:A:82:ARG:NH1	1:A:83:MET:HE2	2.34	0.42
1:A:136:PHE:O	1:A:137:ASP:HB2	2.20	0.42
1:A:150:GLU:O	1:A:153:ASP:HB2	2.19	0.42
1:B:107:GLU:C	1:B:109:GLU:N	2.78	0.42
1:B:116:VAL:C	3:B:529:HOH:O	2.63	0.42
1:C:209:ILE:O	1:C:213:MET:HG2	2.18	0.42
1:B:26:GLN:HA	1:B:30:SER:OG	2.20	0.42
1:B:53:ARG:NH1	1:B:181:GLU:OE2	2.47	0.42
1:B:77:GLN:OE1	1:B:77:GLN:HA	2.19	0.42
1:C:85:ALA:CB	1:C:125:MET:HE3	2.50	0.42
1:A:121:LEU:HD22	1:B:290:LEU:CD1	2.48	0.41
1:A:144:PHE:C	1:A:146:ASN:N	2.75	0.41
1:A:311:TYR:CD2	1:A:311:TYR:C	2.97	0.41
1:C:23:ARG:HD3	1:D:90:LYS:O	2.20	0.41
1:C:71:VAL:HG22	1:C:96:VAL:HB	2.01	0.41
1:C:109:GLU:OE1	1:C:109:GLU:HA	2.20	0.41
1:C:219:GLN:OE1	1:C:219:GLN:N	2.42	0.41
1:C:264:PHE:CZ	1:C:302:GLY:HA2	2.55	0.41
1:D:180:ASP:OD2	1:D:215:GLN:NE2	2.52	0.41
1:D:187:VAL:O	1:D:187:VAL:CG1	2.68	0.41
1:A:68:THR:OG1	1:A:69:HIS:CD2	2.74	0.41
1:A:74:GLY:O	1:A:99:GLN:HA	2.20	0.41
1:A:75:GLY:H	1:A:78:SER:HB2	1.85	0.41
1:A:279:ALA:O	1:A:280:ILE:C	2.63	0.41
1:B:39:GLU:C	1:B:41:CYS:H	2.28	0.41
1:C:142:LYS:O	1:C:146:ASN:ND2	2.53	0.41
1:A:69:HIS:NE2	1:A:156:HIS:CG	2.88	0.41
1:A:105:ILE:CG2	1:A:110:LYS:HA	2.48	0.41
1:A:124:ILE:C	1:A:126:GLY:N	2.75	0.41
1:C:82:ARG:HA	1:C:122:SER:OG	2.20	0.41
1:A:309:GLU:O	1:A:310:ASP:C	2.63	0.41
1:C:53:ARG:CB	3:C:720:HOH:O	2.61	0.41
1:C:122:SER:O	1:C:127:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HG13	1:C:228:SER:HB3	2.02	0.41
1:C:293:PRO:HD3	1:C:329:LEU:CD2	2.50	0.41
1:C:293:PRO:HD3	1:C:329:LEU:HD23	2.01	0.41
3:C:721:HOH:O	1:D:23:ARG:HD2	2.20	0.41
1:D:181:GLU:O	1:D:185:GLN:HG3	2.21	0.41
1:A:75:GLY:C	1:A:77:GLN:N	2.78	0.41
1:B:131:VAL:C	1:B:132:ILE:HG12	2.46	0.41
1:B:217:GLY:C	1:B:219:GLN:HE22	2.29	0.41
1:D:163:ALA:C	1:D:165:CYS:N	2.78	0.41
1:D:55:LEU:HD13	1:D:87:LEU:CD2	2.51	0.41
1:D:290:LEU:O	1:D:322:HIS:CE1	2.74	0.41
1:A:99:GLN:NE2	1:A:99:GLN:CA	2.84	0.41
1:A:156:HIS:C	1:A:157:LYS:HD2	2.45	0.41
1:A:290:LEU:HG	1:B:46:ALA:HA	2.03	0.41
1:B:235:LYS:HE3	1:B:260:LEU:HB3	2.03	0.41
1:C:43:SER:HB3	1:C:52:LEU:CD2	2.50	0.41
1:C:305:ALA:O	1:C:306:LEU:C	2.62	0.41
1:A:99:GLN:HE21	1:A:99:GLN:CA	2.29	0.41
1:A:137:ASP:HA	1:A:233:LYS:NZ	2.36	0.41
1:A:177:GLY:O	1:A:180:ASP:HB2	2.20	0.41
1:B:42:ASN:HD22	1:B:49:GLY:CA	2.33	0.41
1:B:67:TYR:CE1	1:B:159:TYR:CD1	3.07	0.41
1:D:58:ILE:HG23	3:D:837:HOH:O	2.19	0.41
1:A:96:VAL:HA	1:A:128:ASP:HB3	2.03	0.41
1:B:18:ILE:CG1	1:B:37:LYS:HG3	2.50	0.41
1:B:77:GLN:O	1:B:78:SER:C	2.62	0.41
1:B:97:LEU:HD12	1:B:122:SER:HB3	2.03	0.41
1:B:185:GLN:HA	1:B:188:GLU:OE2	2.20	0.41
1:B:236:GLU:OE1	1:B:236:GLU:C	2.64	0.41
1:B:281:ARG:HH21	1:B:336:PHE:HA	1.86	0.41
1:C:8:LYS:HD3	1:C:57:TYR:CE1	2.56	0.41
1:C:112:VAL:HG13	1:C:116:VAL:CG2	2.51	0.41
1:C:162:PRO:HG3	3:C:656:HOH:O	2.20	0.41
1:C:167:GLU:HG3	3:C:642:HOH:O	2.21	0.41
1:C:282:THR:O	1:C:286:GLN:HG2	2.21	0.41
1:D:58:ILE:HA	3:D:837:HOH:O	2.20	0.41
1:D:76:ARG:HA	1:D:76:ARG:HD3	1.80	0.41
1:D:226:ASP:CB	1:D:260:LEU:HD11	2.38	0.41
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.86	0.41
1:A:105:ILE:O	1:A:106:PRO:C	2.63	0.41
1:A:170:TYR:O	1:A:172:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:OD1	1:B:327:PRO:HB2	2.21	0.41
1:C:43:SER:CB	1:C:52:LEU:HD23	2.51	0.41
1:C:45:LEU:HD21	1:C:90:LYS:HD3	2.03	0.41
1:D:96:VAL:HG21	1:D:151:LEU:HD21	2.01	0.41
1:D:176:VAL:HG11	1:D:249:ILE:HG21	2.02	0.41
1:A:325:GLY:C	1:A:327:PRO:CD	2.94	0.40
1:B:202:THR:OG1	2:B:501:PLP:O3P	2.38	0.40
1:C:69:HIS:ND1	1:C:94:LYS:CB	2.84	0.40
1:C:324:GLY:HA2	3:C:622:HOH:O	2.20	0.40
1:B:73:ILE:HB	1:B:144:PHE:HD1	1.85	0.40
1:B:305:ALA:O	1:B:308:LYS:HB2	2.21	0.40
1:D:51:THR:HG21	1:D:80:GLN:CB	2.51	0.40
1:D:168:HIS:ND1	1:D:168:HIS:C	2.80	0.40
1:A:310:ASP:HA	3:A:403:HOH:O	2.21	0.40
1:B:70:LEU:HD11	1:B:87:LEU:CD1	2.46	0.40
1:B:88:ALA:CB	1:B:95:CYS:HB2	2.52	0.40
1:C:38:ARG:HH12	1:D:44:GLY:HA3	1.86	0.40
1:C:42:ASN:HB2	3:C:708:HOH:O	2.21	0.40
1:C:229:PHE:CB	1:C:268:CYS:HA	2.51	0.40
1:D:264:PHE:HB3	1:D:301:GLN:NE2	2.36	0.40
1:D:279:ALA:HB2	1:D:301:GLN:HA	2.03	0.40
1:B:198:VAL:HB	1:B:321:VAL:HB	2.02	0.40
1:D:80:GLN:HB3	3:D:743:HOH:O	2.22	0.40
1:D:306:LEU:HD12	1:D:306:LEU:HA	1.82	0.40
1:A:78:SER:C	1:A:118:ASN:HD22	2.29	0.40
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.94	0.40
1:B:80:GLN:OE1	1:B:164:GLY:HA2	2.20	0.40
1:B:170:TYR:N	1:B:170:TYR:CD2	2.89	0.40
1:C:206:THR:HG22	1:C:210:LEU:HG	2.04	0.40
1:D:3:VAL:C	1:D:5:LYS:N	2.80	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	339/341 (99%)	271 (80%)	51 (15%)	17 (5%)	1	2
1	B	339/341 (99%)	257 (76%)	63 (19%)	19 (6%)	1	2
1	C	339/341 (99%)	303 (89%)	34 (10%)	2 (1%)	21	38
1	D	339/341 (99%)	296 (87%)	36 (11%)	7 (2%)	5	11
All	All	1356/1364 (99%)	1127 (83%)	184 (14%)	45 (3%)	3	5

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	232	GLU
1	B	204	SER
1	B	231	SER
1	B	267	PRO
1	D	30	SER
1	A	76	ARG
1	A	113	TYR
1	A	137	ASP
1	A	144	PHE
1	A	145	ALA
1	A	171	GLY
1	A	231	SER
1	B	109	GLU
1	B	259	THR
1	B	261	ASP
1	B	296	GLU
1	B	335	PHE
1	D	337	PRO
1	A	10	PRO
1	A	64	GLU
1	A	162	PRO
1	A	253	HIS
1	B	232	GLU
1	C	112	VAL
1	C	231	SER
1	D	66	ASP
1	D	100	GLU
1	D	231	SER
1	A	309	GLU

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Mol	Chain	Res	Type
1	B	253	HIS
1	B	274	GLU
1	B	309	GLU
1	D	132	ILE
1	B	2	GLY
1	B	77	GLN
1	B	201	VAL
1	B	21	LEU
1	B	105	ILE
1	B	138	ILE
1	A	92	GLY
1	A	272	PRO
1	B	223	ILE
1	D	116	VAL
1	A	29	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	275/275 (100%)	266 (97%)	9 (3%)	33	57
1	B	275/275 (100%)	263 (96%)	12 (4%)	25	47
1	C	275/275 (100%)	264 (96%)	11 (4%)	28	50
1	D	275/275 (100%)	262 (95%)	13 (5%)	23	45
All	All	1100/1100 (100%)	1055 (96%)	45 (4%)	27	49

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	20	ASN
1	A	52	LEU
1	A	60	PRO
1	A	107	GLU
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	273	ASN
1	A	291	THR
1	A	303	LEU
1	B	23	ARG
1	B	52	LEU
1	B	71	VAL
1	B	99	GLN
1	B	107	GLU
1	B	141	ARG
1	B	201	VAL
1	B	236	GLU
1	B	247	LYS
1	B	252	GLU
1	B	273	ASN
1	B	296	GLU
1	C	52	LEU
1	C	76	ARG
1	C	87	LEU
1	C	99	GLN
1	C	112	VAL
1	C	236	GLU
1	C	239	LEU
1	C	273	ASN
1	C	303	LEU
1	C	306	LEU
1	C	327	PRO
1	D	31	LYS
1	D	51	THR
1	D	52	LEU
1	D	77	GLN
1	D	151	LEU
1	D	231	SER
1	D	232	GLU
1	D	239	LEU
1	D	296	GLU
1	D	303	LEU
1	D	306	LEU
1	D	338	THR
1	D	339	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	77	GLN
1	A	99	GLN
1	A	118	ASN
1	A	146	ASN
1	A	184	ASN
1	A	215	GLN
1	A	219	GLN
1	A	273	ASN
1	A	322	HIS
1	B	20	ASN
1	B	26	GLN
1	B	42	ASN
1	B	77	GLN
1	B	114	ASN
1	B	146	ASN
1	B	156	HIS
1	B	215	GLN
1	B	219	GLN
1	B	273	ASN
1	B	301	GLN
1	B	322	HIS
1	C	20	ASN
1	C	69	HIS
1	C	77	GLN
1	C	146	ASN
1	C	149	GLN
1	C	156	HIS
1	C	273	ASN
1	C	301	GLN
1	C	322	HIS
1	D	20	ASN
1	D	69	HIS
1	D	77	GLN
1	D	184	ASN
1	D	253	HIS
1	D	273	ASN
1	D	322	HIS

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	D	701	-	15,15,16	1.57	3 (20%)	21,22,23	2.03	3 (14%)
2	PLP	A	401	-	15,15,16	1.77	4 (26%)	21,22,23	1.82	3 (14%)
2	PLP	B	501	-	15,15,16	1.80	4 (26%)	21,22,23	1.87	3 (14%)
2	PLP	C	601	-	15,15,16	1.69	4 (26%)	21,22,23	1.98	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	701	-	-	0/6/6/8	0/1/1/1
2	PLP	A	401	-	-	0/6/6/8	0/1/1/1
2	PLP	B	501	-	-	2/6/6/8	0/1/1/1
2	PLP	C	601	-	-	0/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLP	C5-C4	3.64	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	PLP	C5-C4	3.46	1.44	1.40
2	A	401	PLP	C5-C4	3.43	1.44	1.40
2	B	501	PLP	C2-N1	3.23	1.39	1.33
2	A	401	PLP	C2-N1	3.21	1.39	1.33
2	D	701	PLP	C5-C4	3.20	1.44	1.40
2	C	601	PLP	C2-N1	2.97	1.39	1.33
2	B	501	PLP	C2A-C2	2.54	1.54	1.50
2	C	601	PLP	P-O3P	-2.48	1.45	1.54
2	D	701	PLP	P-O3P	-2.41	1.45	1.54
2	B	501	PLP	P-O3P	-2.39	1.45	1.54
2	A	401	PLP	C2A-C2	2.35	1.54	1.50
2	A	401	PLP	P-O3P	-2.31	1.46	1.54
2	D	701	PLP	C2-N1	2.23	1.37	1.33
2	C	601	PLP	C2A-C2	2.22	1.53	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	PLP	O4P-C5A-C5	7.15	122.76	109.36
2	C	601	PLP	O4P-C5A-C5	6.45	121.45	109.36
2	B	501	PLP	O4P-C5A-C5	6.10	120.80	109.36
2	A	401	PLP	O4P-C5A-C5	5.77	120.17	109.36
2	C	601	PLP	C5A-C5-C6	-2.43	115.41	119.36
2	B	501	PLP	C5-C6-N1	-2.35	120.00	123.83
2	A	401	PLP	C5-C6-N1	-2.34	120.03	123.83
2	D	701	PLP	C5A-C5-C6	-2.23	115.73	119.36
2	C	601	PLP	C5-C6-N1	-2.22	120.22	123.83
2	D	701	PLP	C5-C6-N1	-2.20	120.25	123.83
2	A	401	PLP	C5A-C5-C6	-2.16	115.84	119.36
2	B	501	PLP	C5A-C5-C6	-2.15	115.85	119.36
2	C	601	PLP	C4A-C4-C5	2.11	123.11	120.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C4-C5-C5A-O4P
2	B	501	PLP	C6-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	PLP	1	0
2	A	401	PLP	1	0
2	B	501	PLP	2	0
2	C	601	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.