



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:18 PM UTC

PDB ID : 3Q0K / pdb_00003q0k
Title : Crystal structure of Human PACSIN 2 F-BAR
Authors : Bai, X.; Meng, G.; Zheng, X.
Deposited on : 2010-12-15
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

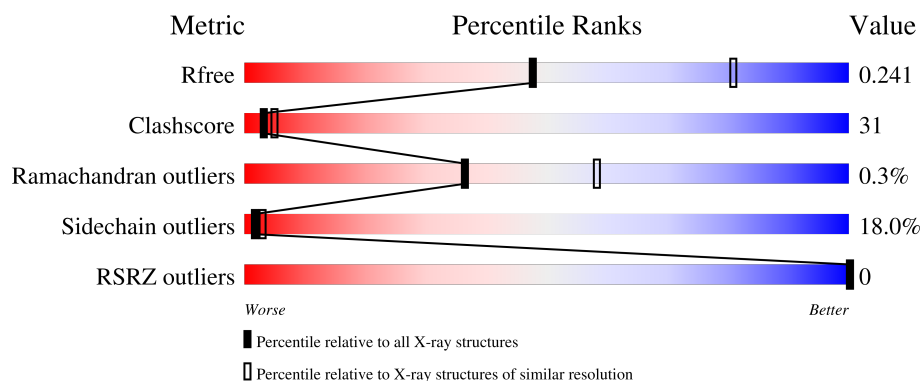
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9729 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 Protein kinase C and casein kinase substrate in neurons protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2380	1499	427	439	15			
1	B	287	Total	C	N	O	S	0	0	0
			2373	1493	427	438	15			
1	C	287	Total	C	N	O	S	0	0	0
			2379	1494	428	442	15			
1	D	289	Total	C	N	O	S	0	0	0
			2391	1504	429	443	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

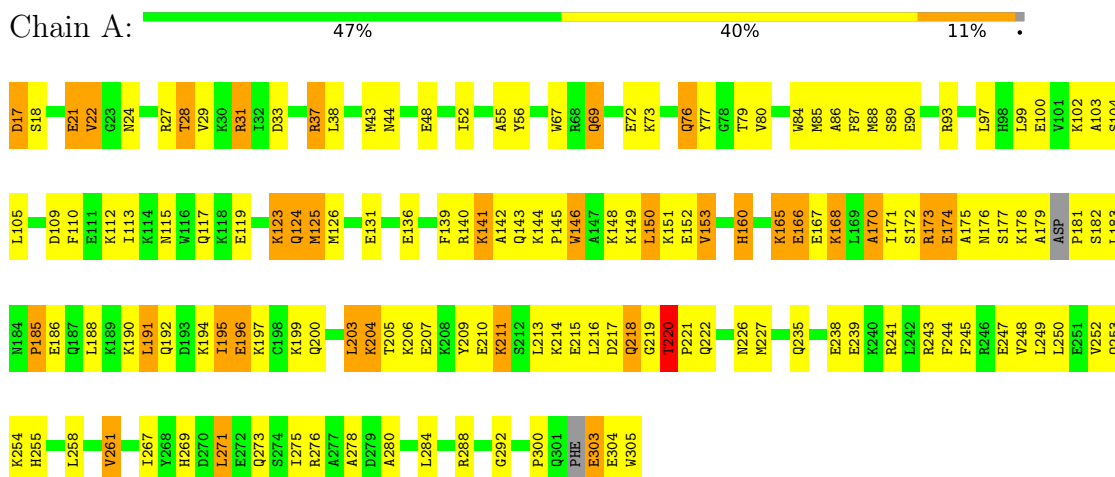
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	43	Total	O	0	0
			43	43		
3	C	42	Total	O	0	0
			42	42		
3	D	56	Total	O	0	0
			56	56		

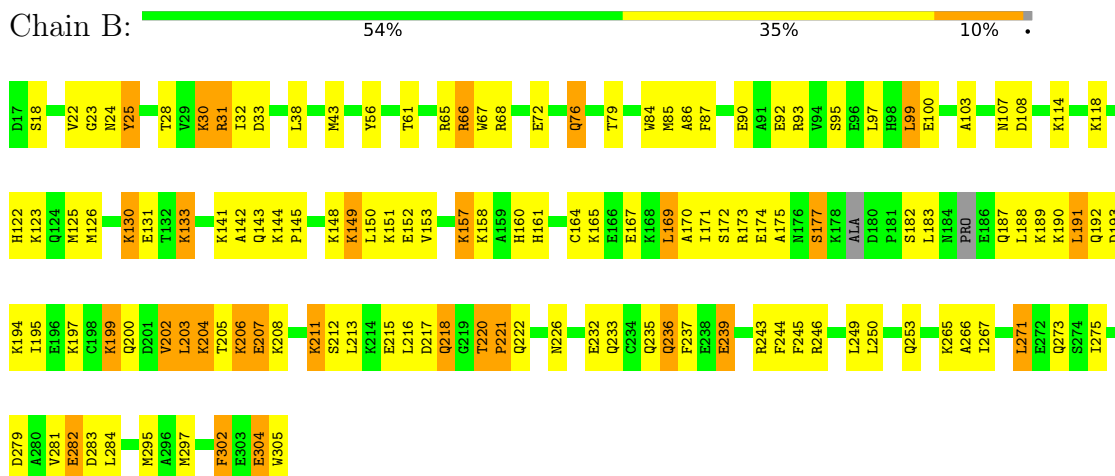
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 2

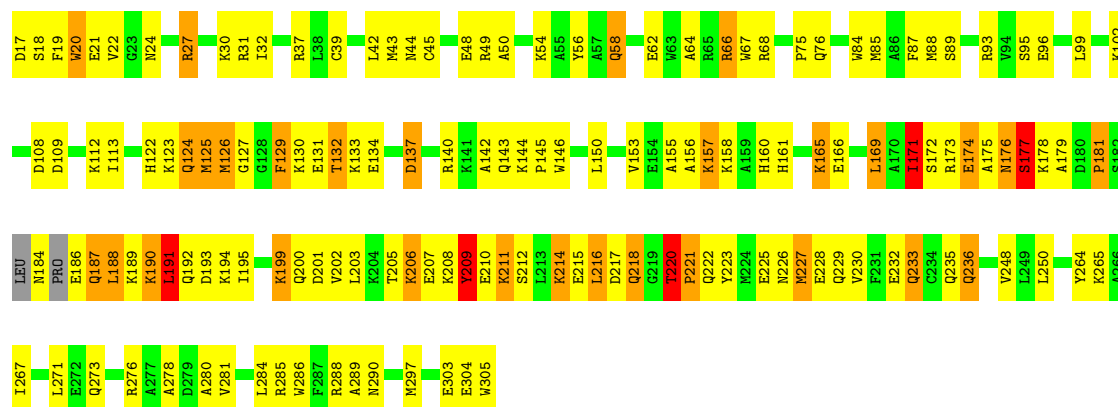


- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 2



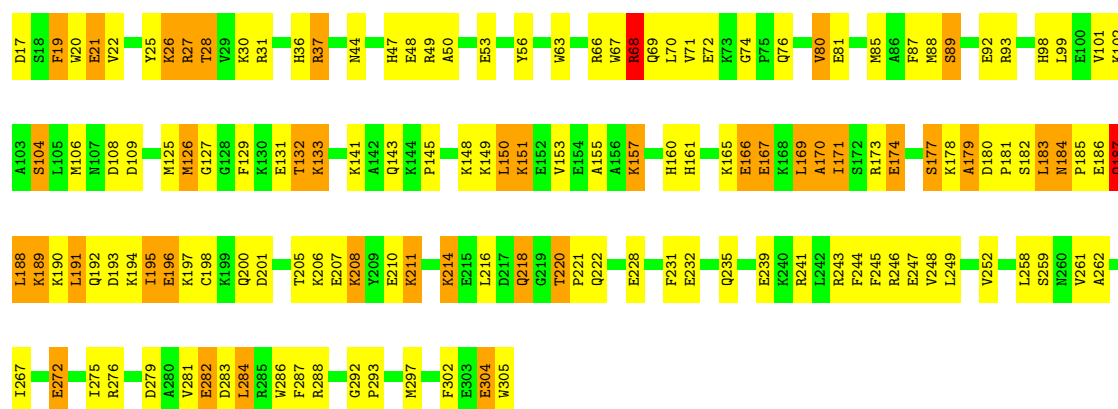
- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 2





- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 2

Chain D: 50% 36% 13% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	31.56Å 353.59Å 86.05Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	29.63 – 2.60 29.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	80.7 (29.63-2.60) 80.6 (29.63-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.201 , 0.292 0.204 , 0.241	Depositor DCC
R_{free} test set	2358 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 13.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9729	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.35	1/2429 (0.0%)	1.24	22/3249 (0.7%)
1	B	1.32	2/2421 (0.1%)	1.22	17/3238 (0.5%)
1	C	1.35	2/2426 (0.1%)	1.30	25/3244 (0.8%)
1	D	1.27	0/2442	1.27	24/3272 (0.7%)
All	All	1.32	5/9718 (0.1%)	1.26	88/13003 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	218	GLN	C-O	6.25	1.31	1.24
1	B	218	GLN	C-O	5.44	1.30	1.24
1	A	55	ALA	CA-CB	-5.24	1.44	1.53
1	C	37	ARG	C-O	-5.24	1.17	1.24
1	B	266	ALA	C-O	-5.00	1.17	1.24

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	155	ALA	N-CA-C	-9.83	100.52	111.14
1	D	68	ARG	N-CA-C	-9.13	101.27	111.14
1	B	108	ASP	N-CA-C	9.06	124.74	111.96
1	C	191	LEU	N-CA-C	8.42	120.08	111.07
1	A	21	GLU	N-CA-C	-8.29	98.01	110.28
1	C	99	LEU	N-CA-C	-8.14	103.48	113.50
1	D	74	GLY	CA-C-N	8.04	128.23	119.87
1	D	74	GLY	C-N-CA	8.04	128.23	119.87
1	A	99	LEU	N-CA-C	-8.03	102.11	112.23
1	D	101	VAL	N-CA-C	-7.93	102.96	110.42
1	D	170	ALA	N-CA-C	-7.69	102.98	111.36
1	B	220	THR	CA-C-N	-7.62	110.59	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	THR	C-N-CA	-7.62	110.59	119.05
1	A	171	ILE	N-CA-C	7.56	118.35	110.72
1	D	80	VAL	N-CA-C	-7.54	103.95	113.22
1	D	183	LEU	N-CA-C	7.53	119.57	111.36
1	C	68	ARG	N-CA-C	-7.52	103.08	111.28
1	A	220	THR	CA-C-N	-7.47	111.20	118.97
1	A	220	THR	C-N-CA	-7.47	111.20	118.97
1	D	70	LEU	N-CA-C	7.29	119.31	111.36
1	D	179	ALA	N-CA-C	-7.26	98.74	110.20
1	C	75	PRO	N-CA-C	7.21	122.18	114.68
1	D	151	LYS	N-CA-C	-7.04	103.66	111.82
1	B	182	SER	N-CA-C	7.03	118.94	111.28
1	D	267	ILE	N-CA-C	-6.90	104.05	110.53
1	C	171	ILE	CB-CA-C	-6.79	103.28	111.97
1	C	108	ASP	N-CA-C	6.75	121.66	112.68
1	B	130	LYS	N-CA-C	-6.73	103.87	111.07
1	B	125	MET	N-CA-C	6.68	119.40	111.71
1	C	199	LYS	N-CA-C	-6.63	104.05	111.28
1	C	209	TYR	N-CA-C	-6.56	105.38	113.19
1	C	220	THR	CA-C-N	-6.56	111.77	119.05
1	C	220	THR	C-N-CA	-6.56	111.77	119.05
1	A	110	PHE	N-CA-C	-6.34	104.46	111.82
1	A	86	ALA	N-CA-C	-6.30	104.51	111.82
1	B	161	HIS	N-CA-C	-6.28	105.62	113.28
1	B	33	ASP	N-CA-C	-6.22	104.40	112.23
1	D	81	GLU	N-CA-C	-6.21	104.40	112.23
1	C	176	ASN	CA-C-N	-6.20	112.41	122.26
1	C	176	ASN	C-N-CA	-6.20	112.41	122.26
1	B	267	ILE	CB-CA-C	-6.12	104.14	111.97
1	C	285	ARG	N-CA-C	-5.96	104.79	111.28
1	B	221	PRO	CA-C-N	-5.95	112.30	120.28
1	B	221	PRO	C-N-CA	-5.95	112.30	120.28
1	A	141	LYS	O-C-N	5.95	128.44	122.08
1	C	32	ILE	N-CA-C	5.93	116.05	110.30
1	A	52	ILE	N-CA-C	5.93	116.58	110.36
1	B	183	LEU	N-CA-C	5.77	117.03	108.60
1	C	289	ALA	N-CA-C	5.75	117.63	111.36
1	D	99	LEU	N-CA-C	-5.72	105.18	111.82
1	D	189	LYS	N-CA-C	-5.72	105.05	111.28
1	A	125	MET	N-CA-C	-5.72	102.18	110.24
1	B	218	GLN	CA-C-O	5.71	126.60	120.55
1	B	25	TYR	N-CA-C	-5.70	106.36	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	ASP	CA-C-N	5.67	128.15	120.38
1	D	109	ASP	C-N-CA	5.67	128.15	120.38
1	C	137	ASP	N-CA-C	-5.65	105.89	112.89
1	C	211	LYS	N-CA-C	-5.58	105.20	111.28
1	A	247	GLU	CA-C-N	5.55	128.31	120.42
1	A	247	GLU	C-N-CA	5.55	128.31	120.42
1	D	262	ALA	N-CA-C	-5.55	101.16	109.15
1	A	194	LYS	N-CA-C	-5.53	105.40	111.82
1	A	292	GLY	CA-C-N	5.49	125.16	119.56
1	A	292	GLY	C-N-CA	5.49	125.16	119.56
1	A	172	SER	N-CA-C	5.46	117.23	111.28
1	C	130	LYS	N-CA-C	-5.43	105.36	111.28
1	D	286	TRP	N-CA-C	-5.42	105.28	111.14
1	C	250	LEU	N-CA-C	-5.41	105.46	111.36
1	C	20	TRP	N-CA-C	5.41	119.14	112.54
1	D	304	GLU	N-CA-C	5.38	119.85	113.12
1	D	222	GLN	N-CA-C	-5.38	105.58	111.82
1	B	202	VAL	N-CA-C	-5.37	105.26	110.42
1	D	187	GLN	N-CA-C	-5.36	106.59	113.02
1	A	269	HIS	N-CA-C	-5.35	105.35	111.07
1	A	170	ALA	O-C-N	-5.30	115.75	122.27
1	A	67	TRP	N-CA-C	5.28	117.95	111.82
1	D	208	LYS	N-CA-C	5.25	116.81	111.14
1	C	129	PHE	N-CA-C	5.22	118.00	109.59
1	C	67	TRP	N-CA-C	5.22	117.88	111.82
1	C	177	SER	N-CA-C	-5.17	106.99	113.72
1	A	90	GLU	N-CA-C	5.12	116.86	111.28
1	A	151	LYS	N-CA-C	-5.12	105.78	112.23
1	C	221	PRO	CA-C-N	-5.08	113.84	120.44
1	C	221	PRO	C-N-CA	-5.08	113.84	120.44
1	B	190	LYS	N-CA-C	-5.05	105.77	111.28
1	A	160	HIS	N-CA-C	5.04	116.86	111.36
1	D	127	GLY	N-CA-C	-5.03	107.17	111.95
1	B	65	ARG	N-CA-C	-5.00	105.74	111.14

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	2380	0	2334	179	1
1	B	2373	0	2314	142	1
1	C	2379	0	2319	159	2
1	D	2391	0	2334	148	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	61	0	0	3	0
3	B	43	0	0	4	0
3	C	42	0	0	8	0
3	D	56	0	0	1	0
All	All	9729	0	9301	583	3

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 31.

All (583) 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:188:LEU:O	1:A:188:LEU:HD23	1.34	1.25
1:B:217:ASP:O	1:B:220:THR:HG22	1.38	1.23
1:B:217:ASP:O	1:B:221:PRO:HD3	1.37	1.23
1:A:177:SER:HB3	1:A:178:LYS:C	1.62	1.23
1:B:218:GLN:O	1:B:221:PRO:HD2	1.33	1.23
1:A:213:LEU:CD2	1:B:302:PHE:HD2	1.52	1.22
1:A:217:ASP:O	1:A:221:PRO:HD3	1.33	1.22
1:A:177:SER:HB3	1:A:179:ALA:N	1.55	1.20
1:A:218:GLN:O	1:A:221:PRO:HD2	1.38	1.20
1:A:141:LYS:O	1:A:145:PRO:HD3	1.41	1.16
1:A:166:GLU:OE2	1:A:166:GLU:HA	1.47	1.14
1:B:174:GLU:HA	1:B:177:SER:OG	1.45	1.12
1:A:167:GLU:HG2	1:A:168:LYS:HE3	1.23	1.11
1:A:146:TRP:HZ3	1:A:220:THR:HG22	0.95	1.10
1:A:146:TRP:CZ3	1:A:220:THR:HG22	1.86	1.10
1:B:187:GLN:H	1:B:187:GLN:NE2	1.50	1.09
1:C:126:MET:HE3	1:C:126:MET:HA	1.27	1.09
1:D:188:LEU:HD12	1:D:188:LEU:C	1.75	1.09
1:C:169:LEU:O	1:C:169:LEU:HD23	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLU:OE1	1:D:166:GLU:HA	1.47	1.07
1:A:177:SER:H	1:A:178:LYS:CA	1.66	1.06
1:A:181:PRO:HA	1:A:182:SER:HB3	1.07	1.06
1:A:177:SER:H	1:A:178:LYS:HA	0.99	1.06
1:B:157:LYS:NZ	1:B:157:LYS:HB3	1.66	1.06
1:D:214:LYS:HD2	1:D:214:LYS:O	1.56	1.05
1:C:125:MET:O	1:C:126:MET:HE3	1.56	1.04
1:D:188:LEU:C	1:D:188:LEU:CD1	2.30	1.04
1:B:174:GLU:HB2	1:B:191:LEU:HD21	1.39	1.04
1:A:177:SER:N	1:A:178:LYS:HA	1.68	1.03
1:D:160:HIS:HE1	1:D:206:LYS:HB2	1.21	1.03
1:A:177:SER:CB	1:A:178:LYS:C	2.30	1.03
1:C:218:GLN:O	1:C:221:PRO:HD2	1.58	1.03
1:C:171:ILE:HD12	1:C:195:ILE:HD12	1.40	1.03
1:C:265:LYS:HE3	3:C:515:HOH:O	1.58	1.02
1:C:171:ILE:HD12	1:C:195:ILE:CD1	1.89	1.02
1:D:214:LYS:HD2	1:D:214:LYS:C	1.84	1.02
1:A:188:LEU:HD23	1:A:188:LEU:C	1.85	1.02
1:A:213:LEU:CD2	1:B:302:PHE:CD2	2.45	1.00
1:A:213:LEU:HD23	1:B:302:PHE:HD2	1.23	0.98
1:B:99:LEU:HD13	1:B:99:LEU:O	1.61	0.98
1:B:157:LYS:HB3	1:B:157:LYS:HZ3	1.19	0.98
1:A:213:LEU:HD23	1:B:302:PHE:CD2	2.01	0.96
1:D:37:ARG:HG2	1:D:37:ARG:HH11	1.28	0.95
1:A:200:GLN:HA	1:A:203:LEU:HD23	1.46	0.95
1:B:174:GLU:HB2	1:B:191:LEU:CD2	1.96	0.95
1:C:143:GLN:C	1:C:145:PRO:HD2	1.92	0.95
1:A:181:PRO:CA	1:A:182:SER:HB3	1.96	0.94
1:C:54:LYS:NZ	1:C:58:GLN:HE22	1.64	0.94
1:A:175:ALA:O	1:A:177:SER:HA	1.68	0.94
1:C:126:MET:HA	1:C:126:MET:CE	1.97	0.93
1:D:153:VAL:O	1:D:157:LYS:HG2	1.68	0.93
1:C:286:TRP:CE2	1:C:290:ASN:ND2	2.36	0.92
1:B:174:GLU:CB	1:B:191:LEU:HD21	2.00	0.92
1:C:216:LEU:O	1:C:220:THR:HG23	1.70	0.91
1:D:37:ARG:HH11	1:D:37:ARG:CG	1.81	0.91
1:B:169:LEU:HD13	1:B:172:SER:OG	1.70	0.91
1:A:177:SER:HB3	1:A:179:ALA:CA	1.99	0.91
1:A:181:PRO:HA	1:A:182:SER:CB	1.95	0.91
1:C:218:GLN:C	1:C:221:PRO:HD2	1.96	0.91
1:A:146:TRP:HZ3	1:A:220:THR:CG2	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HD13	1:A:195:ILE:N	1.86	0.90
1:D:129:PHE:HB2	1:D:132:THR:HG22	1.54	0.89
1:B:79:THR:HG21	1:B:279:ASP:H	1.35	0.89
1:C:58:GLN:O	1:C:62:GLU:HG3	1.71	0.89
1:A:142:ALA:HB1	1:A:226:ASN:HB3	1.53	0.88
1:C:169:LEU:C	1:C:169:LEU:CD2	2.47	0.88
1:D:31:ARG:HH22	1:D:235:GLN:NE2	1.71	0.88
1:D:31:ARG:HH22	1:D:235:GLN:HE22	0.92	0.88
1:B:157:LYS:NZ	1:B:157:LYS:CB	2.37	0.88
1:B:122:HIS:HD2	1:B:131:GLU:OE1	1.57	0.87
1:C:217:ASP:O	1:C:221:PRO:HD3	1.74	0.86
1:D:126:MET:SD	1:D:126:MET:N	2.48	0.86
1:D:44:ASN:O	1:D:48:GLU:HG3	1.76	0.86
1:A:222:GLN:HA	1:A:222:GLN:HE21	1.41	0.85
1:D:188:LEU:O	1:D:188:LEU:HD13	1.75	0.85
1:C:54:LYS:CE	1:C:58:GLN:HE22	1.89	0.85
1:A:44:ASN:O	1:A:48:GLU:HG3	1.78	0.84
1:B:174:GLU:CA	1:B:191:LEU:HD21	2.08	0.84
1:C:303:GLU:O	1:D:161:HIS:CE1	2.30	0.84
1:A:195:ILE:N	1:A:195:ILE:CD1	2.40	0.84
1:B:218:GLN:C	1:B:221:PRO:HD2	2.02	0.84
1:D:31:ARG:NH2	1:D:235:GLN:HE22	1.74	0.83
1:A:191:LEU:O	1:A:195:ILE:HD13	1.77	0.83
1:C:169:LEU:HD23	1:C:169:LEU:C	2.03	0.83
1:D:184:ASN:N	1:D:185:PRO:HD3	1.93	0.82
1:C:127:GLY:HA2	3:C:6:HOH:O	1.77	0.82
1:C:21:GLU:HG3	1:D:297:MET:HE1	1.62	0.82
1:D:160:HIS:CE1	1:D:206:LYS:HB2	2.11	0.82
1:D:145:PRO:HA	1:D:148:LYS:HE3	1.62	0.82
1:A:209:TYR:O	1:A:213:LEU:HD13	1.78	0.82
1:C:171:ILE:HG22	1:C:172:SER:N	1.95	0.81
1:C:232:GLU:O	1:C:236:GLN:HG2	1.79	0.81
1:B:304:GLU:O	1:B:305:TRP:HB3	1.80	0.81
1:D:214:LYS:NZ	1:D:218:GLN:HB3	1.96	0.81
1:C:218:GLN:O	1:C:221:PRO:CD	2.30	0.80
1:C:217:ASP:O	1:C:221:PRO:CD	2.30	0.80
1:A:209:TYR:O	1:A:213:LEU:CD1	2.30	0.80
1:C:177:SER:O	1:C:181:PRO:CB	2.30	0.80
1:B:188:LEU:HG	1:B:189:LYS:N	1.97	0.80
1:D:182:SER:OG	1:D:183:LEU:CD1	2.30	0.80
1:A:303:GLU:HB2	1:B:157:LYS:CE	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:O	1:C:220:THR:CG2	2.30	0.79
1:B:304:GLU:O	1:B:305:TRP:CB	2.30	0.79
1:A:304:GLU:O	1:A:305:TRP:HB2	1.80	0.79
1:B:187:GLN:NE2	1:B:187:GLN:N	2.30	0.79
1:C:156:ALA:HB1	1:C:209:TYR:HB2	1.65	0.79
1:C:125:MET:O	1:C:126:MET:CE	2.30	0.79
1:C:174:GLU:O	1:C:178:LYS:CB	2.30	0.79
1:D:183:LEU:HD12	1:D:183:LEU:N	1.95	0.79
1:D:188:LEU:CD1	1:D:188:LEU:O	2.30	0.79
1:C:171:ILE:CD1	1:C:195:ILE:HD12	2.12	0.78
1:D:214:LYS:HZ2	1:D:218:GLN:HB3	1.48	0.78
1:A:141:LYS:O	1:A:145:PRO:CD	2.29	0.78
1:D:160:HIS:HE1	1:D:206:LYS:CB	1.95	0.78
1:D:214:LYS:C	1:D:214:LYS:CD	2.56	0.78
1:C:169:LEU:O	1:C:169:LEU:CD2	2.30	0.77
1:D:182:SER:OG	1:D:183:LEU:HD13	1.84	0.77
1:D:192:GLN:O	1:D:195:ILE:HG12	1.86	0.76
1:D:214:LYS:O	1:D:214:LYS:CD	2.32	0.76
1:A:177:SER:N	1:A:178:LYS:CA	2.30	0.76
1:A:85:MET:HA	1:A:88:MET:HE2	1.66	0.75
1:A:195:ILE:HD13	1:A:195:ILE:H	1.47	0.75
1:D:71:VAL:HB	1:D:85:MET:HE2	1.67	0.75
1:D:188:LEU:HD12	1:D:189:LYS:N	2.00	0.75
1:A:218:GLN:O	1:A:221:PRO:CD	2.30	0.75
1:C:31:ARG:NH1	1:D:287:PHE:CD1	2.55	0.75
1:A:188:LEU:C	1:A:188:LEU:CD2	2.57	0.74
1:C:265:LYS:CE	3:C:515:HOH:O	2.22	0.74
1:A:303:GLU:HB2	1:B:157:LYS:HE2	1.69	0.74
1:B:79:THR:CG2	1:B:279:ASP:H	2.00	0.74
1:B:174:GLU:HA	1:B:191:LEU:HD21	1.69	0.74
1:B:31:ARG:HH12	1:B:235:GLN:NE2	1.86	0.74
1:A:143:GLN:O	1:A:144:LYS:C	2.31	0.73
1:A:37:ARG:NH2	3:A:320:HOH:O	2.20	0.73
1:D:160:HIS:CE1	1:D:206:LYS:CB	2.71	0.73
1:D:248:VAL:O	1:D:252:VAL:HG23	1.87	0.73
1:B:217:ASP:O	1:B:220:THR:CG2	2.30	0.73
1:D:72:GLU:HG3	1:D:85:MET:CE	2.18	0.73
1:A:136:GLU:O	1:A:140:ARG:HD3	1.89	0.72
1:B:174:GLU:CA	1:B:177:SER:OG	2.30	0.72
1:B:169:LEU:CD1	1:B:172:SER:OG	2.36	0.72
1:A:166:GLU:OE2	1:A:166:GLU:CA	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLN:HA	1:A:222:GLN:NE2	2.04	0.72
1:A:177:SER:CA	1:A:178:LYS:C	2.62	0.72
1:B:99:LEU:HD13	1:B:99:LEU:C	2.13	0.72
1:C:303:GLU:O	1:D:161:HIS:NE2	2.22	0.72
1:D:183:LEU:CD1	1:D:183:LEU:N	2.53	0.72
1:D:68:ARG:HH12	1:D:92:GLU:CD	1.98	0.71
1:A:191:LEU:O	1:A:195:ILE:CD1	2.37	0.71
1:C:126:MET:HE3	1:C:126:MET:CA	2.14	0.71
1:B:217:ASP:O	1:B:221:PRO:CD	2.30	0.71
1:A:175:ALA:O	1:A:177:SER:CA	2.37	0.70
1:B:157:LYS:CB	1:B:157:LYS:HZ2	2.04	0.70
1:B:114:LYS:O	1:B:118:LYS:HG3	1.90	0.70
1:B:23:GLY:H	1:B:143:GLN:HE22	1.37	0.70
1:A:17:ASP:HA	1:A:24:ASN:HD21	1.56	0.70
1:A:150:LEU:HD23	1:A:216:LEU:HD11	1.73	0.70
1:C:76:GLN:OE1	1:D:241:ARG:NH1	2.23	0.70
1:D:191:LEU:O	1:D:195:ILE:HG23	1.92	0.70
1:A:185:PRO:CD	1:A:186:GLU:H	2.04	0.69
1:C:203:LEU:HD21	1:C:207:GLU:OE2	1.93	0.69
1:A:177:SER:CB	1:A:178:LYS:O	2.41	0.69
1:C:144:LYS:N	1:C:145:PRO:CD	2.56	0.69
1:D:36:HIS:HE1	3:D:490:HOH:O	1.75	0.69
1:A:218:GLN:C	1:A:221:PRO:HD2	2.17	0.68
1:B:187:GLN:N	1:B:187:GLN:CD	2.52	0.68
1:B:200:GLN:O	1:B:203:LEU:HD23	1.94	0.68
1:C:216:LEU:HD13	1:C:220:THR:HG22	1.76	0.68
1:A:185:PRO:HD2	1:A:186:GLU:H	1.57	0.68
1:B:220:THR:HG22	1:B:221:PRO:HD3	1.76	0.68
1:C:54:LYS:NZ	1:C:58:GLN:NE2	2.41	0.67
1:B:169:LEU:HD13	1:B:169:LEU:O	1.94	0.67
1:D:22:VAL:HA	1:D:143:GLN:NE2	2.10	0.67
1:A:181:PRO:HB2	1:A:182:SER:C	2.20	0.67
1:C:124:GLN:HG3	1:C:126:MET:H	1.59	0.67
1:A:215:GLU:O	1:A:218:GLN:HG2	1.94	0.67
1:B:79:THR:HG22	1:B:283:ASP:CG	2.20	0.66
1:C:22:VAL:O	1:C:22:VAL:HG13	1.94	0.66
1:C:125:MET:HE2	1:C:125:MET:H	1.60	0.66
1:D:72:GLU:HG3	1:D:85:MET:HE1	1.75	0.66
1:D:166:GLU:OE1	1:D:166:GLU:CA	2.30	0.66
1:B:169:LEU:HD13	1:B:172:SER:HG	1.57	0.66
1:C:214:LYS:HD2	1:C:214:LYS:C	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TRP:CD1	1:A:146:TRP:C	2.73	0.66
1:C:54:LYS:HZ3	1:C:58:GLN:HE22	1.44	0.66
1:C:214:LYS:HD2	1:C:214:LYS:O	1.96	0.66
1:A:238:GLU:OE1	1:A:241:ARG:NH2	2.30	0.65
1:B:239:GLU:OE2	1:B:243:ARG:NH1	2.30	0.65
1:A:213:LEU:HD22	1:B:302:PHE:HD2	1.53	0.65
1:A:218:GLN:O	1:A:219:GLY:C	2.38	0.65
1:A:239:GLU:HG3	1:B:284:LEU:HD11	1.79	0.65
1:B:204:LYS:HG2	1:B:208:LYS:HE3	1.78	0.65
1:D:184:ASN:N	1:D:184:ASN:OD1	2.30	0.65
1:C:66:ARG:HG2	3:C:518:HOH:O	1.96	0.65
1:C:142:ALA:HB1	1:C:226:ASN:HB3	1.79	0.65
1:C:174:GLU:OE1	1:C:175:ALA:HA	1.96	0.65
1:B:211:LYS:HG3	1:B:212:SER:N	2.12	0.64
1:C:31:ARG:NH1	1:D:287:PHE:CG	2.66	0.64
1:C:174:GLU:OE1	1:C:175:ALA:N	2.30	0.64
1:A:177:SER:HB3	1:A:178:LYS:O	1.94	0.64
1:B:187:GLN:H	1:B:187:GLN:CD	2.05	0.64
1:C:184:ASN:HB3	1:C:187:GLN:HB2	1.79	0.64
1:A:174:GLU:OE2	1:A:175:ALA:N	2.30	0.64
1:A:304:GLU:O	1:A:305:TRP:CB	2.45	0.64
1:C:174:GLU:OE1	1:C:174:GLU:C	2.40	0.64
1:A:206:LYS:O	1:A:210:GLU:CG	2.46	0.64
1:A:211:LYS:O	1:A:215:GLU:HG3	1.97	0.64
1:C:143:GLN:HG3	1:C:223:TYR:HE1	1.63	0.64
1:D:180:ASP:OD1	1:D:184:ASN:ND2	2.30	0.64
1:A:177:SER:CB	1:A:179:ALA:N	2.47	0.63
1:C:191:LEU:N	1:C:191:LEU:HD23	2.14	0.63
1:A:84:TRP:O	1:A:87:PHE:HB2	1.99	0.63
1:B:169:LEU:O	1:B:173:ARG:HG2	1.99	0.63
1:D:184:ASN:N	1:D:185:PRO:CD	2.62	0.63
1:A:93:ARG:NH1	1:A:267:ILE:HA	2.14	0.62
1:B:144:LYS:HB3	1:B:145:PRO:HD3	1.81	0.62
1:B:99:LEU:C	1:B:99:LEU:CD1	2.73	0.62
1:B:31:ARG:HH12	1:B:235:GLN:HE22	1.47	0.62
1:D:22:VAL:HA	1:D:143:GLN:HE22	1.65	0.61
1:A:181:PRO:CB	1:A:182:SER:C	2.73	0.61
1:C:85:MET:HA	1:C:88:MET:HE2	1.82	0.61
1:C:286:TRP:CD2	1:C:290:ASN:ND2	2.63	0.61
1:D:31:ARG:HH12	1:D:235:GLN:HE21	1.48	0.61
1:A:43:MET:HE2	1:A:113:ILE:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLU:HA	1:C:191:LEU:CD1	2.30	0.61
1:D:89:SER:O	1:D:93:ARG:HG2	2.01	0.61
1:D:195:ILE:HG13	1:D:196:GLU:N	2.16	0.61
1:D:160:HIS:CE1	1:D:206:LYS:CA	2.84	0.60
1:B:169:LEU:CD1	1:B:169:LEU:O	2.49	0.60
1:B:220:THR:CG2	1:B:221:PRO:HD3	2.30	0.60
1:C:144:LYS:N	1:C:145:PRO:HD2	2.16	0.60
1:D:287:PHE:O	1:D:288:ARG:C	2.43	0.60
1:C:17:ASP:N	3:C:519:HOH:O	2.34	0.60
1:A:206:LYS:O	1:A:210:GLU:HG2	2.01	0.60
1:A:31:ARG:HH22	1:A:235:GLN:NE2	2.00	0.60
1:C:203:LEU:O	1:C:207:GLU:HG3	2.01	0.60
1:D:185:PRO:HG2	1:D:187:GLN:NE2	2.17	0.59
1:A:31:ARG:HH22	1:A:235:GLN:HE21	1.50	0.59
1:A:144:LYS:O	1:A:145:PRO:C	2.43	0.59
1:C:174:GLU:OE1	1:C:175:ALA:CA	2.50	0.59
1:C:218:GLN:O	1:C:221:PRO:CG	2.51	0.59
1:B:143:GLN:HG2	1:B:143:GLN:O	2.02	0.59
1:D:80:VAL:HG23	1:D:283:ASP:OD2	2.03	0.59
1:A:28:THR:HG22	3:B:506:HOH:O	2.03	0.59
1:D:167:GLU:HA	1:D:198:CYS:HB3	1.83	0.59
1:D:214:LYS:NZ	1:D:218:GLN:CB	2.66	0.59
1:A:33:ASP:HB3	3:A:505:HOH:O	2.03	0.59
1:A:258:LEU:HA	1:A:261:VAL:HG22	1.85	0.59
1:B:217:ASP:C	1:B:220:THR:HG22	2.27	0.59
1:C:172:SER:O	1:C:176:ASN:HB2	2.03	0.59
1:D:31:ARG:HH12	1:D:235:GLN:NE2	2.00	0.59
1:A:38:LEU:HD13	1:B:76:GLN:HG2	1.85	0.58
1:A:18:SER:O	1:A:24:ASN:ND2	2.31	0.58
1:B:157:LYS:HB3	1:B:157:LYS:HZ2	1.59	0.58
1:D:68:ARG:NH2	1:D:92:GLU:OE2	2.33	0.58
1:C:187:GLN:CA	1:C:187:GLN:HE21	2.16	0.58
1:B:174:GLU:HB2	1:B:191:LEU:HD23	1.84	0.58
1:C:44:ASN:O	1:C:48:GLU:HG3	2.04	0.58
1:C:175:ALA:O	1:C:179:ALA:N	2.37	0.58
1:B:79:THR:HG21	1:B:279:ASP:N	2.14	0.57
1:C:122:HIS:HD2	1:C:131:GLU:OE2	1.87	0.57
1:C:187:GLN:HE21	1:C:187:GLN:N	2.02	0.57
1:C:39:CYS:O	1:C:43:MET:HG3	2.05	0.57
1:B:160:HIS:CE1	1:B:206:LYS:HB2	2.39	0.56
1:C:22:VAL:O	1:C:22:VAL:CG1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:HA	1:B:295:MET:HE1	1.86	0.56
1:A:76:GLN:HG2	1:B:38:LEU:HD13	1.87	0.56
1:D:279:ASP:HB3	1:D:282:GLU:HB2	1.87	0.56
1:A:303:GLU:CB	1:B:157:LYS:HE2	2.34	0.56
1:B:149:LYS:O	1:B:153:VAL:HG23	2.04	0.56
1:A:209:TYR:O	1:A:213:LEU:HD12	2.06	0.56
1:A:271:LEU:HD13	1:B:253:GLN:HB2	1.88	0.56
1:B:68:ARG:NH2	1:B:92:GLU:OE2	2.39	0.56
1:C:169:LEU:C	1:C:169:LEU:HD22	2.30	0.56
1:C:209:TYR:HE2	1:D:302:PHE:HD1	1.51	0.56
1:A:143:GLN:O	1:A:146:TRP:N	2.39	0.56
1:C:304:GLU:HG3	1:C:305:TRP:H	1.71	0.56
1:D:26:LYS:HG2	1:D:27:ARG:N	2.21	0.56
1:C:42:LEU:HD23	1:C:113:ILE:HD13	1.87	0.56
1:A:115:ASN:O	1:A:119:GLU:HG3	2.06	0.56
1:B:79:THR:HG22	1:B:283:ASP:OD1	2.06	0.56
1:C:31:ARG:HH22	1:C:235:GLN:HE21	1.54	0.56
1:B:149:LYS:HE3	1:B:215:GLU:HB3	1.87	0.55
1:D:30:LYS:O	1:D:30:LYS:HG2	2.06	0.55
1:A:37:ARG:CD	1:A:37:ARG:C	2.79	0.55
1:A:185:PRO:CD	1:A:186:GLU:N	2.68	0.55
1:C:146:TRP:HE1	1:C:220:THR:HG22	1.71	0.55
1:D:17:ASP:CG	1:D:21:GLU:OE2	2.50	0.55
1:A:170:ALA:HB1	1:A:195:ILE:HD12	1.89	0.55
1:A:177:SER:H	1:A:178:LYS:C	2.13	0.55
1:C:190:LYS:O	1:C:193:ASP:HB2	2.07	0.55
1:D:183:LEU:C	1:D:184:ASN:OD1	2.50	0.55
1:B:22:VAL:HA	1:B:143:GLN:NE2	2.22	0.55
1:B:172:SER:O	1:B:175:ALA:HB3	2.06	0.55
1:D:190:LYS:O	1:D:194:LYS:N	2.32	0.55
1:D:185:PRO:CG	1:D:187:GLN:HE22	2.20	0.54
1:D:193:ASP:O	1:D:197:LYS:HG2	2.07	0.54
1:B:122:HIS:CD2	1:B:131:GLU:OE1	2.50	0.54
1:B:188:LEU:CG	1:B:189:LYS:N	2.70	0.54
1:D:76:GLN:NE2	1:D:80:VAL:HB	2.22	0.54
1:D:150:LEU:O	1:D:150:LEU:HG	2.05	0.54
1:A:175:ALA:O	1:A:177:SER:C	2.50	0.54
1:D:179:ALA:O	1:D:181:PRO:HD3	2.08	0.54
1:C:17:ASP:N	3:C:375:HOH:O	2.40	0.54
1:C:278:ALA:HB3	1:D:246:ARG:HG3	1.89	0.54
1:A:181:PRO:HB2	1:A:183:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASP:O	1:C:205:THR:HG23	2.08	0.54
1:D:194:LYS:HA	1:D:197:LYS:HG3	1.90	0.53
1:C:155:ALA:HA	1:C:158:LYS:HE3	1.91	0.53
1:B:85:MET:C	1:B:87:PHE:H	2.15	0.53
1:C:54:LYS:HZ3	1:C:58:GLN:NE2	2.04	0.53
1:C:217:ASP:O	1:C:221:PRO:HD2	2.08	0.53
1:A:188:LEU:HD21	1:A:192:GLN:HG3	1.90	0.53
1:C:216:LEU:HD13	1:C:220:THR:CG2	2.39	0.53
1:A:21:GLU:OE1	1:B:297:MET:HE1	2.08	0.53
1:D:207:GLU:HA	1:D:210:GLU:OE2	2.08	0.53
1:D:47:HIS:HD2	1:D:106:MET:SD	2.32	0.53
1:C:276:ARG:HA	1:D:246:ARG:NH1	2.25	0.52
1:C:19:PHE:CD1	1:D:292:GLY:HA2	2.44	0.52
1:C:153:VAL:HG22	1:C:212:SER:HB3	1.90	0.52
1:C:216:LEU:O	1:C:216:LEU:HD13	2.09	0.52
1:C:297:MET:HB2	1:D:20:TRP:HB2	1.90	0.52
1:C:112:LYS:HD3	1:C:248:VAL:HG22	1.90	0.52
1:D:160:HIS:CE1	1:D:206:LYS:HA	2.44	0.52
1:A:177:SER:N	1:A:178:LYS:C	2.67	0.52
1:A:200:GLN:HA	1:A:203:LEU:CD2	2.32	0.52
1:C:156:ALA:HB1	1:C:209:TYR:CB	2.38	0.52
1:D:239:GLU:O	1:D:243:ARG:HG3	2.10	0.52
1:A:93:ARG:HD3	1:A:267:ILE:HG12	1.93	0.51
1:D:145:PRO:O	1:D:148:LYS:HG3	2.10	0.51
1:B:203:LEU:HG	1:B:204:LYS:N	2.22	0.51
1:A:173:ARG:O	1:A:176:ASN:O	2.28	0.51
1:D:37:ARG:CG	1:D:37:ARG:NH1	2.51	0.51
1:C:304:GLU:O	1:C:305:TRP:CB	2.58	0.51
1:B:100:GLU:HA	1:B:103:ALA:HB3	1.92	0.51
1:A:97:LEU:HD22	1:A:258:LEU:HD22	1.92	0.51
1:C:125:MET:H	1:C:125:MET:CE	2.24	0.51
1:A:124:GLN:O	1:A:125:MET:C	2.51	0.51
1:C:87:PHE:CE2	1:D:249:LEU:HD22	2.46	0.51
1:A:174:GLU:OE2	1:A:174:GLU:C	2.54	0.51
1:A:258:LEU:HA	1:A:261:VAL:CG2	2.41	0.51
1:B:187:GLN:H	1:B:187:GLN:HE21	1.50	0.51
1:C:174:GLU:HA	1:C:191:LEU:HD12	1.93	0.51
1:C:218:GLN:O	1:C:221:PRO:HG2	2.11	0.51
1:C:228:GLU:OE2	1:D:288:ARG:NH2	2.43	0.51
1:C:165:LYS:HD3	1:C:165:LYS:N	2.25	0.51
1:C:280:ALA:O	1:C:284:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASP:OD1	1:D:21:GLU:OE2	2.28	0.50
1:C:157:LYS:CG	1:C:209:TYR:HE1	2.25	0.50
1:A:218:GLN:C	1:A:221:PRO:CD	2.84	0.50
1:D:72:GLU:HG3	1:D:85:MET:HE3	1.92	0.50
1:D:85:MET:SD	1:D:88:MET:HE2	2.51	0.50
1:A:250:LEU:O	1:A:253:GLN:HB3	2.11	0.50
1:A:213:LEU:HD22	1:B:302:PHE:CD2	2.37	0.50
1:D:174:GLU:OE2	1:D:174:GLU:O	2.30	0.50
1:D:214:LYS:HZ3	1:D:218:GLN:CB	2.23	0.50
1:B:169:LEU:HD13	1:B:169:LEU:C	2.35	0.50
1:B:220:THR:HG23	1:B:221:PRO:N	2.26	0.50
1:C:64:ALA:HA	1:C:88:MET:HG3	1.94	0.50
1:A:196:GLU:OE1	1:A:196:GLU:O	2.30	0.50
1:C:27:ARG:NH1	3:C:508:HOH:O	2.44	0.50
1:D:181:PRO:O	1:D:184:ASN:OD1	2.30	0.50
1:A:176:ASN:O	1:A:176:ASN:OD1	2.30	0.50
1:D:50:ALA:HB1	1:D:102:LYS:HG2	1.93	0.50
1:A:125:MET:O	1:A:125:MET:HG3	2.10	0.50
1:B:174:GLU:O	1:B:177:SER:HB2	2.12	0.49
1:C:216:LEU:HD13	1:C:216:LEU:C	2.37	0.49
1:A:146:TRP:CD1	1:A:146:TRP:O	2.66	0.49
1:A:103:ALA:O	1:A:104:SER:C	2.53	0.49
1:A:152:GLU:O	1:A:153:VAL:C	2.55	0.49
1:A:216:LEU:O	1:A:219:GLY:N	2.46	0.49
1:C:304:GLU:HG3	1:C:305:TRP:N	2.28	0.49
1:A:168:LYS:HA	1:A:168:LYS:HE2	1.94	0.49
1:B:85:MET:C	1:B:87:PHE:N	2.69	0.49
1:D:196:GLU:O	1:D:200:GLN:OE1	2.30	0.49
1:A:87:PHE:CE2	1:B:249:LEU:HD22	2.48	0.49
1:C:165:LYS:HE2	1:D:305:TRP:CZ3	2.47	0.49
1:C:206:LYS:O	1:C:207:GLU:C	2.53	0.49
1:D:231:PHE:CD1	1:D:231:PHE:C	2.91	0.49
1:A:276:ARG:O	1:B:246:ARG:NH2	2.46	0.48
1:B:173:ARG:O	1:B:177:SER:OG	2.30	0.48
1:B:233:GLN:HA	1:B:236:GLN:HB2	1.96	0.48
1:A:216:LEU:O	1:A:220:THR:HG23	2.13	0.48
1:D:85:MET:HA	1:D:88:MET:HE2	1.95	0.48
1:D:182:SER:C	1:D:183:LEU:HD12	2.38	0.48
1:C:89:SER:O	1:C:93:ARG:HG2	2.13	0.48
1:A:206:LYS:O	1:A:210:GLU:HG3	2.14	0.48
1:A:177:SER:HB2	1:A:179:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:O	1:A:207:GLU:HG2	2.13	0.48
1:A:220:THR:O	1:A:221:PRO:C	2.53	0.48
1:D:169:LEU:O	1:D:173:ARG:HG2	2.14	0.48
1:A:252:VAL:HG12	1:B:87:PHE:HE2	1.79	0.48
1:A:109:ASP:OD2	1:A:255:HIS:HD2	1.97	0.48
1:A:146:TRP:O	1:A:146:TRP:CG	2.64	0.48
1:D:281:VAL:HA	1:D:284:LEU:HB2	1.95	0.48
1:A:125:MET:O	1:A:126:MET:HB2	2.14	0.47
1:D:185:PRO:HG2	1:D:187:GLN:HE22	1.79	0.47
1:A:18:SER:HA	1:B:295:MET:CE	2.44	0.47
1:B:170:ALA:O	1:B:173:ARG:HB2	2.15	0.47
1:D:31:ARG:NH2	1:D:235:GLN:NE2	2.48	0.47
1:D:19:PHE:CD2	1:D:19:PHE:C	2.92	0.47
1:B:142:ALA:HB1	1:B:226:ASN:HB3	1.95	0.47
1:B:103:ALA:O	1:B:107:ASN:HB2	2.13	0.47
1:B:123:LYS:HD3	3:B:504:HOH:O	2.15	0.47
1:C:214:LYS:HE3	1:C:218:GLN:NE2	2.28	0.47
1:C:304:GLU:O	1:C:305:TRP:HB3	2.15	0.47
1:D:25:TYR:O	1:D:28:THR:HG23	2.15	0.47
1:D:185:PRO:CG	1:D:187:GLN:NE2	2.76	0.47
1:A:76:GLN:OE1	1:A:77:TYR:O	2.33	0.47
1:A:148:LYS:NZ	3:A:511:HOH:O	2.48	0.47
1:A:160:HIS:NE2	1:A:206:LYS:HB2	2.30	0.47
1:B:66:ARG:HG2	1:B:67:TRP:CD1	2.50	0.47
1:C:157:LYS:HG2	1:C:209:TYR:CE1	2.50	0.47
1:D:148:LYS:HG3	1:D:149:LYS:N	2.29	0.47
1:A:21:GLU:O	1:A:22:VAL:C	2.58	0.47
1:D:208:LYS:O	1:D:211:LYS:HB3	2.15	0.47
1:A:136:GLU:OE1	1:A:140:ARG:HD2	2.15	0.47
1:B:174:GLU:CB	1:B:191:LEU:CD2	2.74	0.47
1:C:209:TYR:HE2	1:D:302:PHE:CD1	2.31	0.47
1:B:237:PHE:HE2	3:B:508:HOH:O	1.96	0.46
1:B:174:GLU:HA	1:B:177:SER:CB	2.42	0.46
1:B:194:LYS:HA	1:B:194:LYS:HD3	1.77	0.46
1:C:42:LEU:HD23	1:C:113:ILE:CD1	2.45	0.46
1:C:30:LYS:HD2	1:C:30:LYS:HA	1.80	0.46
1:C:189:LYS:O	1:C:190:LYS:C	2.58	0.46
1:B:281:VAL:O	1:B:282:GLU:C	2.54	0.46
1:D:182:SER:OG	1:D:183:LEU:HD12	2.13	0.46
1:D:67:TRP:O	1:D:71:VAL:HG23	2.15	0.46
1:D:272:GLU:HG3	1:D:272:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLN:HG2	1:A:218:GLN:H	1.42	0.46
1:D:19:PHE:O	1:D:19:PHE:CG	2.66	0.46
1:A:123:LYS:HA	1:A:123:LYS:HD2	1.85	0.46
1:A:204:LYS:NZ	1:A:204:LYS:HB3	2.30	0.46
1:B:169:LEU:CD1	1:B:169:LEU:C	2.86	0.46
1:C:56:TYR:HB2	1:D:56:TYR:CD1	2.50	0.46
1:D:167:GLU:HA	1:D:198:CYS:CB	2.45	0.46
1:B:188:LEU:HD23	1:B:188:LEU:H	1.81	0.46
1:A:177:SER:OG	1:A:178:LYS:O	2.30	0.46
1:B:79:THR:HG22	1:B:283:ASP:OD2	2.15	0.46
1:B:244:PHE:O	1:B:245:PHE:C	2.56	0.46
1:D:228:GLU:O	1:D:232:GLU:HB2	2.16	0.46
1:C:188:LEU:O	1:C:189:LYS:C	2.59	0.46
1:C:202:VAL:O	1:C:203:LEU:C	2.57	0.46
1:A:76:GLN:NE2	1:A:80:VAL:CG1	2.79	0.45
1:A:217:ASP:HA	1:A:220:THR:HG23	1.99	0.45
1:C:137:ASP:HA	1:C:140:ARG:HD3	1.98	0.45
1:C:199:LYS:O	1:C:200:GLN:C	2.58	0.45
1:A:188:LEU:CD2	1:A:192:GLN:HG3	2.46	0.45
1:A:244:PHE:O	1:A:248:VAL:HG23	2.15	0.45
1:B:79:THR:CG2	1:B:279:ASP:N	2.74	0.45
1:C:31:ARG:NH1	1:D:287:PHE:CE1	2.83	0.45
1:B:131:GLU:H	1:B:131:GLU:CD	2.23	0.45
1:D:180:ASP:OD1	1:D:184:ASN:HB3	2.16	0.45
1:A:177:SER:CB	1:A:179:ALA:HB2	2.47	0.45
1:C:217:ASP:C	1:C:220:THR:HG23	2.41	0.45
1:D:186:GLU:OE2	1:D:186:GLU:O	2.34	0.45
1:D:201:ASP:O	1:D:205:THR:HG23	2.17	0.45
1:C:217:ASP:CA	1:C:220:THR:HG23	2.46	0.45
1:D:181:PRO:HG2	1:D:184:ASN:H	1.81	0.45
1:C:50:ALA:HB1	1:C:102:LYS:HG2	1.98	0.45
1:A:17:ASP:CA	1:A:24:ASN:HD21	2.27	0.45
1:A:165:LYS:HD2	1:A:165:LYS:HA	1.44	0.45
1:B:31:ARG:HE	1:B:31:ARG:HB3	1.35	0.45
1:B:199:LYS:HE3	1:B:199:LYS:HB2	1.35	0.45
1:B:204:LYS:HG2	1:B:208:LYS:CE	2.47	0.45
1:C:206:LYS:C	1:C:208:LYS:N	2.74	0.45
1:A:275:ILE:CG2	1:B:250:LEU:HG	2.47	0.45
1:C:227:MET:O	1:C:228:GLU:C	2.59	0.45
1:B:220:THR:CG2	1:B:221:PRO:CD	2.95	0.44
1:A:176:ASN:O	1:A:176:ASN:CG	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:HA	1:C:233:GLN:NE2	2.33	0.44
1:B:204:LYS:O	1:B:205:THR:C	2.60	0.44
1:C:286:TRP:CZ2	1:C:290:ASN:ND2	2.84	0.44
1:D:133:LYS:HD2	1:D:133:LYS:HA	1.76	0.44
1:A:190:LYS:HD2	1:A:190:LYS:HA	1.58	0.44
1:B:93:ARG:HA	1:B:93:ARG:HD3	1.74	0.44
1:C:49:ARG:HB2	1:D:63:TRP:CZ2	2.52	0.44
1:A:105:LEU:O	1:A:109:ASP:HB2	2.18	0.44
1:C:157:LYS:HG2	1:C:209:TYR:HE1	1.83	0.44
1:D:104:SER:O	1:D:108:ASP:HB2	2.17	0.44
1:A:176:ASN:HA	1:A:177:SER:HA	1.79	0.44
1:C:133:LYS:HE3	1:C:137:ASP:OD2	2.16	0.44
1:A:253:GLN:CG	1:B:271:LEU:HD13	2.48	0.44
1:B:174:GLU:O	1:B:174:GLU:HG3	2.18	0.44
1:D:71:VAL:HG21	1:D:88:MET:HE1	2.00	0.44
1:A:87:PHE:CE2	1:A:275:ILE:HD11	2.52	0.43
1:A:143:GLN:C	1:A:145:PRO:HD2	2.43	0.43
1:B:87:PHE:CE1	1:B:275:ILE:HD11	2.53	0.43
1:D:129:PHE:HB2	1:D:132:THR:CG2	2.35	0.43
1:A:69:GLN:HG3	1:A:73:LYS:HD2	2.01	0.43
1:A:245:PHE:O	1:A:249:LEU:HG	2.18	0.43
1:A:56:TYR:HB2	1:B:56:TYR:CD1	2.54	0.43
1:B:25:TYR:CD1	1:B:25:TYR:C	2.97	0.43
1:B:144:LYS:CB	1:B:145:PRO:HD3	2.48	0.43
1:D:235:GLN:HE21	1:D:235:GLN:HA	1.83	0.43
1:A:139:PHE:CD1	1:A:227:MET:HE3	2.54	0.43
1:C:129:PHE:HB2	1:C:132:THR:OG1	2.19	0.43
1:C:160:HIS:CD2	1:C:205:THR:OG1	2.72	0.43
1:D:25:TYR:C	1:D:25:TYR:CD1	2.96	0.43
1:B:18:SER:O	1:B:24:ASN:ND2	2.32	0.43
1:C:211:LYS:O	1:C:215:GLU:HG3	2.18	0.43
1:A:185:PRO:CG	1:A:186:GLU:N	2.81	0.43
1:D:87:PHE:CE1	1:D:275:ILE:HD11	2.54	0.43
1:B:148:LYS:HD3	3:B:510:HOH:O	2.17	0.43
1:B:206:LYS:HD2	1:B:207:GLU:N	2.34	0.43
1:C:31:ARG:HA	3:C:508:HOH:O	2.18	0.43
1:C:221:PRO:HG2	1:C:222:GLN:H	1.83	0.43
1:A:181:PRO:CA	1:A:182:SER:CB	2.72	0.43
1:C:143:GLN:HG3	1:C:223:TYR:CE1	2.48	0.43
1:A:204:LYS:HB2	1:A:204:LYS:HE3	1.85	0.42
1:D:292:GLY:O	1:D:293:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:O	1:A:216:LEU:C	2.61	0.42
1:B:84:TRP:O	1:B:87:PHE:HB2	2.19	0.42
1:C:85:MET:HA	1:C:88:MET:CE	2.48	0.42
1:D:98:HIS:CE1	1:D:258:LEU:HD11	2.54	0.42
1:A:37:ARG:C	1:A:37:ARG:HD2	2.44	0.42
1:C:20:TRP:CZ2	1:D:293:PRO:HA	2.54	0.42
1:D:149:LYS:HB3	1:D:216:LEU:HD12	2.01	0.42
1:B:169:LEU:HD13	1:B:169:LEU:HA	1.67	0.42
1:C:208:LYS:C	1:C:210:GLU:H	2.27	0.42
1:A:79:THR:HB	1:A:278:ALA:HA	2.02	0.42
1:A:173:ARG:H	1:A:173:ARG:HG2	1.61	0.42
1:D:173:ARG:O	1:D:177:SER:OG	2.37	0.42
1:A:203:LEU:HG	1:A:204:LYS:N	2.35	0.42
1:C:174:GLU:O	1:C:175:ALA:C	2.61	0.42
1:B:222:GLN:O	1:B:222:GLN:HG3	2.20	0.42
1:D:149:LYS:HB3	1:D:216:LEU:CD1	2.50	0.42
1:B:174:GLU:HA	1:B:191:LEU:CD2	2.44	0.42
1:C:172:SER:O	1:C:173:ARG:C	2.59	0.42
1:C:188:LEU:HD12	1:C:188:LEU:HA	1.74	0.42
1:C:264:TYR:O	1:C:267:ILE:HB	2.20	0.42
1:D:145:PRO:O	1:D:148:LYS:CG	2.67	0.42
1:A:181:PRO:HB2	1:A:183:LEU:HA	2.01	0.42
1:C:157:LYS:O	1:C:161:HIS:HB2	2.20	0.42
1:A:167:GLU:HG2	1:A:168:LYS:CE	2.17	0.42
1:A:280:ALA:O	1:A:284:LEU:HG	2.20	0.41
1:B:200:GLN:HG2	1:B:203:LEU:HD22	2.02	0.41
1:C:18:SER:O	1:C:24:ASN:ND2	2.41	0.41
1:C:174:GLU:HA	1:C:191:LEU:HD13	2.01	0.41
1:C:216:LEU:C	1:C:216:LEU:CD1	2.92	0.41
1:A:207:GLU:O	1:A:210:GLU:HB2	2.20	0.41
1:C:125:MET:C	1:C:126:MET:HE3	2.36	0.41
1:C:220:THR:O	1:C:221:PRO:C	2.60	0.41
1:B:85:MET:O	1:B:87:PHE:N	2.53	0.41
1:D:183:LEU:C	1:D:185:PRO:HD3	2.43	0.41
1:B:133:LYS:HD2	1:B:133:LYS:HA	1.87	0.41
1:B:239:GLU:O	1:B:243:ARG:HG3	2.21	0.41
1:A:142:ALA:CB	1:A:226:ASN:HB3	2.37	0.41
1:B:30:LYS:HE3	1:B:30:LYS:HB3	1.72	0.41
1:A:300:PRO:HG2	1:B:216:LEU:HD21	2.02	0.41
1:B:249:LEU:HD23	1:B:249:LEU:HA	1.90	0.41
1:D:220:THR:N	1:D:221:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:O	1:B:99:LEU:CD1	2.49	0.41
1:B:141:LYS:O	1:B:141:LYS:HG2	2.21	0.41
1:B:207:GLU:O	1:B:211:LYS:HB3	2.20	0.41
1:A:136:GLU:HG3	1:A:140:ARG:HD2	2.02	0.41
1:A:140:ARG:O	1:A:144:LYS:N	2.40	0.41
1:A:220:THR:OG1	1:A:221:PRO:N	2.54	0.41
1:C:165:LYS:HE2	1:D:305:TRP:HZ3	1.86	0.41
1:C:225:GLU:O	1:C:226:ASN:C	2.62	0.41
1:D:232:GLU:O	1:D:235:GLN:HB2	2.20	0.41
1:D:244:PHE:O	1:D:245:PHE:C	2.64	0.41
1:C:45:CYS:HA	1:D:67:TRP:CZ2	2.56	0.41
1:C:143:GLN:O	1:C:145:PRO:HD2	2.17	0.41
1:C:155:ALA:O	1:C:158:LYS:HB3	2.21	0.41
1:D:49:ARG:NH1	1:D:53:GLU:OE2	2.54	0.41
1:D:171:ILE:HD12	1:D:171:ILE:HA	1.65	0.41
1:C:84:TRP:O	1:C:87:PHE:HB2	2.21	0.40
1:D:87:PHE:CZ	1:D:275:ILE:HD11	2.56	0.40
1:D:195:ILE:CG1	1:D:196:GLU:N	2.84	0.40
1:B:61:THR:HG22	1:B:95:SER:OG	2.22	0.40
1:D:170:ALA:CB	1:D:195:ILE:HA	2.51	0.40
1:D:180:ASP:HA	1:D:181:PRO:HD2	1.91	0.40
1:A:43:MET:HE1	1:A:117:GLN:OE1	2.21	0.40
1:A:112:LYS:HE2	1:A:248:VAL:HG22	2.04	0.40
1:B:220:THR:HG23	1:B:221:PRO:CD	2.51	0.40
1:A:217:ASP:CA	1:A:220:THR:HG23	2.51	0.40
1:A:275:ILE:HG21	1:B:250:LEU:HG	2.03	0.40
1:B:203:LEU:O	1:B:206:LYS:HB3	2.21	0.40
1:A:177:SER:HB3	1:A:179:ALA:CB	2.49	0.40
1:B:220:THR:O	1:B:221:PRO:C	2.58	0.40
1:C:206:LYS:O	1:C:208:LYS:N	2.53	0.40
1:C:216:LEU:O	1:C:220:THR:HG22	2.16	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:O	1:B:192:GLN:OE1[2_455]	1.40	0.80
1:C:181:PRO:O	1:D:178:LYS:NZ[2_546]	1.70	0.50
1:C:181:PRO:N	1:D:178:LYS:NZ[2_546]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/289 (97%)	275 (98%)	5 (2%)	1 (0%)	30	51
1	B	281/289 (97%)	276 (98%)	4 (1%)	1 (0%)	30	51
1	C	282/289 (98%)	272 (96%)	9 (3%)	1 (0%)	30	51
1	D	287/289 (99%)	280 (98%)	7 (2%)	0	100	100
All	All	1131/1156 (98%)	1103 (98%)	25 (2%)	3 (0%)	36	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	PRO
1	A	185	PRO
1	B	86	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/251 (98%)	203 (82%)	44 (18%)	2	3
1	B	245/251 (98%)	198 (81%)	47 (19%)	1	2
1	C	246/251 (98%)	205 (83%)	41 (17%)	2	4
1	D	248/251 (99%)	203 (82%)	45 (18%)	2	3
All	All	986/1004 (98%)	809 (82%)	177 (18%)	2	3

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	22	VAL
1	A	27	ARG
1	A	28	THR
1	A	29	VAL
1	A	31	ARG
1	A	37	ARG
1	A	69	GLN
1	A	72	GLU
1	A	76	GLN
1	A	89	SER
1	A	100	GLU
1	A	102	LYS
1	A	123	LYS
1	A	124	GLN
1	A	131	GLU
1	A	146	TRP
1	A	149	LYS
1	A	150	LEU
1	A	153	VAL
1	A	165	LYS
1	A	166	GLU
1	A	168	LYS
1	A	173	ARG
1	A	174	GLU
1	A	191	LEU
1	A	195	ILE
1	A	196	GLU
1	A	197	LYS
1	A	199	LYS
1	A	203	LEU
1	A	204	LYS
1	A	205	THR
1	A	211	LYS
1	A	214	LYS
1	A	218	GLN
1	A	220	THR
1	A	243	ARG
1	A	254	LYS
1	A	261	VAL
1	A	271	LEU
1	A	273	GLN
1	A	288	ARG

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Mol	Chain	Res	Type
1	A	303	GLU
1	B	28	THR
1	B	30	LYS
1	B	31	ARG
1	B	32	ILE
1	B	43	MET
1	B	66	ARG
1	B	72	GLU
1	B	76	GLN
1	B	90	GLU
1	B	97	LEU
1	B	99	LEU
1	B	126	MET
1	B	130	LYS
1	B	133	LYS
1	B	149	LYS
1	B	150	LEU
1	B	151	LYS
1	B	152	GLU
1	B	157	LYS
1	B	158	LYS
1	B	164	CYS
1	B	165	LYS
1	B	167	GLU
1	B	169	LEU
1	B	171	ILE
1	B	177	SER
1	B	191	LEU
1	B	193	ASP
1	B	195	ILE
1	B	197	LYS
1	B	199	LYS
1	B	202	VAL
1	B	203	LEU
1	B	204	LYS
1	B	206	LYS
1	B	207	GLU
1	B	211	LYS
1	B	213	LEU
1	B	232	GLU
1	B	236	GLN
1	B	239	GLU

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Mol	Chain	Res	Type
1	B	265	LYS
1	B	271	LEU
1	B	273	GLN
1	B	282	GLU
1	B	302	PHE
1	B	304	GLU
1	C	27	ARG
1	C	58	GLN
1	C	66	ARG
1	C	95	SER
1	C	96	GLU
1	C	109	ASP
1	C	123	LYS
1	C	124	GLN
1	C	125	MET
1	C	126	MET
1	C	132	THR
1	C	134	GLU
1	C	150	LEU
1	C	157	LYS
1	C	165	LYS
1	C	166	GLU
1	C	169	LEU
1	C	171	ILE
1	C	174	GLU
1	C	177	SER
1	C	186	GLU
1	C	187	GLN
1	C	188	LEU
1	C	190	LYS
1	C	191	LEU
1	C	192	GLN
1	C	194	LYS
1	C	206	LYS
1	C	209	TYR
1	C	214	LYS
1	C	216	LEU
1	C	220	THR
1	C	227	MET
1	C	229	GLN
1	C	230	VAL
1	C	233	GLN

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Mol	Chain	Res	Type
1	C	236	GLN
1	C	271	LEU
1	C	273	GLN
1	C	281	VAL
1	C	288	ARG
1	D	19	PHE
1	D	21	GLU
1	D	26	LYS
1	D	27	ARG
1	D	28	THR
1	D	37	ARG
1	D	66	ARG
1	D	68	ARG
1	D	69	GLN
1	D	89	SER
1	D	104	SER
1	D	125	MET
1	D	126	MET
1	D	131	GLU
1	D	132	THR
1	D	133	LYS
1	D	141	LYS
1	D	150	LEU
1	D	151	LYS
1	D	157	LYS
1	D	165	LYS
1	D	166	GLU
1	D	167	GLU
1	D	169	LEU
1	D	171	ILE
1	D	174	GLU
1	D	177	SER
1	D	184	ASN
1	D	187	GLN
1	D	188	LEU
1	D	191	LEU
1	D	195	ILE
1	D	196	GLU
1	D	211	LYS
1	D	214	LYS
1	D	218	GLN
1	D	220	THR

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Mol	Chain	Res	Type
1	D	247	GLU
1	D	259	SER
1	D	261	VAL
1	D	272	GLU
1	D	276	ARG
1	D	282	GLU
1	D	284	LEU
1	D	304	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	ASN
1	A	47	HIS
1	A	115	ASN
1	A	160	HIS
1	A	192	GLN
1	A	200	GLN
1	A	222	GLN
1	A	235	GLN
1	A	298	ASN
1	B	36	HIS
1	B	44	ASN
1	B	58	GLN
1	B	69	GLN
1	B	122	HIS
1	B	143	GLN
1	B	161	HIS
1	B	187	GLN
1	B	192	GLN
1	B	218	GLN
1	B	235	GLN
1	B	301	GLN
1	C	44	ASN
1	C	58	GLN
1	C	59	GLN
1	C	115	ASN
1	C	117	GLN
1	C	122	HIS
1	C	161	HIS
1	C	187	GLN

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Mol	Chain	Res	Type
1	C	200	GLN
1	C	235	GLN
1	C	255	HIS
1	C	290	ASN
1	C	291	HIS
1	D	36	HIS
1	D	44	ASN
1	D	47	HIS
1	D	58	GLN
1	D	143	GLN
1	D	187	GLN
1	D	233	GLN
1	D	235	GLN
1	D	236	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/289 (99%)	-1.52	0 100 100	20, 39, 106, 115	0
1	B	287/289 (99%)	-1.52	0 100 100	21, 41, 114, 121	0
1	C	287/289 (99%)	-1.53	0 100 100	24, 40, 113, 119	0
1	D	289/289 (100%)	-1.54	0 100 100	24, 41, 114, 122	0
All	All	1150/1156 (99%)	-1.53	0 100 100	20, 41, 111, 122	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	488	1/1	1.00	0.02	35,35,35,35	0
2	CA	B	488	1/1	1.00	0.02	42,42,42,42	0
2	CA	C	488	1/1	1.00	0.01	33,33,33,33	0
2	CA	D	488	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.