



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:40 PM UTC

PDB ID : 1S26 / pdb_00001s26
Title : Structure of Anthrax Edema Factor-Calmodulin-alpha,beta-methyleneadenosine 5'-triphosphate Complex Reveals an Alternative Mode of ATP Binding to the Catalytic Site
Authors : Shen, Y.; Zhukovskaya, N.L.; Bohm, A.; Tang, W.-J.
Deposited on : 2004-01-08
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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:

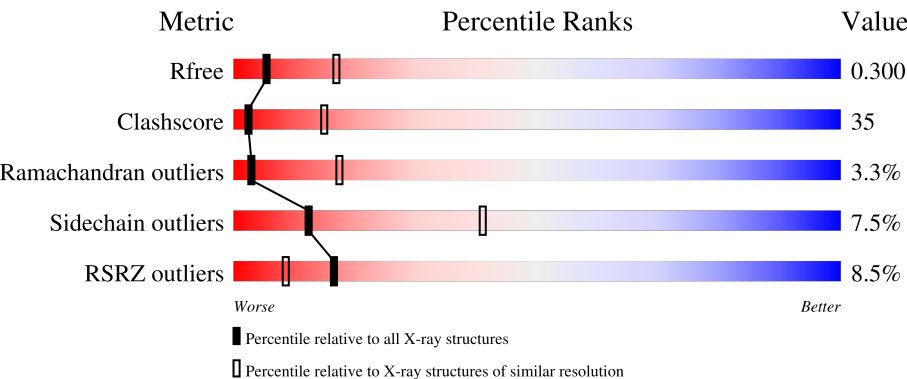
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	510	4% 53% 35% 7% 5%
1	B	510	8% 34% 46% 11% 9%
1	C	510	4% 55% 35% 8% 2%
2	D	148	19% 40% 47% 9% 5%

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Mol	Chain	Length	Quality of chain
2	E	148	22%39%49%7% . .
2	F	148	12%37%51%7% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15317 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 Calmodulin-sensitive adenylyate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	465	Total	C	N	O	S	113	0	0
			3794	2431	642	718	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

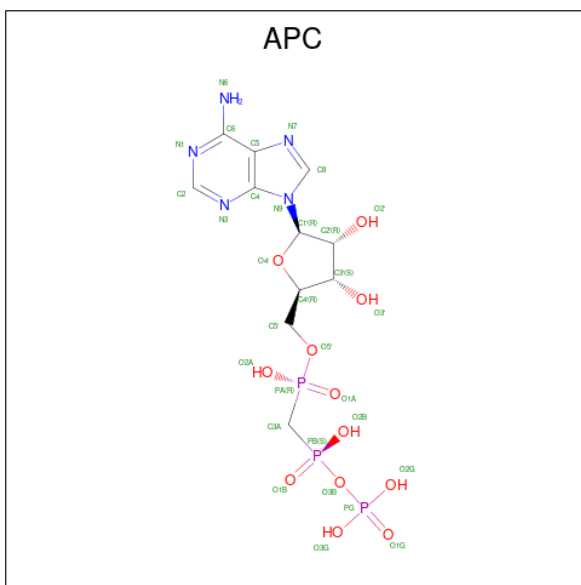
- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Yb	0	0
			1	1		
3	B	1	Total	Yb	0	0
			1	1		
3	C	1	Total	Yb	0	0
			1	1		

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	C	1	Total 31	C 11	N 5	O 12	P 3	0	0

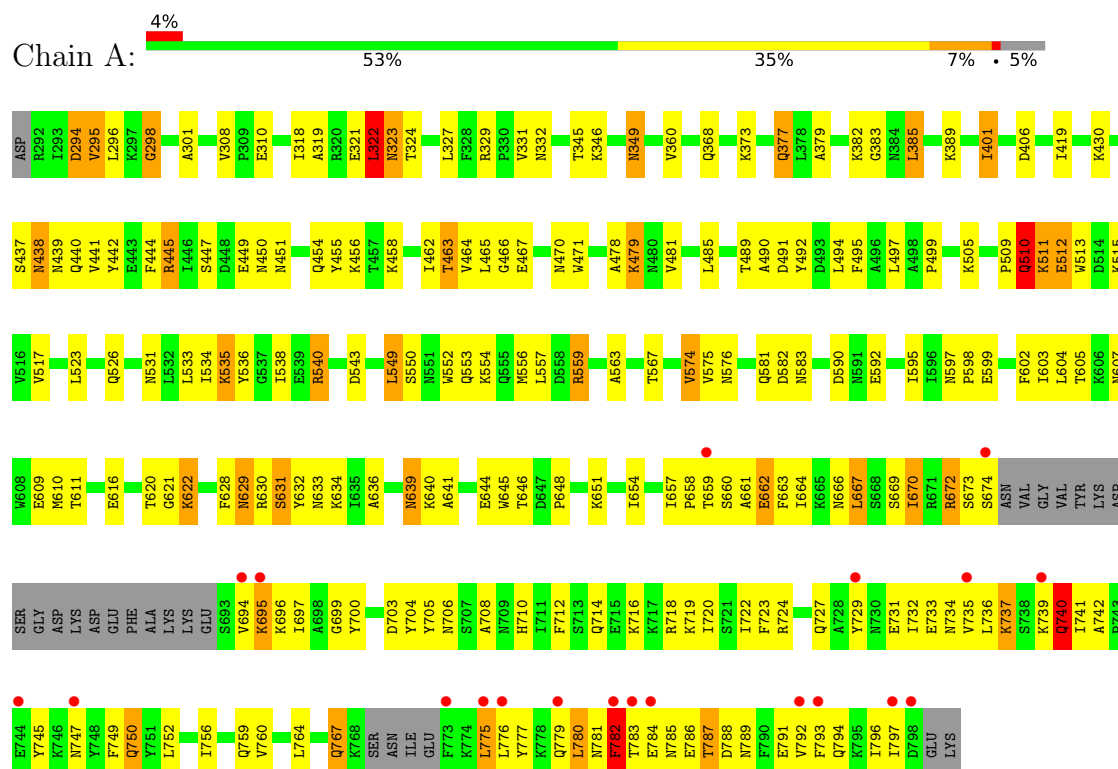
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Ca 2 2	0	0
5	E	2	Total Ca 2 2	0	0
5	F	2	Total Ca 2 2	0	0

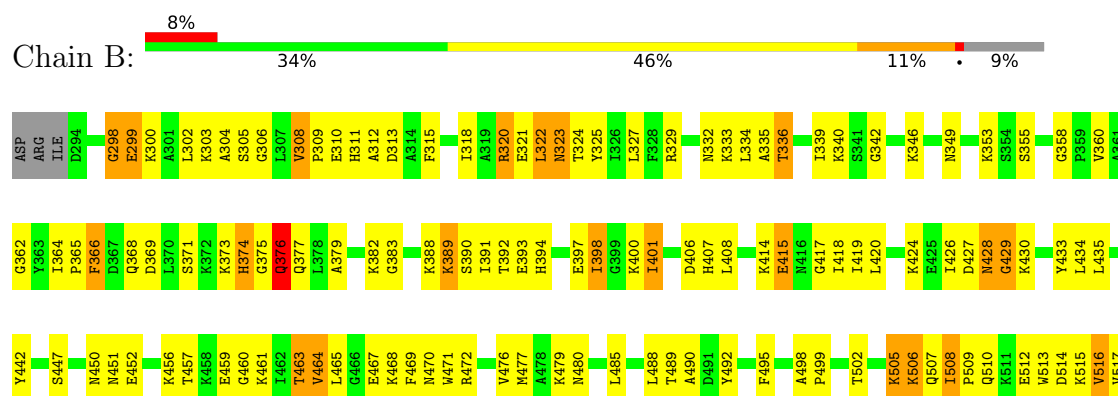
3 Residue-property plots

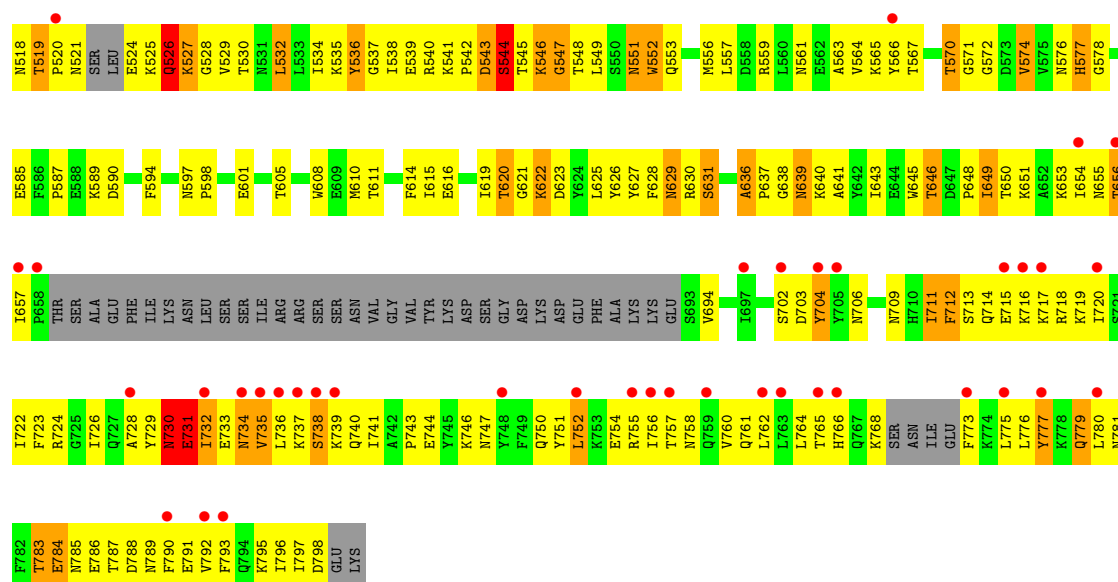
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

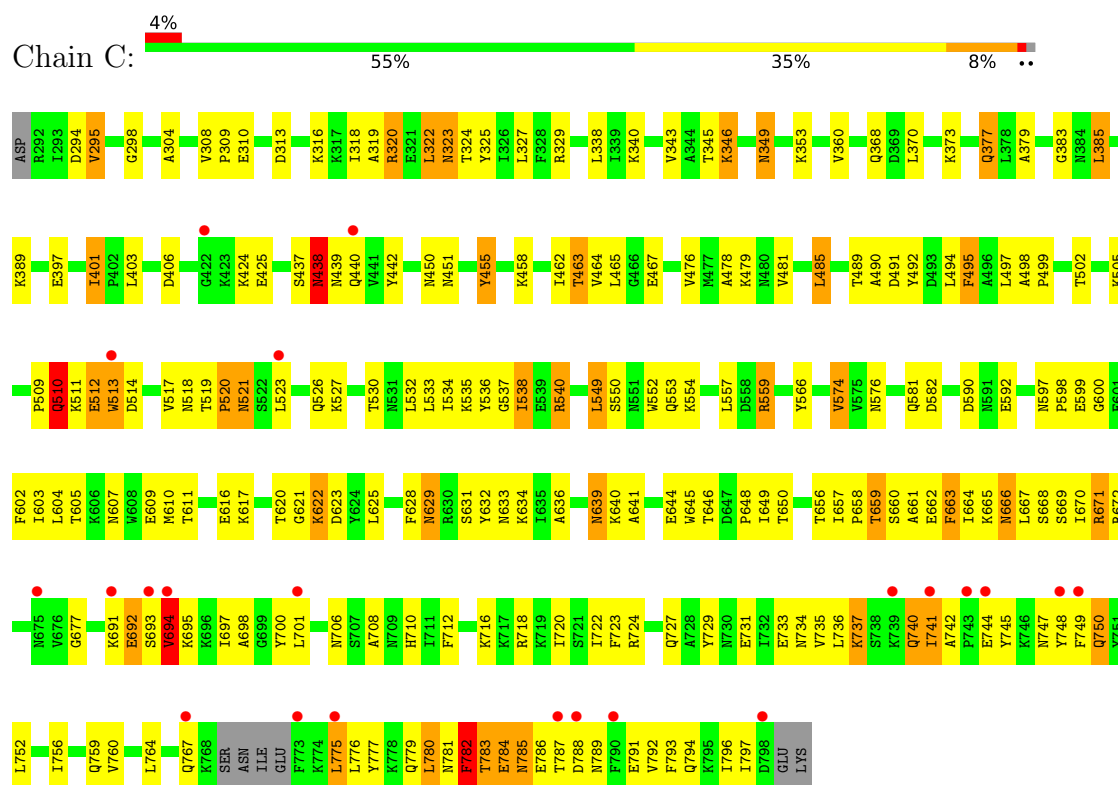


• Molecule 1: Calmodulin-sensitive adenylate cyclase

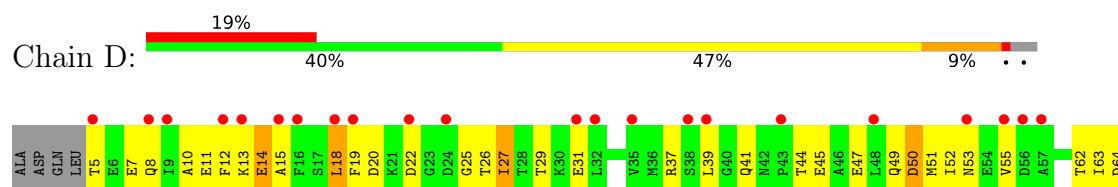




• Molecule 1: Calmodulin-sensitive adenylate cyclase

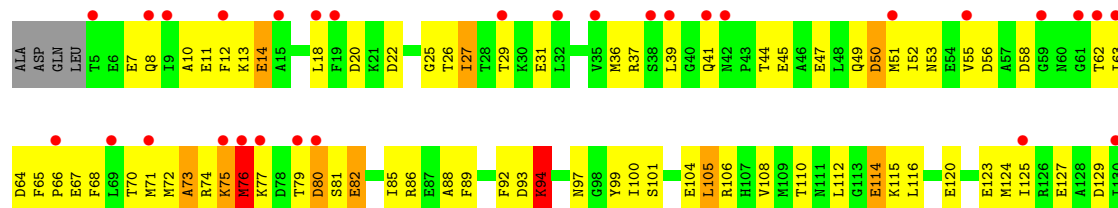
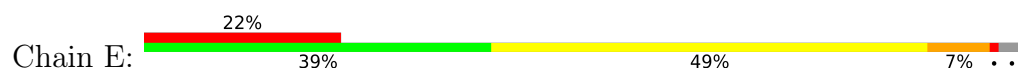


• Molecule 2: Calmodulin

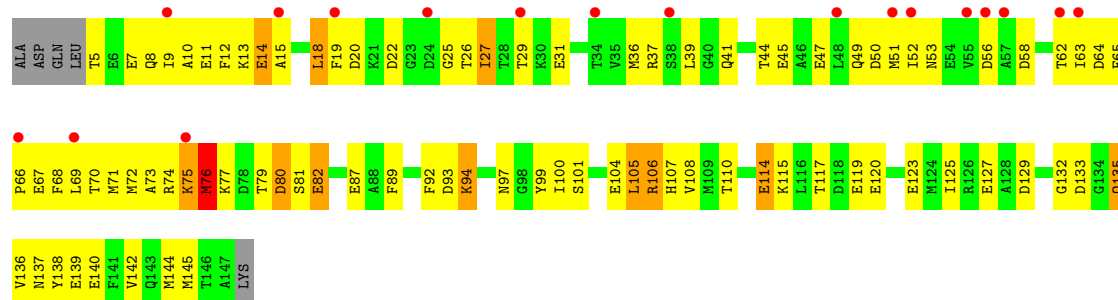




• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 167.60Å 345.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 3.00 29.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.78-3.00) 99.6 (29.78-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.304 0.261 , 0.300	Depositor DCC
R_{free} test set	3610 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15317	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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

5.1 Standard geometry

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

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	0.59	1/4027 (0.0%)	1.09	33/5419 (0.6%)
1	B	0.63	6/3867 (0.2%)	1.14	37/5204 (0.7%)
1	C	0.62	7/4172 (0.2%)	1.15	37/5613 (0.7%)
2	D	0.44	0/1137	0.85	1/1527 (0.1%)
2	E	0.40	0/1137	0.82	1/1527 (0.1%)
2	F	0.43	0/1137	0.86	2/1527 (0.1%)
All	All	0.58	14/15477 (0.1%)	1.07	111/20817 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	783	THR	C-N	-11.80	1.22	1.33
1	C	784	GLU	CA-C	-9.09	1.42	1.53
1	B	731	GLU	C-N	-6.77	1.25	1.33
1	B	656	THR	N-CA	6.76	1.54	1.46
1	C	785	ASN	CA-C	-6.48	1.43	1.52
1	B	544	SER	C-N	-6.35	1.24	1.33
1	B	731	GLU	CA-C	-5.91	1.44	1.52
1	C	785	ASN	N-CA	-5.76	1.39	1.46
1	C	783	THR	N-CA	-5.66	1.39	1.46
1	C	785	ASN	C-N	-5.53	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	322	LEU	C-N	-5.41	1.25	1.33
1	B	376	GLN	C-N	5.35	1.40	1.33
1	B	731	GLU	N-CA	5.29	1.53	1.46
1	A	784	GLU	CA-C	-5.27	1.46	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	784	GLU	N-CA-C	-13.78	90.41	108.19
1	C	322	LEU	CA-C-N	-12.63	104.08	122.77
1	C	322	LEU	C-N-CA	-12.63	104.08	122.77
1	C	782	PHE	N-CA-C	-12.56	98.60	114.56
1	C	783	THR	N-CA-C	11.88	125.70	111.33
1	A	322	LEU	N-CA-C	-11.48	92.06	110.20
1	C	785	ASN	CA-C-N	-10.49	101.50	121.54
1	C	785	ASN	C-N-CA	-10.49	101.50	121.54
1	B	740	GLN	OE1-CD-NE2	-10.34	112.26	122.60
1	B	376	GLN	OE1-CD-NE2	-10.34	112.26	122.60
1	C	784	GLU	CA-C-N	-10.16	102.09	121.81
1	C	784	GLU	C-N-CA	-10.16	102.09	121.81
1	A	740	GLN	OE1-CD-NE2	-9.90	112.69	122.60
1	A	510	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	767	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	C	510	GLN	OE1-CD-NE2	-9.71	112.89	122.60
1	C	740	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	C	767	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	B	622	LYS	N-CA-C	9.35	124.66	111.30
1	A	785	ASN	N-CA-C	9.28	124.51	112.26
1	B	375	GLY	CA-C-N	-9.12	110.29	122.42
1	B	375	GLY	C-N-CA	-9.12	110.29	122.42
1	C	511	LYS	N-CA-C	-8.88	103.03	114.04
1	B	730	ASN	O-C-N	-8.41	112.06	122.24
1	B	543	ASP	CA-C-N	-8.33	107.96	122.79
1	B	543	ASP	C-N-CA	-8.33	107.96	122.79
1	B	732	ILE	N-CA-C	-8.24	104.85	112.43
1	C	785	ASN	N-CA-C	8.01	122.45	111.71
1	A	672	ARG	N-CA-C	-8.01	101.16	112.13
1	A	785	ASN	CA-CB-CG	-7.72	104.88	112.60
1	A	783	THR	N-CA-C	7.72	124.03	111.37
1	B	740	GLN	CG-CD-NE2	7.46	127.59	116.40
1	A	784	GLU	CA-C-N	-7.35	111.62	122.86
1	A	784	GLU	C-N-CA	-7.35	111.62	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	LEU	N-CA-C	-7.25	98.74	110.20
1	A	767	GLN	CG-CD-NE2	7.22	127.22	116.40
1	B	777	TYR	N-CA-C	-7.21	104.36	113.02
1	B	730	ASN	CA-C-N	-7.21	107.78	121.54
1	B	730	ASN	C-N-CA	-7.21	107.78	121.54
1	B	779	GLN	N-CA-C	-7.02	104.29	112.92
1	A	667	LEU	N-CA-C	-7.00	102.83	113.89
1	A	740	GLN	CG-CD-NE2	6.90	126.75	116.40
1	A	510	GLN	CG-CD-NE2	6.76	126.54	116.40
1	C	767	GLN	CG-CD-NE2	6.75	126.53	116.40
1	A	535	LYS	N-CA-C	6.69	118.57	111.28
1	A	784	GLU	N-CA-C	-6.67	98.90	109.23
1	A	783	THR	CA-C-O	-6.61	113.29	121.02
1	B	366	PHE	N-CA-C	-6.50	104.12	111.14
1	A	695	LYS	N-CA-C	-6.49	105.35	113.20
1	B	546	LYS	N-CA-C	-6.48	99.07	109.96
1	B	532	LEU	N-CA-C	-6.44	103.50	112.45
1	B	376	GLN	CG-CD-NE2	6.40	126.00	116.40
1	B	656	THR	CB-CA-C	-6.33	101.47	110.34
1	C	740	GLN	CG-CD-NE2	6.30	125.84	116.40
1	C	592	GLU	N-CA-C	6.28	119.14	108.90
1	A	512	GLU	N-CA-C	-6.28	103.73	112.45
2	F	106	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	C	510	GLN	CG-CD-NE2	6.24	125.76	116.40
1	B	374	HIS	CA-C-N	-6.15	109.36	121.41
1	B	374	HIS	C-N-CA	-6.15	109.36	121.41
1	B	342	GLY	N-CA-C	6.13	123.20	115.42
1	C	783	THR	CA-C-O	-6.09	114.06	120.63
1	B	401	ILE	CA-C-N	-6.08	113.71	119.85
1	B	401	ILE	C-N-CA	-6.08	113.71	119.85
1	A	669	SER	N-CA-C	-6.04	106.07	113.50
1	B	576	ASN	N-CA-C	6.01	120.77	113.38
1	A	322	LEU	CB-CA-C	5.99	119.65	109.53
1	A	592	GLU	N-CA-C	5.97	118.68	109.07
2	F	106	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	C	322	LEU	CA-C-O	-5.92	114.30	121.05
1	B	308	VAL	CA-C-N	5.92	127.24	119.84
1	B	308	VAL	C-N-CA	5.92	127.24	119.84
1	C	442	TYR	N-CA-C	5.92	118.84	110.14
1	C	538	ILE	N-CA-C	5.85	117.22	111.67
1	C	346	LYS	N-CA-C	5.80	119.17	109.95
1	A	441	VAL	N-CA-C	5.80	117.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	LYS	N-CA-C	5.79	118.91	109.59
1	B	495	PHE	N-CA-C	-5.72	105.13	111.36
1	C	512	GLU	N-CA-C	-5.71	105.03	112.23
1	A	377	GLN	N-CA-C	5.70	120.78	111.37
1	A	308	VAL	N-CA-C	-5.69	103.37	108.95
1	C	495	PHE	N-CA-C	-5.68	104.47	111.40
1	C	513	TRP	N-CA-C	-5.67	106.21	113.01
1	C	671	ARG	N-CA-C	-5.66	105.96	112.92
1	C	576	ASN	N-CA-C	5.58	120.08	112.88
1	B	358	GLY	CA-C-N	5.58	125.24	119.05
1	B	358	GLY	C-N-CA	5.58	125.24	119.05
2	D	94	LYS	N-CA-C	5.58	118.12	111.71
1	C	377	GLN	N-CA-C	5.56	120.55	111.37
1	C	750	GLN	N-CA-C	-5.54	105.34	111.71
1	A	782	PHE	N-CA-C	-5.50	99.08	110.80
1	A	740	GLN	N-CA-C	-5.49	99.10	110.80
1	C	783	THR	CA-C-N	-5.43	112.09	122.08
1	C	783	THR	C-N-CA	-5.43	112.09	122.08
1	A	576	ASN	N-CA-C	5.36	119.80	112.88
1	C	308	VAL	N-CA-C	-5.35	103.71	108.95
1	B	731	GLU	O-C-N	5.33	129.67	122.59
1	B	783	THR	N-CA-C	-5.32	108.05	114.75
1	A	575	VAL	N-CA-C	-5.30	100.01	107.75
1	B	577	HIS	N-CA-C	5.27	115.49	108.38
1	B	636	ALA	CA-C-N	5.23	125.03	119.28
1	B	636	ALA	C-N-CA	5.23	125.03	119.28
1	C	532	LEU	N-CA-C	-5.17	105.34	111.69
1	B	505	LYS	N-CA-C	-5.16	105.57	111.14
1	A	750	GLN	N-CA-C	-5.12	105.83	111.71
1	C	511	LYS	CA-C-O	5.09	125.42	119.06
1	C	672	ARG	N-CA-C	-5.08	106.77	113.17
1	A	533	LEU	N-CA-C	-5.03	105.70	111.14
1	A	595	ILE	N-CA-C	5.02	115.81	108.53
1	B	548	THR	N-CA-C	-5.02	102.43	109.96
2	E	94	LYS	N-CA-C	5.02	118.17	111.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	730	ASN	Mainchain
1	C	566	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3952	0	3999	219	0
1	B	3794	0	3828	371	0
1	C	4094	0	4134	232	0
2	D	1125	0	1049	95	0
2	E	1125	0	1049	89	0
2	F	1125	0	1049	98	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	3	0
4	C	31	0	12	2	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	15317	0	15144	1042	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 35.

All (1042) 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:489:THR:HG22	1:B:490:ALA:H	1.08	1.11
1:B:616:GLU:HA	1:B:620:THR:HG22	1.40	1.03
1:B:543:ASP:OD1	1:B:544:SER:N	1.93	1.02
1:B:629:ASN:HD22	1:B:631:SER:H	1.04	1.02
1:B:535:LYS:HE2	1:B:535:LYS:HA	1.38	1.01
1:B:726:ILE:HA	1:B:729:TYR:HB2	1.39	1.01
1:B:366:PHE:HD1	1:B:477:MET:HE1	1.28	0.99
1:B:731:GLU:HG3	1:B:732:ILE:H	1.28	0.97
1:B:353:LYS:N	1:B:368:GLN:HE22	1.63	0.95
1:B:605:THR:HG21	1:B:611:THR:OG1	1.65	0.95
1:B:353:LYS:H	1:B:368:GLN:NE2	1.65	0.95
1:A:510:GLN:O	1:A:510:GLN:HG3	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ASN:HD22	1:B:551:ASN:N	1.66	0.93
1:B:489:THR:HG22	1:B:490:ALA:N	1.81	0.92
2:E:97:ASN:HD21	2:E:99:TYR:HB2	1.34	0.92
2:D:26:THR:HG22	2:D:64:ASP:HB3	1.51	0.92
1:B:324:THR:HG22	1:B:499:PRO:HA	1.48	0.92
2:F:26:THR:HG22	2:F:64:ASP:HB3	1.52	0.92
2:E:26:THR:HG22	2:E:64:ASP:HB3	1.52	0.91
1:B:714:GLN:HE22	1:B:715:GLU:HG3	1.35	0.91
1:B:514:ASP:HA	1:B:517:VAL:HG12	1.51	0.90
1:A:719:LYS:HE3	1:A:767:GLN:HE22	1.35	0.90
1:C:664:ILE:HG21	2:F:15:ALA:HB2	1.51	0.90
1:A:445:ARG:HH21	1:A:471:TRP:NE1	1.71	0.89
1:C:629:ASN:HD22	1:C:631:SER:H	1.14	0.88
1:B:518:ASN:C	1:B:520:PRO:HD3	1.99	0.88
1:B:551:ASN:H	1:B:551:ASN:ND2	1.70	0.87
1:C:697:ILE:HD11	1:C:735:VAL:HG21	1.57	0.87
1:B:551:ASN:HD22	1:B:551:ASN:H	0.92	0.86
1:C:633:ASN:HD21	1:C:645:TRP:H	1.22	0.85
1:B:709:ASN:HD21	1:B:720:ILE:HD11	1.40	0.85
1:C:559:ARG:HH11	1:C:559:ARG:HB3	1.40	0.85
1:C:658:PRO:HG3	1:C:752:LEU:HD22	1.59	0.84
1:A:633:ASN:HD21	1:A:645:TRP:H	1.23	0.84
1:C:692:GLU:O	1:C:735:VAL:HG22	1.77	0.84
1:B:597:ASN:HD21	1:B:601:GLU:HB2	1.42	0.84
1:C:657:ILE:HG13	1:C:759:GLN:HG2	1.60	0.84
1:A:629:ASN:HD22	1:A:631:SER:H	1.21	0.83
1:C:629:ASN:ND2	1:C:631:SER:H	1.78	0.82
1:B:322:LEU:HD12	1:B:556:MET:HE1	1.61	0.82
1:C:349:ASN:HD22	1:C:349:ASN:H	1.28	0.82
1:C:510:GLN:HG3	1:C:510:GLN:O	1.79	0.82
1:A:349:ASN:H	1:A:349:ASN:HD22	1.24	0.82
1:B:427:ASP:O	1:B:429:GLY:N	2.12	0.82
1:B:654:ILE:HA	1:B:755:ARG:CD	2.10	0.82
1:B:427:ASP:O	1:B:428:ASN:C	2.22	0.82
2:D:70:THR:O	2:D:73:ALA:HB3	1.77	0.82
1:B:714:GLN:NE2	1:B:715:GLU:HG3	1.94	0.82
1:A:777:TYR:HA	1:A:780:LEU:HD21	1.61	0.81
1:B:709:ASN:ND2	1:B:720:ILE:HD11	1.95	0.81
2:F:97:ASN:HD21	2:F:99:TYR:HB2	1.46	0.81
1:B:489:THR:CG2	1:B:490:ALA:H	1.90	0.81
1:A:463:THR:HG22	1:A:465:LEU:H	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HG22	1:C:465:LEU:H	1.46	0.80
1:B:711:ILE:HG13	1:B:712:PHE:HD1	1.46	0.80
1:B:791:GLU:HG3	1:B:792:VAL:H	1.45	0.80
1:B:366:PHE:HA	1:B:477:MET:HE3	1.62	0.80
1:B:712:PHE:HD1	1:B:712:PHE:H	1.26	0.80
1:B:735:VAL:HG22	1:B:738:SER:HB2	1.61	0.80
1:B:353:LYS:H	1:B:368:GLN:HE22	0.82	0.80
1:C:777:TYR:HA	1:C:780:LEU:HD21	1.62	0.79
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.17	0.79
1:C:616:GLU:HA	1:C:620:THR:HG22	1.64	0.79
1:A:616:GLU:HA	1:A:620:THR:HG22	1.63	0.79
1:C:519:THR:OG1	1:C:520:PRO:HD2	1.83	0.79
1:A:444:PHE:C	1:A:445:ARG:HH11	1.90	0.78
1:A:523:LEU:HD13	2:D:127:GLU:HB3	1.66	0.78
1:B:535:LYS:HE2	1:B:535:LYS:CA	2.14	0.78
1:B:775:LEU:HD22	1:B:775:LEU:H	1.48	0.78
1:B:712:PHE:HB3	1:B:716:LYS:CG	2.14	0.77
1:B:322:LEU:O	1:B:324:THR:HG23	1.84	0.77
1:B:720:ILE:O	1:B:724:ARG:HG2	1.83	0.77
1:B:320:ARG:HG3	1:B:321:GLU:N	1.99	0.77
1:B:731:GLU:CG	1:B:732:ILE:H	1.88	0.77
1:A:349:ASN:HD22	1:A:349:ASN:N	1.82	0.77
1:C:329:ARG:HD2	1:C:590:ASP:OD2	1.85	0.76
2:E:138:TYR:O	2:E:142:VAL:HG23	1.85	0.76
2:D:133:ASP:OD2	2:D:135:GLN:HG3	1.85	0.76
1:A:510:GLN:O	1:A:510:GLN:CG	2.32	0.76
1:B:366:PHE:CD1	1:B:477:MET:HE1	2.17	0.76
1:A:559:ARG:HB3	1:A:559:ARG:HH11	1.50	0.76
1:B:312:ALA:O	1:B:315:PHE:HB2	1.86	0.76
1:B:629:ASN:ND2	1:B:631:SER:HB2	2.01	0.75
1:B:561:ASN:O	1:B:564:VAL:HG22	1.85	0.75
1:B:712:PHE:HB3	1:B:716:LYS:HG2	1.69	0.74
1:A:719:LYS:HE3	1:A:767:GLN:NE2	2.01	0.74
1:A:445:ARG:HD3	1:A:454:GLN:HB2	1.69	0.74
2:F:68:PHE:HA	2:F:71:MET:HE3	1.70	0.74
1:C:349:ASN:HD22	1:C:349:ASN:N	1.83	0.74
1:B:526:GLN:HE21	2:E:124:MET:HE2	1.53	0.74
1:A:706:ASN:HD21	1:A:708:ALA:HB3	1.53	0.74
1:B:526:GLN:NE2	2:E:124:MET:HE2	2.03	0.74
1:B:308:VAL:HB	1:B:311:HIS:ND1	2.02	0.73
1:A:345:THR:HB	1:A:491:ASP:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:TYR:O	1:A:780:LEU:HD11	1.88	0.73
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.70	0.73
2:E:70:THR:O	2:E:73:ALA:HB3	1.89	0.73
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.71	0.73
2:D:68:PHE:HA	2:D:71:MET:HE3	1.69	0.73
1:B:639:ASN:ND2	1:B:641:ALA:H	1.87	0.72
1:B:648:PRO:HA	1:B:651:LYS:HB2	1.71	0.72
1:A:445:ARG:HH21	1:A:471:TRP:HE1	1.34	0.72
1:A:639:ASN:ND2	1:A:641:ALA:H	1.86	0.72
1:B:597:ASN:ND2	1:B:601:GLU:HB2	2.04	0.72
2:E:68:PHE:HA	2:E:71:MET:HE3	1.71	0.72
1:B:777:TYR:HA	1:B:780:LEU:HD12	1.71	0.72
1:C:668:SER:HB2	2:F:14:GLU:HG3	1.72	0.72
1:A:445:ARG:NH2	1:A:471:TRP:NE1	2.37	0.71
1:B:306:GLY:O	1:B:336:THR:HB	1.90	0.71
1:B:318:ILE:HD12	1:B:318:ILE:H	1.55	0.71
1:C:639:ASN:ND2	1:C:641:ALA:H	1.89	0.71
2:F:133:ASP:OD2	2:F:135:GLN:HG3	1.90	0.71
1:B:730:ASN:O	1:B:731:GLU:C	2.24	0.71
1:B:565:LYS:C	1:B:567:THR:H	1.98	0.71
1:C:633:ASN:ND2	1:C:644:GLU:HA	2.06	0.71
1:A:445:ARG:NE	1:A:471:TRP:CE2	2.59	0.71
1:C:438:ASN:C	1:C:438:ASN:HD22	1.98	0.71
1:A:792:VAL:O	1:A:796:ILE:HG12	1.90	0.70
1:A:629:ASN:ND2	1:A:631:SER:H	1.89	0.70
1:A:706:ASN:ND2	1:A:708:ALA:HB3	2.06	0.70
1:B:300:LYS:HA	1:B:303:LYS:NZ	2.06	0.70
1:B:335:ALA:HB1	1:B:489:THR:CG2	2.21	0.70
1:B:792:VAL:O	1:B:796:ILE:HG12	1.91	0.70
1:C:722:ILE:HD13	1:C:764:LEU:HD23	1.73	0.70
1:B:369:ASP:OD2	1:B:442:TYR:OH	2.09	0.70
1:C:509:PRO:HG2	1:C:512:GLU:HB2	1.72	0.70
1:C:706:ASN:HD21	1:C:708:ALA:HB3	1.56	0.70
1:A:445:ARG:NH2	1:A:471:TRP:HE1	1.89	0.70
1:B:505:LYS:C	1:B:507:GLN:H	1.99	0.70
2:F:70:THR:O	2:F:73:ALA:HB3	1.89	0.70
2:E:136:VAL:HA	2:E:140:GLU:OE1	1.92	0.70
2:F:138:TYR:O	2:F:142:VAL:HG23	1.92	0.70
2:F:68:PHE:O	2:F:72:MET:HG2	1.92	0.70
1:A:438:ASN:HD22	1:A:438:ASN:C	2.00	0.69
1:A:456:LYS:HD3	1:A:471:TRP:HD1	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:VAL:HA	2:D:140:GLU:OE1	1.93	0.69
1:A:633:ASN:ND2	1:A:644:GLU:HA	2.07	0.69
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.72	0.69
1:B:389:LYS:HB2	1:B:389:LYS:NZ	2.08	0.69
1:C:706:ASN:ND2	1:C:708:ALA:HB3	2.07	0.69
1:C:792:VAL:O	1:C:796:ILE:HG12	1.92	0.69
1:C:777:TYR:O	1:C:780:LEU:HD11	1.92	0.68
2:E:10:ALA:O	2:E:14:GLU:HB2	1.94	0.68
1:A:463:THR:HG22	1:A:465:LEU:N	2.08	0.68
1:C:559:ARG:HB3	1:C:559:ARG:NH1	2.09	0.68
1:A:695:LYS:HD2	2:D:19:PHE:HB2	1.76	0.68
1:B:332:ASN:C	1:B:332:ASN:HD22	2.01	0.68
1:B:629:ASN:HD22	1:B:631:SER:N	1.86	0.68
1:C:659:THR:HG22	1:C:661:ALA:H	1.59	0.68
1:B:654:ILE:HA	1:B:755:ARG:HD2	1.76	0.68
1:B:797:ILE:HG13	1:B:798:ASP:N	2.08	0.68
1:C:633:ASN:HD21	1:C:645:TRP:N	1.92	0.68
2:D:97:ASN:HD21	2:D:99:TYR:HB2	1.59	0.67
2:D:68:PHE:O	2:D:72:MET:HG2	1.95	0.67
2:F:10:ALA:O	2:F:14:GLU:HB2	1.94	0.67
1:B:538:ILE:CD1	1:B:625:LEU:HD11	2.24	0.67
1:B:535:LYS:HZ1	1:B:539:GLU:HB2	1.60	0.67
1:C:775:LEU:HD23	1:C:775:LEU:H	1.59	0.67
2:D:8:GLN:HA	2:D:8:GLN:HE21	1.60	0.67
1:A:695:LYS:HG3	2:D:18:LEU:HD13	1.76	0.67
1:C:667:LEU:HA	1:C:670:ILE:HG22	1.77	0.67
1:B:389:LYS:HB2	1:B:389:LYS:HZ2	1.60	0.67
1:B:362:GLY:O	1:B:489:THR:HG23	1.96	0.66
1:C:660:SER:O	1:C:663:PHE:HB3	1.94	0.66
1:A:775:LEU:HD23	1:A:775:LEU:H	1.60	0.66
1:B:459:GLU:O	1:B:461:LYS:N	2.27	0.66
2:D:10:ALA:O	2:D:14:GLU:HB2	1.96	0.66
2:E:80:ASP:C	2:E:82:GLU:H	2.04	0.66
1:C:327:LEU:N	1:C:327:LEU:HD12	2.10	0.66
2:E:13:LYS:HG3	2:E:65:PHE:CE2	2.31	0.66
1:B:346:LYS:NZ	4:B:2139:APC:H3A2	2.10	0.66
1:B:322:LEU:HD12	1:B:556:MET:CE	2.26	0.66
1:B:509:PRO:HG2	1:B:512:GLU:HB3	1.78	0.66
1:B:540:ARG:HD2	1:B:627:TYR:CZ	2.31	0.66
1:C:463:THR:HG22	1:C:465:LEU:N	2.10	0.66
1:C:517:VAL:HG13	1:C:518:ASN:ND2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:THR:HG22	1:C:661:ALA:N	2.11	0.66
1:C:440:GLN:CD	1:C:440:GLN:H	2.03	0.66
1:B:551:ASN:N	1:B:551:ASN:ND2	2.35	0.66
1:A:456:LYS:HD3	1:A:471:TRP:CD1	2.31	0.65
1:B:549:LEU:HD12	1:B:553:GLN:HE21	1.61	0.65
1:C:621:GLY:O	1:C:622:LYS:HE3	1.96	0.65
2:D:13:LYS:HG3	2:D:65:PHE:CE2	2.31	0.65
1:C:663:PHE:HA	1:C:748:TYR:OH	1.96	0.65
1:B:418:ILE:HG22	1:B:419:ILE:HG23	1.77	0.65
2:F:13:LYS:HG3	2:F:65:PHE:CE2	2.32	0.65
1:A:445:ARG:HE	1:A:471:TRP:NE1	1.94	0.65
1:A:492:TYR:CD2	1:A:574:VAL:CG1	2.80	0.65
2:D:76:MET:HE3	2:D:79:THR:HG21	1.77	0.65
1:B:394:HIS:HB3	1:B:397:GLU:HB2	1.78	0.65
1:C:700:TYR:CD1	1:C:727:GLN:HB3	2.32	0.65
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.32	0.65
1:C:629:ASN:HD22	1:C:631:SER:N	1.93	0.65
1:A:327:LEU:N	1:A:327:LEU:HD12	2.12	0.64
1:A:445:ARG:HG3	1:A:471:TRP:CZ2	2.31	0.64
1:C:657:ILE:HG13	1:C:759:GLN:CG	2.27	0.64
1:A:440:GLN:H	1:A:440:GLN:CD	2.04	0.64
1:B:722:ILE:HG23	1:B:760:VAL:HG11	1.78	0.64
2:E:25:GLY:O	2:E:64:ASP:HA	1.96	0.64
2:F:25:GLY:O	2:F:64:ASP:HA	1.97	0.64
1:A:445:ARG:HH21	1:A:471:TRP:CD1	2.14	0.64
1:B:324:THR:HG22	1:B:499:PRO:CA	2.24	0.64
1:B:525:LYS:HZ3	2:E:116:LEU:HD21	1.63	0.64
2:D:5:THR:OG1	2:D:8:GLN:HG2	1.98	0.64
2:F:136:VAL:HA	2:F:140:GLU:OE1	1.96	0.64
1:B:368:GLN:HG3	1:B:383:GLY:HA3	1.78	0.64
1:B:538:ILE:HD11	1:B:625:LEU:HD11	1.79	0.64
1:C:349:ASN:H	1:C:349:ASN:ND2	1.96	0.64
2:D:25:GLY:O	2:D:64:ASP:HA	1.96	0.64
2:D:80:ASP:C	2:D:82:GLU:H	2.04	0.64
2:E:133:ASP:OD2	2:E:135:GLN:HG3	1.98	0.64
1:B:535:LYS:C	1:B:536:TYR:HD2	2.05	0.64
1:B:656:THR:HG22	1:B:752:LEU:HD21	1.80	0.64
2:E:68:PHE:O	2:E:72:MET:HG2	1.97	0.63
1:B:376:GLN:HB2	1:B:379:ALA:CB	2.28	0.63
1:B:320:ARG:CB	1:B:320:ARG:HH21	2.10	0.63
1:C:598:PRO:HG2	1:C:599:GLU:OE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:ASN:ND2	2:E:99:TYR:HB2	2.12	0.63
1:C:505:LYS:HE3	1:C:513:TRP:CG	2.33	0.63
1:A:723:PHE:HB2	1:A:793:PHE:CE2	2.34	0.63
1:C:734:ASN:HA	1:C:737:LYS:HB2	1.80	0.63
2:E:8:GLN:HE21	2:E:8:GLN:HA	1.63	0.63
2:F:80:ASP:C	2:F:82:GLU:H	2.06	0.63
1:A:633:ASN:HD21	1:A:645:TRP:N	1.97	0.63
1:B:795:LYS:HA	1:B:798:ASP:OD2	1.99	0.63
1:B:320:ARG:HH21	1:B:320:ARG:HB3	1.64	0.63
1:B:722:ILE:HG23	1:B:760:VAL:CG1	2.28	0.63
1:A:540:ARG:NH2	2:D:87:GLU:OE1	2.32	0.62
1:A:639:ASN:C	1:A:639:ASN:HD22	2.07	0.62
1:C:345:THR:HB	1:C:491:ASP:HB3	1.81	0.62
1:B:534:ILE:HG22	1:B:535:LYS:CE	2.29	0.62
1:A:734:ASN:HA	1:A:737:LYS:HB2	1.81	0.62
1:A:736:LEU:HD21	1:A:749:PHE:HB2	1.81	0.62
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.33	0.62
2:D:138:TYR:O	2:D:142:VAL:HG23	1.99	0.62
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.81	0.62
1:A:657:ILE:HG23	1:A:759:GLN:HG2	1.82	0.62
2:D:74:ARG:O	2:D:77:LYS:HB2	1.99	0.62
1:A:559:ARG:HB3	1:A:559:ARG:NH1	2.15	0.62
1:B:629:ASN:ND2	1:B:631:SER:H	1.87	0.62
1:B:722:ILE:HD13	1:B:764:LEU:HD21	1.80	0.62
2:F:8:GLN:HE21	2:F:8:GLN:HA	1.65	0.62
1:B:450:ASN:O	1:B:451:ASN:HB2	1.99	0.62
1:C:616:GLU:HA	1:C:620:THR:CG2	2.29	0.62
1:C:695:LYS:CB	2:F:18:LEU:HD22	2.30	0.62
1:B:716:LYS:O	1:B:720:ILE:HG23	1.99	0.62
1:C:510:GLN:O	1:C:510:GLN:CG	2.46	0.62
1:B:519:THR:N	1:B:520:PRO:HD3	2.15	0.61
2:E:110:THR:HG22	2:E:115:LYS:HD2	1.82	0.61
2:F:63:ILE:N	2:F:63:ILE:HD12	2.15	0.61
1:A:670:ILE:HD12	1:A:745:TYR:CE1	2.35	0.61
1:B:722:ILE:O	1:B:726:ILE:HG13	2.00	0.61
2:E:65:PHE:HB2	2:E:66:PRO:HD3	1.82	0.61
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.36	0.61
1:B:459:GLU:C	1:B:461:LYS:H	2.08	0.61
1:B:536:TYR:N	1:B:536:TYR:CD2	2.69	0.61
1:B:758:ASN:HA	1:B:761:GLN:HB3	1.82	0.61
1:C:550:SER:H	1:C:553:GLN:NE2	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:GLU:O	1:C:735:VAL:HG23	2.00	0.61
1:B:320:ARG:HG3	1:B:321:GLU:H	1.65	0.61
1:B:565:LYS:O	1:B:567:THR:N	2.33	0.61
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.83	0.61
1:B:299:GLU:O	1:B:303:LYS:HG3	2.01	0.61
1:B:305:SER:HB3	1:B:594:PHE:CD1	2.36	0.61
1:B:734:ASN:C	1:B:736:LEU:H	2.06	0.61
1:C:535:LYS:HD2	1:C:536:TYR:CE2	2.35	0.61
1:A:444:PHE:C	1:A:445:ARG:NH1	2.59	0.61
1:C:736:LEU:HD21	1:C:749:PHE:HB2	1.83	0.61
1:C:783:THR:O	1:C:784:GLU:OE1	2.19	0.60
2:F:110:THR:HG22	2:F:115:LYS:HD2	1.82	0.60
1:A:329:ARG:HD2	1:A:590:ASP:OD2	2.01	0.60
1:B:736:LEU:O	1:B:741:ILE:HD12	2.01	0.60
1:A:598:PRO:HG2	1:A:599:GLU:OE2	2.01	0.60
2:D:49:GLN:O	2:D:52:ILE:HG22	2.02	0.60
2:D:101:SER:OG	2:D:104:GLU:HG3	2.02	0.60
2:E:74:ARG:O	2:E:77:LYS:HB2	2.00	0.60
2:F:49:GLN:O	2:F:52:ILE:HG22	2.01	0.60
1:B:622:LYS:O	1:B:623:ASP:HB2	2.00	0.60
1:B:629:ASN:HD21	1:B:631:SER:HB2	1.67	0.60
1:B:649:ILE:HG22	1:B:649:ILE:O	2.02	0.60
1:B:726:ILE:HA	1:B:729:TYR:CB	2.23	0.60
1:B:744:GLU:OE1	1:B:744:GLU:HA	2.00	0.60
1:B:525:LYS:NZ	2:E:116:LEU:HD21	2.16	0.60
1:A:349:ASN:H	1:A:349:ASN:ND2	1.95	0.60
2:E:49:GLN:O	2:E:52:ILE:HG22	2.02	0.60
2:D:44:THR:HG22	2:D:47:GLU:OE1	2.02	0.60
2:F:74:ARG:O	2:F:77:LYS:HB2	2.02	0.60
1:B:639:ASN:C	1:B:639:ASN:HD22	2.09	0.59
1:B:703:ASP:O	1:B:704:TYR:C	2.44	0.59
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.31	0.59
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.32	0.59
2:E:76:MET:HE3	2:E:79:THR:HG21	1.83	0.59
1:B:764:LEU:O	1:B:768:LYS:HB2	2.03	0.59
2:F:44:THR:HG22	2:F:47:GLU:OE1	2.02	0.59
1:A:712:PHE:CD2	1:A:716:LYS:HG2	2.37	0.59
1:B:534:ILE:HG22	1:B:535:LYS:HE3	1.85	0.59
1:B:320:ARG:HB3	1:B:320:ARG:NH2	2.17	0.59
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.38	0.59
2:F:76:MET:HE3	2:F:79:THR:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLU:O	1:A:735:VAL:HG23	2.03	0.59
1:B:516:VAL:HA	1:B:520:PRO:HG2	1.85	0.59
1:C:663:PHE:O	1:C:667:LEU:HG	2.03	0.59
1:B:302:LEU:C	1:B:304:ALA:H	2.11	0.59
1:C:747:ASN:HA	1:C:750:GLN:HG2	1.83	0.59
1:B:728:ALA:HA	1:B:731:GLU:CD	2.27	0.59
1:A:697:ILE:HD13	1:A:732:ILE:HG12	1.85	0.58
2:D:7:GLU:HA	2:D:10:ALA:HB3	1.84	0.58
2:F:7:GLU:HA	2:F:10:ALA:HB3	1.86	0.58
1:C:295:VAL:HG21	1:C:603:ILE:HG22	1.84	0.58
1:C:514:ASP:HA	1:C:517:VAL:HG12	1.84	0.58
1:A:540:ARG:HH22	2:D:87:GLU:CD	2.11	0.58
1:A:345:THR:HB	1:A:491:ASP:CB	2.34	0.58
1:A:747:ASN:HA	1:A:750:GLN:HG2	1.85	0.58
1:B:508:ILE:HG21	1:B:532:LEU:HD22	1.86	0.58
1:C:691:LYS:O	1:C:692:GLU:C	2.47	0.58
1:B:479:LYS:HG2	1:B:488:LEU:HD21	1.85	0.58
1:B:732:ILE:O	1:B:735:VAL:HG12	2.03	0.58
2:D:25:GLY:HA3	2:D:65:PHE:HE1	1.67	0.58
2:E:63:ILE:HD12	2:E:63:ILE:N	2.19	0.58
1:B:364:ILE:HB	1:B:477:MET:HB2	1.86	0.58
1:B:791:GLU:HG3	1:B:792:VAL:N	2.18	0.58
1:A:621:GLY:O	1:A:622:LYS:HE3	2.04	0.58
1:B:791:GLU:CG	1:B:792:VAL:H	2.15	0.58
1:C:639:ASN:C	1:C:639:ASN:HD22	2.11	0.58
2:D:63:ILE:N	2:D:63:ILE:HD12	2.19	0.58
2:E:75:LYS:O	2:E:79:THR:HG22	2.04	0.58
1:B:543:ASP:CG	1:B:544:SER:N	2.62	0.58
1:B:762:LEU:HA	1:B:765:THR:OG1	2.04	0.58
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.39	0.58
1:B:706:ASN:O	1:B:709:ASN:HB2	2.03	0.57
1:B:715:GLU:O	1:B:719:LYS:HB2	2.03	0.57
1:A:581:GLN:NE2	1:A:629:ASN:H	2.01	0.57
1:B:390:SER:HB3	1:B:398:ILE:HG21	1.86	0.57
1:B:565:LYS:C	1:B:567:THR:N	2.62	0.57
1:C:492:TYR:CD2	1:C:574:VAL:CG1	2.87	0.57
1:C:666:ASN:N	1:C:666:ASN:HD22	2.02	0.57
1:C:657:ILE:HG13	1:C:759:GLN:CB	2.34	0.57
1:B:648:PRO:C	1:B:650:THR:H	2.11	0.57
1:C:523:LEU:HD22	2:F:127:GLU:HB3	1.86	0.57
1:C:742:ALA:HB3	1:C:745:TYR:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:THR:O	1:A:787:THR:HG22	2.04	0.57
1:C:670:ILE:HG23	1:C:745:TYR:CZ	2.39	0.57
1:B:625:LEU:HD12	1:B:626:TYR:H	1.70	0.57
1:C:661:ALA:O	1:C:663:PHE:N	2.36	0.57
1:C:747:ASN:O	1:C:750:GLN:HG2	2.04	0.57
2:E:129:ASP:OD1	2:E:132:GLY:N	2.34	0.57
1:B:536:TYR:HD2	1:B:536:TYR:N	2.03	0.57
2:E:7:GLU:O	2:E:11:GLU:HG3	2.04	0.57
1:A:438:ASN:C	1:A:438:ASN:ND2	2.63	0.57
1:C:513:TRP:HZ2	2:F:114:GLU:H	1.51	0.56
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.87	0.56
1:B:318:ILE:HD12	1:B:318:ILE:N	2.20	0.56
1:B:776:LEU:HD13	1:B:779:GLN:CD	2.30	0.56
1:C:346:LYS:NZ	4:C:3139:APC:H3A2	2.19	0.56
2:E:123:GLU:O	2:E:127:GLU:HG2	2.05	0.56
2:F:7:GLU:O	2:F:11:GLU:HG3	2.05	0.56
1:B:318:ILE:O	1:B:322:LEU:HG	2.05	0.56
1:B:419:ILE:O	1:B:420:LEU:HD23	2.05	0.56
1:B:722:ILE:HG12	1:B:760:VAL:HG13	1.85	0.56
1:C:540:ARG:NH2	2:F:87:GLU:OE1	2.37	0.56
1:C:787:THR:O	1:C:787:THR:HG22	2.05	0.56
2:E:25:GLY:HA3	2:E:65:PHE:HE1	1.71	0.56
1:B:505:LYS:C	1:B:507:GLN:N	2.64	0.56
1:B:335:ALA:O	1:B:339:ILE:HG13	2.06	0.56
1:B:735:VAL:HG13	1:B:735:VAL:O	2.04	0.56
1:B:737:LYS:O	1:B:738:SER:C	2.47	0.56
1:C:373:LYS:HG2	1:C:379:ALA:HB1	1.86	0.56
1:C:438:ASN:C	1:C:438:ASN:ND2	2.63	0.56
1:B:469:PHE:CD1	1:B:472:ARG:HD2	2.39	0.56
1:C:668:SER:CB	2:F:14:GLU:HG3	2.35	0.56
2:D:8:GLN:HA	2:D:8:GLN:NE2	2.20	0.56
2:F:123:GLU:O	2:F:127:GLU:HG2	2.05	0.56
1:A:672:ARG:NH2	2:D:7:GLU:HG2	2.21	0.56
1:A:695:LYS:HB2	2:D:18:LEU:HD22	1.86	0.56
1:C:712:PHE:CD2	1:C:716:LYS:HG2	2.40	0.56
1:A:492:TYR:CD2	1:A:574:VAL:HG13	2.41	0.56
1:B:615:ILE:HD12	1:B:645:TRP:HH2	1.71	0.56
1:C:617:LYS:O	1:C:617:LYS:HD3	2.06	0.56
1:B:648:PRO:C	1:B:650:THR:N	2.63	0.56
1:B:723:PHE:HB2	1:B:793:PHE:HE2	1.70	0.56
1:B:322:LEU:HD21	1:B:559:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLN:HB2	1:B:379:ALA:HB3	1.87	0.56
1:B:538:ILE:O	1:B:540:ARG:HD3	2.06	0.56
1:B:626:TYR:CD2	1:B:627:TYR:N	2.73	0.56
1:C:491:ASP:C	1:C:491:ASP:OD2	2.49	0.56
1:B:639:ASN:HD22	1:B:641:ALA:H	1.52	0.55
1:B:738:SER:O	1:B:739:LYS:HG2	2.06	0.55
2:F:25:GLY:HA3	2:F:65:PHE:HE1	1.70	0.55
1:A:695:LYS:CD	2:D:19:PHE:HB2	2.36	0.55
1:A:697:ILE:HG12	1:A:731:GLU:HB2	1.87	0.55
1:A:712:PHE:HD2	1:A:716:LYS:HG2	1.72	0.55
1:C:304:ALA:HB3	1:C:604:LEU:HD13	1.88	0.55
2:F:8:GLN:HA	2:F:8:GLN:NE2	2.22	0.55
1:A:310:GLU:OE2	1:A:310:GLU:N	2.31	0.55
1:A:517:VAL:HG13	2:D:114:GLU:OE2	2.06	0.55
1:B:534:ILE:HG22	1:B:535:LYS:N	2.19	0.55
2:E:8:GLN:HA	2:E:8:GLN:NE2	2.20	0.55
1:A:513:TRP:O	1:A:517:VAL:HG23	2.07	0.55
2:F:75:LYS:O	2:F:79:THR:HG22	2.06	0.55
1:A:430:LYS:HD2	1:A:449:GLU:OE1	2.05	0.55
1:A:534:ILE:HA	1:A:538:ILE:HB	1.88	0.55
1:B:723:PHE:HB2	1:B:793:PHE:CE2	2.41	0.55
1:B:382:LYS:NZ	4:B:2139:APC:N6	2.55	0.55
1:B:516:VAL:O	1:B:520:PRO:HD2	2.07	0.55
1:C:779:GLN:OE1	1:C:796:ILE:HD12	2.07	0.55
1:B:450:ASN:OD1	1:B:452:GLU:HG3	2.07	0.55
1:C:540:ARG:HH22	2:F:87:GLU:CD	2.15	0.55
1:A:607:ASN:ND2	1:A:609:GLU:HB2	2.21	0.55
2:D:26:THR:HA	2:D:63:ILE:O	2.07	0.55
2:F:92:PHE:CE2	2:F:108:VAL:HG11	2.42	0.55
1:B:323:ASN:HD22	1:B:598:PRO:HB2	1.72	0.55
1:A:550:SER:H	1:A:553:GLN:NE2	2.05	0.54
2:D:75:LYS:O	2:D:79:THR:HG22	2.07	0.54
2:E:136:VAL:HG13	2:E:140:GLU:HB2	1.89	0.54
2:F:129:ASP:OD1	2:F:132:GLY:N	2.40	0.54
1:B:335:ALA:HB1	1:B:489:THR:HG21	1.88	0.54
1:B:549:LEU:HD13	1:B:578:GLY:HA2	1.89	0.54
1:B:712:PHE:CD1	1:B:712:PHE:N	2.73	0.54
1:C:633:ASN:HD22	1:C:644:GLU:HA	1.72	0.54
1:A:659:THR:HG23	1:A:662:GLU:H	1.71	0.54
1:A:747:ASN:O	1:A:750:GLN:HG2	2.07	0.54
1:C:695:LYS:HB2	2:F:18:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LYS:NZ	1:B:539:GLU:HB2	2.21	0.54
1:B:639:ASN:HD22	1:B:640:LYS:N	2.05	0.54
1:B:733:GLU:C	1:B:735:VAL:H	2.16	0.54
1:C:494:LEU:HD23	1:C:497:LEU:HG	1.89	0.54
1:B:650:THR:HA	1:B:653:LYS:HB2	1.89	0.54
1:B:329:ARG:HD2	1:B:590:ASP:OD2	2.07	0.54
1:B:784:GLU:HG2	1:B:788:ASP:OD2	2.07	0.54
2:E:44:THR:HG22	2:E:47:GLU:OE1	2.07	0.54
1:A:742:ALA:HB3	1:A:745:TYR:CD1	2.43	0.54
1:B:788:ASP:O	1:B:791:GLU:HG2	2.08	0.54
1:C:437:SER:C	1:C:439:ASN:H	2.16	0.54
2:E:7:GLU:HA	2:E:10:ALA:HB3	1.89	0.54
2:F:26:THR:HA	2:F:63:ILE:O	2.08	0.54
1:B:415:GLU:C	1:B:417:GLY:H	2.15	0.53
1:A:779:GLN:OE1	1:A:796:ILE:HD12	2.08	0.53
1:A:331:VAL:O	1:A:332:ASN:C	2.52	0.53
1:B:400:LYS:HA	1:B:476:VAL:O	2.09	0.53
2:D:75:LYS:C	2:D:77:LYS:H	2.16	0.53
2:D:129:ASP:OD1	2:D:132:GLY:N	2.41	0.53
2:F:12:PHE:HD1	2:F:39:LEU:HD21	1.73	0.53
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.90	0.53
1:B:758:ASN:HA	1:B:761:GLN:CB	2.38	0.53
1:C:668:SER:O	1:C:671:ARG:HB3	2.09	0.53
2:D:12:PHE:HD1	2:D:39:LEU:HD21	1.74	0.53
1:B:323:ASN:HD22	1:B:598:PRO:CB	2.20	0.53
1:B:450:ASN:CG	1:B:452:GLU:HG3	2.34	0.53
1:B:428:ASN:O	1:B:430:LYS:N	2.41	0.53
1:C:310:GLU:OE2	1:C:310:GLU:N	2.31	0.53
1:A:535:LYS:NZ	1:A:536:TYR:CZ	2.75	0.53
1:B:729:TYR:HE2	1:B:773:PHE:CE1	2.27	0.53
1:C:695:LYS:HG3	2:F:18:LEU:HD13	1.90	0.53
1:C:775:LEU:HD23	1:C:775:LEU:N	2.24	0.53
2:D:70:THR:O	2:D:73:ALA:CB	2.54	0.53
2:D:110:THR:HG22	2:D:115:LYS:HD2	1.91	0.52
2:F:5:THR:OG1	2:F:8:GLN:HG2	2.10	0.52
1:A:368:GLN:HG3	1:A:383:GLY:C	2.34	0.52
1:A:543:ASP:OD1	1:A:554:LYS:NZ	2.43	0.52
1:B:760:VAL:HB	1:B:773:PHE:CZ	2.45	0.52
1:C:631:SER:O	1:C:634:LYS:HB2	2.10	0.52
2:E:26:THR:HA	2:E:63:ILE:O	2.08	0.52
1:A:373:LYS:HG2	1:A:379:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASN:C	1:B:332:ASN:ND2	2.68	0.52
1:C:657:ILE:HG12	1:C:756:ILE:HD13	1.92	0.52
2:F:97:ASN:ND2	2:F:99:TYR:HB2	2.20	0.52
1:A:491:ASP:OD2	1:A:491:ASP:C	2.48	0.52
2:E:12:PHE:HD1	2:E:39:LEU:HD21	1.74	0.52
2:E:49:GLN:HA	2:E:52:ILE:HG22	1.91	0.52
2:E:75:LYS:C	2:E:77:LYS:H	2.17	0.52
1:B:757:THR:O	1:B:761:GLN:HB2	2.09	0.52
1:B:762:LEU:O	1:B:766:HIS:HB2	2.10	0.52
1:C:463:THR:HB	1:C:467:GLU:H	1.74	0.52
1:A:513:TRP:HZ2	2:D:114:GLU:H	1.56	0.52
1:A:789:ASN:N	1:A:789:ASN:HD22	2.08	0.52
1:B:346:LYS:HZ2	4:B:2139:APC:H3A2	1.73	0.52
1:A:462:ILE:HD12	1:A:467:GLU:O	2.09	0.52
1:A:775:LEU:HD23	1:A:775:LEU:N	2.25	0.52
1:B:519:THR:C	1:B:521:ASN:H	2.17	0.52
1:B:785:ASN:OD1	1:B:787:THR:HG23	2.10	0.52
1:A:616:GLU:HA	1:A:620:THR:CG2	2.35	0.51
2:D:80:ASP:C	2:D:82:GLU:N	2.67	0.51
1:A:445:ARG:NE	1:A:471:TRP:NE1	2.58	0.51
1:B:406:ASP:OD2	1:B:408:LEU:N	2.44	0.51
1:B:463:THR:HG23	1:B:467:GLU:O	2.11	0.51
1:B:518:ASN:O	1:B:519:THR:HG22	2.10	0.51
1:C:385:LEU:CD1	1:C:389:LYS:HE3	2.40	0.51
1:C:540:ARG:HD3	1:C:582:ASP:OD1	2.09	0.51
1:C:659:THR:HB	1:C:662:GLU:HG3	1.92	0.51
1:C:789:ASN:N	1:C:789:ASN:HD22	2.07	0.51
2:D:72:MET:O	2:D:74:ARG:N	2.43	0.51
1:A:695:LYS:CB	2:D:18:LEU:HD22	2.41	0.51
1:B:300:LYS:HA	1:B:303:LYS:HZ2	1.73	0.51
1:C:607:ASN:ND2	1:C:609:GLU:HB2	2.25	0.51
1:C:695:LYS:HD2	2:F:19:PHE:HB2	1.92	0.51
1:A:440:GLN:OE1	1:A:440:GLN:N	2.40	0.51
1:B:298:GLY:O	1:B:300:LYS:N	2.43	0.51
1:B:502:THR:O	1:B:505:LYS:HB3	2.11	0.51
1:C:712:PHE:HB3	1:C:716:LYS:HG2	1.91	0.51
2:D:92:PHE:CE2	2:D:108:VAL:HG11	2.46	0.51
1:A:629:ASN:ND2	1:A:631:SER:HB2	2.26	0.51
1:B:313:ASP:C	1:B:315:PHE:H	2.19	0.51
1:C:581:GLN:NE2	1:C:629:ASN:H	2.08	0.51
2:D:20:ASP:C	2:D:22:ASP:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:ILE:HG13	2:F:52:ILE:O	2.10	0.51
2:F:75:LYS:C	2:F:77:LYS:H	2.17	0.51
1:B:332:ASN:HD22	1:B:333:LYS:N	2.08	0.51
1:B:366:PHE:HD1	1:B:477:MET:CE	2.12	0.51
1:B:376:GLN:HB2	1:B:379:ALA:HB2	1.92	0.51
1:B:407:HIS:H	1:B:407:HIS:CD2	2.24	0.51
1:A:295:VAL:HG21	1:A:603:ILE:HG22	1.93	0.51
1:B:334:LEU:N	1:B:334:LEU:HD22	2.26	0.51
1:B:389:LYS:HG2	1:B:393:GLU:CD	2.36	0.51
1:B:388:LYS:O	1:B:392:THR:HG23	2.11	0.51
2:D:106:ARG:O	2:D:110:THR:HG23	2.10	0.51
1:B:526:GLN:HE21	2:E:124:MET:CE	2.21	0.51
1:B:718:ARG:O	1:B:722:ILE:HG13	2.10	0.51
1:A:629:ASN:HD22	1:A:631:SER:N	2.00	0.51
1:A:792:VAL:HG12	1:A:796:ILE:HD11	1.93	0.51
1:A:445:ARG:HD2	1:A:445:ARG:N	2.26	0.50
1:A:505:LYS:HD3	2:D:112:LEU:O	2.12	0.50
1:B:526:GLN:C	1:B:528:GLY:H	2.19	0.50
1:C:665:LYS:HG2	2:F:11:GLU:HG2	1.93	0.50
2:F:80:ASP:C	2:F:82:GLU:N	2.69	0.50
1:B:625:LEU:HD12	1:B:626:TYR:N	2.26	0.50
1:C:489:THR:OG1	1:C:490:ALA:N	2.45	0.50
2:E:105:LEU:HD12	2:E:125:ILE:CD1	2.40	0.50
2:F:49:GLN:HA	2:F:52:ILE:HG22	1.92	0.50
1:A:437:SER:C	1:A:439:ASN:H	2.19	0.50
1:A:440:GLN:O	1:A:458:LYS:HD2	2.11	0.50
1:A:633:ASN:HD22	1:A:644:GLU:HA	1.73	0.50
1:B:587:PRO:HB2	1:B:643:ILE:HD12	1.92	0.50
1:C:693:SER:O	1:C:697:ILE:HG13	2.11	0.50
1:A:629:ASN:HB3	1:A:632:TYR:CE2	2.47	0.50
1:B:360:VAL:HG21	1:B:365:PRO:HG3	1.94	0.50
1:B:492:TYR:CD2	1:B:574:VAL:HG13	2.45	0.50
1:B:524:GLU:O	1:B:524:GLU:HG3	2.11	0.50
1:B:728:ALA:O	1:B:731:GLU:HG2	2.11	0.50
1:C:440:GLN:O	1:C:458:LYS:HD2	2.12	0.50
1:C:695:LYS:CD	2:F:19:PHE:HB2	2.41	0.50
2:E:92:PHE:O	2:E:94:LYS:N	2.45	0.50
1:A:377:GLN:HB2	1:A:464:VAL:HG12	1.93	0.50
1:A:470:ASN:CG	1:A:471:TRP:H	2.19	0.50
1:A:479:LYS:HD2	1:A:481:VAL:CG2	2.42	0.50
1:B:391:ILE:HD11	1:B:400:LYS:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:PHE:C	1:B:614:PHE:CD2	2.89	0.50
1:B:713:SER:O	1:B:717:LYS:HG3	2.12	0.50
1:C:537:GLY:O	1:C:625:LEU:HD21	2.10	0.50
1:B:628:PHE:CD1	1:B:628:PHE:C	2.90	0.50
1:B:730:ASN:O	1:B:731:GLU:O	2.29	0.50
1:C:462:ILE:HD12	1:C:467:GLU:O	2.11	0.50
1:B:756:ILE:O	1:B:760:VAL:HG23	2.12	0.50
1:C:789:ASN:N	1:C:789:ASN:ND2	2.60	0.50
1:A:733:GLU:O	1:A:737:LYS:HE2	2.11	0.50
1:B:313:ASP:C	1:B:315:PHE:N	2.67	0.50
1:B:514:ASP:O	1:B:516:VAL:N	2.45	0.50
1:C:581:GLN:HE21	1:C:628:PHE:HA	1.76	0.50
2:E:80:ASP:C	2:E:82:GLU:N	2.66	0.50
2:F:105:LEU:HD12	2:F:125:ILE:CD1	2.41	0.50
1:C:602:PHE:O	1:C:603:ILE:HD13	2.12	0.50
1:B:414:LYS:HG3	1:B:420:LEU:HD22	1.94	0.49
1:A:782:PHE:CD1	1:A:782:PHE:N	2.80	0.49
1:B:470:ASN:CG	1:B:471:TRP:H	2.20	0.49
1:B:760:VAL:HG12	1:B:760:VAL:O	2.12	0.49
2:E:27:ILE:HD12	2:E:31:GLU:HG3	1.94	0.49
2:F:20:ASP:C	2:F:22:ASP:H	2.20	0.49
2:F:137:ASN:OD1	2:F:139:GLU:HB2	2.12	0.49
1:B:506:LYS:HG2	1:B:506:LYS:O	2.13	0.49
2:D:27:ILE:HD12	2:D:31:GLU:HG3	1.93	0.49
2:D:49:GLN:HA	2:D:52:ILE:HG22	1.93	0.49
2:E:52:ILE:O	2:E:52:ILE:HG13	2.12	0.49
1:A:509:PRO:HG2	1:A:512:GLU:CB	2.42	0.49
1:B:322:LEU:O	1:B:323:ASN:C	2.55	0.49
1:B:415:GLU:C	1:B:417:GLY:N	2.68	0.49
1:B:419:ILE:HD13	1:B:435:LEU:HD22	1.94	0.49
1:C:694:VAL:HG23	1:C:695:LYS:H	1.78	0.49
1:C:782:PHE:CD1	1:C:782:PHE:N	2.80	0.49
1:A:445:ARG:HG3	1:A:471:TRP:CH2	2.48	0.49
1:A:786:GLU:C	1:A:788:ASP:H	2.20	0.49
1:B:389:LYS:NZ	1:B:389:LYS:CB	2.76	0.49
1:C:668:SER:OG	2:F:10:ALA:HB1	2.12	0.49
1:C:670:ILE:HG23	1:C:745:TYR:CE1	2.47	0.49
2:D:29:THR:OG1	2:D:52:ILE:HG12	2.13	0.49
1:A:318:ILE:HD12	1:A:318:ILE:N	2.27	0.49
1:B:654:ILE:HA	1:B:755:ARG:HD3	1.92	0.49
1:B:762:LEU:HA	1:B:765:THR:HG1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:TYR:HD1	1:B:780:LEU:HD12	1.77	0.49
1:C:499:PRO:HD3	1:C:552:TRP:CH2	2.47	0.49
2:F:101:SER:OG	2:F:104:GLU:HG3	2.11	0.49
1:B:366:PHE:HA	1:B:477:MET:CE	2.39	0.49
1:B:534:ILE:HG22	1:B:535:LYS:HE2	1.95	0.49
1:B:619:ILE:C	1:B:621:GLY:H	2.21	0.49
1:B:746:LYS:O	1:B:750:GLN:HB2	2.12	0.49
1:B:752:LEU:O	1:B:756:ILE:HG13	2.12	0.49
1:C:377:GLN:HB2	1:C:464:VAL:HG12	1.95	0.49
1:C:505:LYS:HE3	1:C:513:TRP:CD1	2.48	0.49
2:E:20:ASP:C	2:E:22:ASP:H	2.20	0.49
2:E:37:ARG:HA	2:E:41:GLN:O	2.12	0.49
2:E:51:MET:C	2:E:53:ASN:H	2.20	0.49
1:B:309:PRO:HG2	1:B:310:GLU:OE2	2.13	0.49
1:B:649:ILE:O	1:B:649:ILE:CG2	2.60	0.49
2:F:36:MET:O	2:F:41:GLN:HB2	2.13	0.49
1:C:520:PRO:HG2	1:C:521:ASN:H	1.78	0.49
1:C:535:LYS:O	1:C:535:LYS:HD3	2.12	0.49
1:C:623:ASP:CG	2:F:94:LYS:HE2	2.37	0.49
1:A:368:GLN:HG3	1:A:383:GLY:HA3	1.95	0.49
1:B:648:PRO:O	1:B:650:THR:N	2.46	0.49
1:A:660:SER:O	1:A:663:PHE:HB3	2.13	0.48
1:B:797:ILE:HG13	1:B:798:ASP:H	1.75	0.48
1:C:628:PHE:CD1	1:C:628:PHE:C	2.91	0.48
1:C:656:THR:HG21	2:F:139:GLU:OE1	2.13	0.48
2:D:123:GLU:O	2:D:127:GLU:HG2	2.12	0.48
2:E:101:SER:OG	2:E:104:GLU:HG3	2.13	0.48
1:A:509:PRO:HG2	1:A:512:GLU:HB2	1.94	0.48
1:A:639:ASN:HD22	1:A:641:ALA:H	1.58	0.48
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.95	0.48
1:B:298:GLY:O	1:B:299:GLU:C	2.55	0.48
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.42	0.48
1:B:508:ILE:HG23	1:B:536:TYR:CE1	2.48	0.48
1:B:514:ASP:HA	1:B:517:VAL:CG1	2.34	0.48
1:B:527:LYS:HG2	1:B:527:LYS:O	2.13	0.48
1:C:345:THR:HB	1:C:491:ASP:CB	2.43	0.48
1:C:669:SER:C	1:C:671:ARG:H	2.21	0.48
1:A:663:PHE:O	1:A:667:LEU:HG	2.13	0.48
1:A:740:GLN:O	1:A:741:ILE:C	2.55	0.48
2:D:7:GLU:O	2:D:11:GLU:HG3	2.12	0.48
1:B:732:ILE:O	1:B:732:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:ILE:HD11	1:C:744:GLU:O	2.13	0.48
1:A:385:LEU:CD1	1:A:389:LYS:HE3	2.44	0.48
1:A:540:ARG:HD3	1:A:582:ASP:OD1	2.12	0.48
1:B:509:PRO:HD2	1:B:536:TYR:HE1	1.78	0.48
1:C:329:ARG:HG2	1:C:495:PHE:HB2	1.96	0.48
1:C:368:GLN:HG3	1:C:383:GLY:C	2.38	0.48
1:C:792:VAL:HG12	1:C:796:ILE:HD11	1.95	0.48
2:F:29:THR:OG1	2:F:52:ILE:HG12	2.14	0.48
1:A:329:ARG:HG2	1:A:495:PHE:HB2	1.95	0.48
1:B:332:ASN:O	1:B:335:ALA:HB3	2.14	0.48
1:B:764:LEU:C	1:B:768:LYS:HB2	2.38	0.48
2:F:64:ASP:OD1	2:F:67:GLU:HG3	2.14	0.48
1:B:570:THR:O	1:B:572:GLY:N	2.47	0.48
1:C:318:ILE:HD12	1:C:318:ILE:N	2.29	0.48
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.95	0.48
1:B:514:ASP:C	1:B:516:VAL:H	2.21	0.48
1:B:628:PHE:CD2	1:B:645:TRP:CD1	3.02	0.48
2:E:85:ILE:O	2:E:88:ALA:HB3	2.13	0.48
1:A:294:ASP:O	1:A:610:MET:HE1	2.13	0.48
1:C:479:LYS:HD2	1:C:481:VAL:CG2	2.43	0.48
2:D:52:ILE:O	2:D:52:ILE:HG13	2.13	0.47
1:A:494:LEU:HD23	1:A:497:LEU:HG	1.96	0.47
1:B:789:ASN:OD1	1:B:792:VAL:HB	2.14	0.47
1:C:401:ILE:HD13	1:C:478:ALA:HB2	1.94	0.47
1:C:607:ASN:HD21	1:C:609:GLU:HB2	1.78	0.47
1:C:700:TYR:N	1:C:700:TYR:CD2	2.82	0.47
2:D:25:GLY:HA3	2:D:65:PHE:CE1	2.47	0.47
2:D:92:PHE:CD2	2:D:108:VAL:HG21	2.49	0.47
2:E:29:THR:OG1	2:E:52:ILE:HG12	2.14	0.47
1:B:505:LYS:O	1:B:507:GLN:N	2.47	0.47
1:C:313:ASP:HA	1:C:316:LYS:HE2	1.96	0.47
2:D:63:ILE:HA	2:D:67:GLU:OE2	2.14	0.47
2:F:89:PHE:CE1	2:F:100:ILE:HG13	2.49	0.47
1:B:369:ASP:OD1	1:B:464:VAL:HG11	2.14	0.47
1:C:733:GLU:O	1:C:737:LYS:HE2	2.14	0.47
1:C:712:PHE:HD2	1:C:716:LYS:HG2	1.78	0.47
2:F:37:ARG:HA	2:F:41:GLN:O	2.15	0.47
1:A:628:PHE:CD1	1:A:628:PHE:C	2.92	0.47
1:A:712:PHE:HB3	1:A:716:LYS:HG2	1.95	0.47
1:A:714:GLN:NE2	2:D:126:ARG:CG	2.77	0.47
1:B:318:ILE:HD11	1:B:563:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ALA:CB	1:B:619:ILE:HD13	2.44	0.47
1:B:525:LYS:O	1:B:526:GLN:C	2.58	0.47
1:B:535:LYS:HD3	1:B:539:GLU:OE1	2.14	0.47
1:B:723:PHE:HE2	1:B:786:GLU:HB3	1.79	0.47
1:B:751:TYR:HA	1:B:754:GLU:OE2	2.14	0.47
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.50	0.47
2:D:44:THR:CG2	2:D:47:GLU:HG3	2.45	0.47
2:E:106:ARG:O	2:E:110:THR:HG23	2.13	0.47
2:E:137:ASN:OD1	2:E:139:GLU:HB2	2.14	0.47
1:B:744:GLU:CD	1:C:397:GLU:HB2	2.40	0.47
1:C:403:LEU:HD13	1:C:476:VAL:HG11	1.97	0.47
1:C:559:ARG:HH11	1:C:559:ARG:CB	2.19	0.47
1:C:629:ASN:ND2	1:C:631:SER:HB2	2.30	0.47
2:D:51:MET:C	2:D:53:ASN:H	2.22	0.47
1:A:534:ILE:HG23	2:D:84:GLU:HB3	1.96	0.47
1:A:639:ASN:ND2	1:A:639:ASN:C	2.73	0.47
1:B:360:VAL:O	1:B:360:VAL:HG22	2.14	0.47
1:B:657:ILE:HG21	2:E:139:GLU:HG3	1.96	0.47
1:C:318:ILE:HD12	1:C:318:ILE:H	1.80	0.47
2:D:44:THR:HG22	2:D:47:GLU:HG3	1.97	0.47
2:E:44:THR:CG2	2:E:47:GLU:HG3	2.45	0.47
1:A:705:TYR:CE2	2:D:139:GLU:HB3	2.50	0.47
1:B:540:ARG:NH2	1:B:630:ARG:CZ	2.77	0.47
1:B:786:GLU:O	1:B:790:PHE:HB2	2.15	0.47
2:D:37:ARG:HA	2:D:41:GLN:O	2.15	0.47
2:E:44:THR:HG22	2:E:47:GLU:HG3	1.96	0.47
2:F:51:MET:C	2:F:53:ASN:H	2.22	0.47
1:B:622:LYS:O	1:B:623:ASP:CB	2.63	0.46
1:A:712:PHE:CD2	1:A:716:LYS:NZ	2.78	0.46
1:C:667:LEU:HB2	2:F:14:GLU:OE2	2.15	0.46
1:C:723:PHE:O	1:C:727:GLN:HG3	2.15	0.46
2:F:44:THR:CG2	2:F:47:GLU:HG3	2.46	0.46
1:A:607:ASN:HD21	1:A:609:GLU:HB2	1.78	0.46
1:A:667:LEU:HA	1:A:670:ILE:HG22	1.97	0.46
1:B:653:LYS:O	1:B:653:LYS:HG3	2.16	0.46
1:B:743:PRO:O	1:B:747:ASN:HB3	2.15	0.46
2:E:44:THR:HG23	2:E:47:GLU:H	1.81	0.46
2:E:80:ASP:O	2:E:82:GLU:N	2.48	0.46
1:A:629:ASN:HB3	1:A:632:TYR:CD2	2.50	0.46
1:B:325:TYR:HB2	1:B:498:ALA:HB3	1.95	0.46
1:B:723:PHE:CE2	1:B:786:GLU:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:LYS:HD2	1:C:536:TYR:CZ	2.49	0.46
1:C:668:SER:CA	2:F:14:GLU:HG3	2.45	0.46
1:B:321:GLU:HB3	1:B:322:LEU:HD23	1.96	0.46
1:B:781:ASN:OD1	1:B:783:THR:HG23	2.15	0.46
1:C:440:GLN:OE1	1:C:440:GLN:N	2.46	0.46
1:C:623:ASP:OD2	2:F:107:HIS:HD2	1.99	0.46
2:D:44:THR:HG23	2:D:47:GLU:H	1.81	0.46
1:A:296:LEU:HD12	1:A:604:LEU:HD22	1.97	0.46
1:A:789:ASN:N	1:A:789:ASN:ND2	2.61	0.46
1:B:524:GLU:HA	1:B:524:GLU:OE2	2.15	0.46
1:C:313:ASP:O	1:C:316:LYS:HB2	2.16	0.46
1:C:621:GLY:HA2	2:F:94:LYS:O	2.16	0.46
1:C:659:THR:CG2	1:C:660:SER:N	2.79	0.46
1:C:698:ALA:O	1:C:701:LEU:HB2	2.15	0.46
2:E:56:ASP:C	2:E:58:ASP:H	2.24	0.46
1:A:295:VAL:HG22	1:A:604:LEU:O	2.16	0.46
1:B:459:GLU:C	1:B:461:LYS:N	2.73	0.46
1:C:691:LYS:HE2	1:C:741:ILE:HG13	1.98	0.46
1:C:700:TYR:N	1:C:700:TYR:HD2	2.14	0.46
2:E:36:MET:O	2:E:41:GLN:HB2	2.15	0.46
2:F:44:THR:HG22	2:F:47:GLU:HG3	1.98	0.46
1:A:657:ILE:HD11	1:A:704:TYR:CG	2.51	0.46
1:B:426:ILE:HA	1:B:430:LYS:O	2.16	0.46
1:B:513:TRP:HD1	1:B:532:LEU:HD13	1.80	0.46
1:B:585:GLU:O	1:B:638:GLY:HA3	2.16	0.46
1:B:605:THR:CG2	1:B:611:THR:OG1	2.53	0.46
1:B:731:GLU:HG2	1:B:731:GLU:H	1.24	0.46
1:C:310:GLU:OE1	1:C:340:LYS:HE3	2.16	0.46
1:B:311:HIS:HD2	1:B:564:VAL:HB	1.81	0.46
1:B:517:VAL:HG22	1:B:517:VAL:O	2.16	0.46
1:B:424:LYS:HE2	1:B:433:TYR:OH	2.15	0.46
1:A:719:LYS:CE	1:A:767:GLN:HE22	2.18	0.45
1:B:720:ILE:HD12	1:B:724:ARG:HH21	1.81	0.45
1:C:316:LYS:HG2	1:C:600:GLY:O	2.15	0.45
1:A:323:ASN:HD22	1:A:598:PRO:CB	2.29	0.45
1:A:463:THR:CG2	1:A:464:VAL:N	2.79	0.45
1:B:320:ARG:CG	1:B:321:GLU:N	2.75	0.45
1:B:322:LEU:HD21	1:B:559:ARG:NH1	2.30	0.45
1:B:456:LYS:HE2	1:B:471:TRP:CZ2	2.50	0.45
1:C:320:ARG:HA	1:C:598:PRO:O	2.16	0.45
1:C:513:TRP:CH2	2:F:114:GLU:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:LEU:HA	1:C:670:ILE:CG2	2.46	0.45
2:D:44:THR:HG22	2:D:47:GLU:CG	2.46	0.45
1:A:454:GLN:OE1	1:A:471:TRP:CE3	2.70	0.45
1:A:463:THR:HB	1:A:467:GLU:H	1.81	0.45
1:A:673:SER:O	1:A:674:SER:HB2	2.16	0.45
1:B:517:VAL:CG2	2:E:114:GLU:HB2	2.45	0.45
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.98	0.45
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.97	0.45
1:B:646:THR:HG21	1:B:651:LYS:NZ	2.32	0.45
1:B:776:LEU:HD13	1:B:779:GLN:NE2	2.31	0.45
1:C:295:VAL:CG2	1:C:603:ILE:HG22	2.45	0.45
1:C:636:ALA:O	1:C:640:LYS:HA	2.17	0.45
2:E:44:THR:HG22	2:E:47:GLU:CG	2.47	0.45
1:B:333:LYS:O	1:B:336:THR:HG22	2.17	0.45
1:C:323:ASN:HD22	1:C:598:PRO:HB3	1.82	0.45
1:C:639:ASN:HD22	1:C:640:LYS:N	2.14	0.45
1:C:661:ALA:C	1:C:663:PHE:N	2.74	0.45
2:F:25:GLY:HA3	2:F:65:PHE:CE1	2.50	0.45
2:F:27:ILE:HD12	2:F:31:GLU:HG3	1.99	0.45
2:F:45:GLU:O	2:F:49:GLN:HG2	2.16	0.45
1:A:445:ARG:HH11	1:A:445:ARG:N	2.14	0.45
1:A:657:ILE:CG2	1:A:756:ILE:HD13	2.46	0.45
1:A:740:GLN:CD	1:A:740:GLN:H	2.23	0.45
1:B:318:ILE:H	1:B:318:ILE:CD1	2.26	0.45
1:C:639:ASN:ND2	1:C:639:ASN:C	2.74	0.45
1:C:748:TYR:O	1:C:752:LEU:HG	2.17	0.45
2:D:44:THR:HG22	2:D:47:GLU:CD	2.42	0.45
1:A:492:TYR:CE2	1:A:574:VAL:HG11	2.52	0.45
1:A:700:TYR:O	1:A:703:ASP:N	2.50	0.45
1:B:734:ASN:C	1:B:736:LEU:N	2.73	0.45
1:C:327:LEU:HD12	1:C:327:LEU:H	1.82	0.45
1:A:463:THR:CG2	1:A:465:LEU:H	2.22	0.45
1:B:649:ILE:CD1	2:E:86:ARG:HG3	2.47	0.45
1:C:712:PHE:CD2	1:C:716:LYS:NZ	2.82	0.45
1:A:602:PHE:O	1:A:603:ILE:HD13	2.17	0.45
1:B:784:GLU:HB2	1:B:788:ASP:CB	2.47	0.45
2:E:64:ASP:OD1	2:E:67:GLU:HG3	2.16	0.45
2:F:44:THR:HG22	2:F:47:GLU:CG	2.47	0.45
2:F:44:THR:HG23	2:F:47:GLU:H	1.81	0.45
1:A:737:LYS:HD3	1:A:737:LYS:HA	1.90	0.45
1:C:776:LEU:N	1:C:776:LEU:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:120:GLU:O	2:E:123:GLU:HB2	2.17	0.45
1:A:697:ILE:HD13	1:A:732:ILE:CG1	2.46	0.44
1:B:308:VAL:HG22	1:B:336:THR:OG1	2.17	0.44
1:B:619:ILE:C	1:B:621:GLY:N	2.75	0.44
1:C:664:ILE:CG2	2:F:15:ALA:HB2	2.35	0.44
2:D:137:ASN:OD1	2:D:139:GLU:HB2	2.16	0.44
2:F:63:ILE:HA	2:F:67:GLU:OE2	2.17	0.44
1:A:385:LEU:HD11	1:A:389:LYS:HE3	2.00	0.44
1:B:514:ASP:C	1:B:516:VAL:N	2.75	0.44
1:C:385:LEU:HD11	1:C:389:LYS:HE3	1.98	0.44
2:F:70:THR:O	2:F:73:ALA:CB	2.62	0.44
1:A:549:LEU:HB2	1:A:553:GLN:HE21	1.81	0.44
1:A:657:ILE:HB	1:A:756:ILE:HD13	1.99	0.44
1:B:508:ILE:HG22	1:B:509:PRO:HD2	1.98	0.44
2:F:44:THR:HG22	2:F:47:GLU:CD	2.43	0.44
1:A:509:PRO:HG3	1:A:512:GLU:OE1	2.16	0.44
1:A:511:LYS:O	1:A:511:LYS:HG2	2.16	0.44
1:A:667:LEU:HA	1:A:670:ILE:CG2	2.47	0.44
1:B:513:TRP:CZ2	2:E:112:LEU:O	2.70	0.44
1:B:775:LEU:H	1:B:775:LEU:CD2	2.25	0.44
1:B:456:LYS:HB3	1:B:470:ASN:C	2.43	0.44
1:B:791:GLU:CG	1:B:792:VAL:N	2.80	0.44
1:C:670:ILE:HG12	1:C:745:TYR:CE1	2.53	0.44
1:B:547:GLY:H	1:B:577:HIS:HB2	1.82	0.44
1:B:732:ILE:O	1:B:735:VAL:CG1	2.64	0.44
1:C:450:ASN:O	1:C:451:ASN:HB2	2.18	0.44
2:D:79:THR:C	2:D:81:SER:H	2.24	0.44
2:E:115:LYS:O	2:E:116:LEU:HD23	2.18	0.44
1:A:360:VAL:O	1:A:360:VAL:HG13	2.18	0.44
1:B:526:GLN:C	1:B:528:GLY:N	2.76	0.44
1:B:655:ASN:O	1:B:656:THR:HG23	2.17	0.44
1:B:738:SER:HB3	1:B:741:ILE:HD11	1.99	0.44
1:B:793:PHE:HA	1:B:796:ILE:CG1	2.47	0.44
1:C:318:ILE:HG23	1:C:322:LEU:HD12	2.00	0.44
2:D:72:MET:C	2:D:74:ARG:N	2.72	0.44
1:A:382:LYS:NZ	4:A:1139:APC:N6	2.66	0.44
1:A:630:ARG:CZ	2:D:83:GLU:HB3	2.48	0.44
1:B:525:LYS:O	1:B:529:VAL:HG22	2.18	0.44
1:C:463:THR:CG2	1:C:464:VAL:N	2.80	0.44
2:F:120:GLU:O	2:F:123:GLU:HB2	2.18	0.44
1:A:318:ILE:HD12	1:A:318:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ILE:C	1:A:666:ASN:H	2.26	0.43
1:A:714:GLN:NE2	2:D:126:ARG:HG3	2.33	0.43
1:A:559:ARG:HH11	1:A:559:ARG:CB	2.27	0.43
1:B:526:GLN:O	1:B:528:GLY:N	2.51	0.43
1:B:549:LEU:CD1	1:B:553:GLN:HB3	2.48	0.43
1:B:751:TYR:O	1:B:754:GLU:HB2	2.18	0.43
1:C:320:ARG:HG3	1:C:598:PRO:O	2.18	0.43
1:C:534:ILE:HA	1:C:538:ILE:HB	1.99	0.43
1:C:667:LEU:O	1:C:671:ARG:HB2	2.18	0.43
2:D:80:ASP:O	2:D:82:GLU:N	2.51	0.43
2:F:129:ASP:OD1	2:F:129:ASP:C	2.61	0.43
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.53	0.43
1:A:787:THR:O	1:A:791:GLU:HG2	2.18	0.43
1:B:552:TRP:CD1	1:B:552:TRP:C	2.94	0.43
1:B:639:ASN:O	1:B:640:LYS:HB2	2.17	0.43
1:B:726:ILE:CA	1:B:729:TYR:HB2	2.29	0.43
1:B:784:GLU:HB2	1:B:788:ASP:HB3	1.98	0.43
1:C:629:ASN:HD22	1:C:629:ASN:C	2.26	0.43
1:A:694:VAL:HG12	1:A:697:ILE:HG13	2.01	0.43
1:C:740:GLN:H	1:C:740:GLN:CD	2.26	0.43
2:F:56:ASP:C	2:F:58:ASP:H	2.25	0.43
1:B:526:GLN:NE2	2:E:124:MET:CE	2.77	0.43
1:B:538:ILE:HD13	1:B:625:LEU:HD11	1.99	0.43
1:B:589:LYS:HZ3	1:B:608:TRP:CG	2.36	0.43
1:B:729:TYR:O	1:B:733:GLU:CD	2.62	0.43
1:C:401:ILE:HG21	1:C:485:LEU:HB3	2.01	0.43
2:D:51:MET:O	2:D:55:VAL:HG12	2.18	0.43
1:A:718:ARG:O	1:A:722:ILE:HG13	2.18	0.43
1:B:302:LEU:C	1:B:304:ALA:N	2.74	0.43
1:B:310:GLU:CD	1:B:310:GLU:H	2.25	0.43
1:B:457:THR:HG21	1:B:468:LYS:HA	2.01	0.43
1:B:605:THR:HG21	1:B:611:THR:HG1	1.76	0.43
1:B:310:GLU:OE1	1:B:340:LYS:HE3	2.19	0.43
1:B:792:VAL:C	1:B:796:ILE:HG12	2.42	0.43
1:C:513:TRP:CZ2	2:F:114:GLU:N	2.85	0.43
2:E:47:GLU:C	2:E:49:GLN:H	2.25	0.43
1:A:583:ASN:ND2	4:A:1139:APC:H3'	2.33	0.43
1:B:709:ASN:OD1	1:B:717:LYS:HG2	2.19	0.43
1:B:744:GLU:OE1	1:C:397:GLU:HB2	2.18	0.43
1:B:779:GLN:HB3	1:B:796:ILE:HG23	2.00	0.43
1:C:294:ASP:O	1:C:610:MET:HE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:LEU:HD23	1:C:497:LEU:CG	2.48	0.43
2:E:50:ASP:OD1	2:E:51:MET:HG3	2.19	0.43
2:E:100:ILE:HD12	2:E:141:PHE:CD1	2.54	0.43
2:F:106:ARG:O	2:F:110:THR:HG23	2.19	0.43
1:A:319:ALA:O	1:A:322:LEU:O	2.37	0.43
1:A:368:GLN:HG3	1:A:383:GLY:CA	2.49	0.43
1:A:605:THR:HG21	1:A:611:THR:HA	2.00	0.43
1:B:549:LEU:HD12	1:B:553:GLN:HB3	2.01	0.43
2:D:72:MET:O	2:D:73:ALA:C	2.61	0.43
1:A:295:VAL:HG23	1:A:605:THR:HA	1.99	0.42
1:B:406:ASP:OD2	1:B:406:ASP:C	2.62	0.42
1:B:530:THR:HG22	2:E:92:PHE:CZ	2.54	0.42
1:C:338:LEU:O	1:C:343:VAL:HG23	2.18	0.42
1:A:294:ASP:O	1:A:610:MET:CE	2.67	0.42
1:A:324:THR:HG21	1:A:556:MET:CE	2.49	0.42
1:A:450:ASN:O	1:A:451:ASN:HB2	2.19	0.42
1:A:489:THR:OG1	1:A:490:ALA:N	2.53	0.42
1:A:697:ILE:C	1:A:699:GLY:H	2.26	0.42
1:A:739:LYS:HB3	1:A:741:ILE:HD13	2.01	0.42
1:B:789:ASN:ND2	1:B:793:PHE:HB2	2.34	0.42
1:C:530:THR:HG21	2:F:145:MET:SD	2.60	0.42
1:C:720:ILE:O	1:C:724:ARG:HG3	2.19	0.42
2:E:63:ILE:HA	2:E:67:GLU:OE2	2.19	0.42
1:A:549:LEU:CD1	1:A:554:LYS:HE2	2.49	0.42
1:A:720:ILE:O	1:A:724:ARG:HG3	2.19	0.42
1:B:733:GLU:O	1:B:735:VAL:N	2.52	0.42
1:C:794:GLN:O	1:C:797:ILE:HG13	2.20	0.42
2:D:105:LEU:HD12	2:D:125:ILE:CD1	2.49	0.42
1:B:653:LYS:O	1:B:755:ARG:HD3	2.19	0.42
1:C:360:VAL:O	1:C:360:VAL:HG13	2.18	0.42
1:C:695:LYS:CG	2:F:18:LEU:HD22	2.49	0.42
1:A:639:ASN:HD22	1:A:640:LYS:N	2.16	0.42
1:B:546:LYS:HA	1:B:577:HIS:CB	2.49	0.42
2:E:25:GLY:HA3	2:E:65:PHE:CE1	2.51	0.42
1:B:313:ASP:O	1:B:315:PHE:N	2.51	0.42
1:B:349:ASN:ND2	1:B:398:ILE:HD13	2.34	0.42
1:B:650:THR:O	1:B:651:LYS:C	2.62	0.42
1:B:654:ILE:HG22	1:B:755:ARG:HG2	2.01	0.42
1:C:499:PRO:HG2	1:C:625:LEU:HB3	2.00	0.42
2:E:20:ASP:OD1	2:E:25:GLY:HA2	2.19	0.42
2:E:51:MET:O	2:E:55:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:80:ASP:O	2:F:82:GLU:N	2.52	0.42
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.82	0.42
1:A:526:GLN:CD	2:D:144:MET:HE2	2.43	0.42
1:A:775:LEU:H	1:A:775:LEU:CD2	2.19	0.42
1:C:526:GLN:CD	2:F:144:MET:HE2	2.44	0.42
1:C:549:LEU:CD1	1:C:554:LYS:HE2	2.48	0.42
1:C:781:ASN:HB2	1:C:789:ASN:HA	2.02	0.42
2:D:20:ASP:OD2	2:D:22:ASP:HB3	2.19	0.42
2:D:47:GLU:C	2:D:49:GLN:H	2.27	0.42
2:D:72:MET:C	2:D:74:ARG:H	2.28	0.42
1:A:631:SER:O	1:A:634:LYS:HB2	2.20	0.42
1:B:789:ASN:C	1:B:791:GLU:N	2.74	0.42
1:C:424:LYS:HG2	1:C:425:GLU:N	2.35	0.42
1:C:648:PRO:O	1:C:649:ILE:C	2.61	0.42
1:B:623:ASP:OD1	2:E:94:LYS:HE2	2.20	0.42
1:B:797:ILE:CG1	1:B:798:ASP:N	2.82	0.42
1:C:492:TYR:CD2	1:C:574:VAL:HG13	2.53	0.42
2:D:13:LYS:HG3	2:D:65:PHE:HE2	1.82	0.42
2:D:89:PHE:CE1	2:D:100:ILE:HG13	2.55	0.42
2:E:27:ILE:O	2:E:62:THR:HA	2.19	0.42
2:E:89:PHE:CE1	2:E:100:ILE:HG13	2.55	0.42
1:B:508:ILE:HG23	1:B:536:TYR:CD1	2.54	0.42
1:B:793:PHE:C	1:B:795:LYS:H	2.27	0.42
2:F:29:THR:O	2:F:29:THR:HG22	2.19	0.42
1:B:731:GLU:CG	1:B:732:ILE:N	2.62	0.41
1:C:295:VAL:HG22	1:C:604:LEU:O	2.20	0.41
1:C:368:GLN:HG3	1:C:383:GLY:HA3	2.02	0.41
1:C:657:ILE:HG12	1:C:756:ILE:HA	2.02	0.41
1:C:670:ILE:CD1	1:C:745:TYR:HA	2.50	0.41
2:E:105:LEU:HD12	2:E:125:ILE:HD13	2.02	0.41
1:A:666:ASN:O	1:A:670:ILE:HB	2.20	0.41
1:C:346:LYS:HZ2	4:C:3139:APC:H3A2	1.83	0.41
1:C:502:THR:O	1:C:505:LYS:HB3	2.20	0.41
2:E:29:THR:HG22	2:E:29:THR:O	2.20	0.41
2:F:47:GLU:C	2:F:49:GLN:H	2.27	0.41
2:F:75:LYS:O	2:F:75:LYS:HD3	2.20	0.41
1:A:696:LYS:HD3	1:A:731:GLU:OE1	2.20	0.41
1:B:355:SER:HB2	1:B:371:SER:HA	2.02	0.41
1:C:324:THR:CB	1:C:499:PRO:HA	2.51	0.41
1:C:497:LEU:HD12	1:C:553:GLN:HG2	2.02	0.41
1:C:527:LYS:HE2	2:F:145:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:THR:HG22	2:D:29:THR:O	2.21	0.41
2:F:27:ILE:O	2:F:62:THR:HA	2.21	0.41
1:A:581:GLN:HE21	1:A:628:PHE:HA	1.85	0.41
1:A:658:PRO:HG3	1:A:752:LEU:HD22	2.01	0.41
1:A:781:ASN:HB2	1:A:789:ASN:HA	2.02	0.41
1:B:333:LYS:C	1:B:335:ALA:H	2.27	0.41
1:C:353:LYS:HG3	1:C:373:LYS:HD3	2.02	0.41
1:C:787:THR:O	1:C:791:GLU:HG2	2.20	0.41
2:D:27:ILE:O	2:D:62:THR:HA	2.21	0.41
2:D:45:GLU:O	2:D:49:GLN:HG2	2.21	0.41
2:D:86:ARG:HA	2:D:138:TYR:HE1	1.85	0.41
2:F:117:THR:C	2:F:119:GLU:N	2.78	0.41
1:A:636:ALA:O	1:A:640:LYS:HA	2.21	0.41
1:B:373:LYS:O	1:B:374:HIS:C	2.61	0.41
1:B:720:ILE:HD12	1:B:724:ARG:NH2	2.35	0.41
1:C:629:ASN:HB3	1:C:632:TYR:CD2	2.55	0.41
1:C:657:ILE:HG23	1:C:658:PRO:HD2	2.02	0.41
1:C:657:ILE:CG1	1:C:759:GLN:HG2	2.38	0.41
1:A:419:ILE:O	1:A:419:ILE:HG13	2.20	0.41
1:A:664:ILE:HD13	2:D:15:ALA:HB2	2.01	0.41
1:A:723:PHE:O	1:A:727:GLN:HG3	2.21	0.41
1:B:761:GLN:O	1:B:765:THR:HG23	2.20	0.41
1:C:370:LEU:HD11	1:C:455:TYR:CE1	2.56	0.41
1:A:581:GLN:HE21	1:A:629:ASN:H	1.67	0.41
1:A:700:TYR:O	1:A:703:ASP:HB2	2.20	0.41
1:B:428:ASN:O	1:B:429:GLY:C	2.64	0.41
1:B:529:VAL:HG23	1:B:530:THR:N	2.36	0.41
1:B:757:THR:HA	1:B:773:PHE:CE1	2.56	0.41
1:B:777:TYR:CD1	1:B:780:LEU:HD12	2.55	0.41
1:C:629:ASN:HD21	1:C:631:SER:HB2	1.86	0.41
1:C:712:PHE:HB3	1:C:716:LYS:CG	2.51	0.41
1:C:786:GLU:C	1:C:788:ASP:H	2.29	0.41
2:E:45:GLU:O	2:E:49:GLN:HG2	2.21	0.41
1:A:654:ILE:O	1:A:654:ILE:HG13	2.19	0.41
1:B:518:ASN:HD22	1:B:518:ASN:HA	1.63	0.41
2:D:86:ARG:HA	2:D:138:TYR:CE1	2.56	0.41
2:F:65:PHE:O	2:F:69:LEU:HG	2.21	0.41
1:A:298:GLY:O	1:A:301:ALA:N	2.52	0.41
1:A:739:LYS:O	1:A:741:ILE:N	2.54	0.41
1:B:322:LEU:HD23	1:B:322:LEU:N	2.36	0.41
1:B:377:GLN:HG3	1:B:465:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:GLN:HA	1:B:761:GLN:NE2	2.35	0.41
1:C:349:ASN:N	1:C:349:ASN:ND2	2.54	0.41
1:C:605:THR:HG21	1:C:611:THR:HA	2.02	0.41
1:C:718:ARG:O	1:C:722:ILE:HG13	2.21	0.41
2:D:20:ASP:C	2:D:22:ASP:N	2.79	0.41
2:D:64:ASP:OD1	2:D:67:GLU:HG3	2.20	0.41
2:D:75:LYS:O	2:D:75:LYS:HD3	2.21	0.41
2:E:20:ASP:O	2:E:22:ASP:N	2.47	0.41
2:F:92:PHE:O	2:F:94:LYS:N	2.53	0.41
1:A:401:ILE:HD13	1:A:478:ALA:HB2	2.02	0.41
1:A:442:TYR:O	1:A:458:LYS:HE3	2.21	0.41
1:B:456:LYS:HA	1:B:469:PHE:CE1	2.56	0.41
1:B:564:VAL:O	1:B:567:THR:HB	2.21	0.41
1:B:636:ALA:HA	1:B:637:PRO:HD3	1.86	0.41
1:B:773:PHE:C	1:B:775:LEU:N	2.78	0.41
1:C:319:ALA:O	1:C:598:PRO:HA	2.21	0.41
1:C:623:ASP:OD1	2:F:94:LYS:HE2	2.21	0.41
2:E:44:THR:HG22	2:E:47:GLU:CD	2.46	0.41
2:E:47:GLU:C	2:E:49:GLN:N	2.79	0.41
1:A:321:GLU:OE2	1:A:559:ARG:NH2	2.54	0.40
1:A:648:PRO:HA	1:A:651:LYS:HD2	2.03	0.40
1:A:660:SER:O	1:A:661:ALA:C	2.64	0.40
1:A:794:GLN:O	1:A:797:ILE:HG13	2.21	0.40
1:B:585:GLU:C	1:B:587:PRO:HD3	2.46	0.40
1:B:605:THR:HG23	1:B:610:MET:HB3	2.04	0.40
2:F:5:THR:O	2:F:9:ILE:HG13	2.20	0.40
1:A:563:ALA:O	1:A:567:THR:HG23	2.20	0.40
1:A:629:ASN:HD21	1:A:631:SER:HB2	1.86	0.40
1:A:776:LEU:HD12	1:A:776:LEU:N	2.36	0.40
1:B:327:LEU:HD12	1:B:327:LEU:N	2.36	0.40
1:B:408:LEU:HA	1:B:408:LEU:HD23	1.76	0.40
1:C:779:GLN:OE1	1:C:796:ILE:HG23	2.20	0.40
1:B:621:GLY:HA2	2:E:94:LYS:O	2.21	0.40
1:B:646:THR:HG21	1:B:651:LYS:HZ3	1.87	0.40
1:C:309:PRO:O	1:C:310:GLU:C	2.64	0.40
1:C:325:TYR:HB2	1:C:498:ALA:HB3	2.03	0.40
2:D:12:PHE:CD1	2:D:39:LEU:HD21	2.55	0.40
2:D:76:MET:HA	2:D:79:THR:CG2	2.51	0.40
2:E:72:MET:O	2:E:74:ARG:N	2.54	0.40
2:E:99:TYR:CE2	2:E:137:ASN:HB3	2.56	0.40
1:A:462:ILE:HG13	1:A:466:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:LYS:HA	1:B:542:PRO:HD3	1.93	0.40
1:B:776:LEU:HD22	1:B:779:GLN:HG3	2.02	0.40
2:E:75:LYS:O	2:E:75:LYS:HD3	2.21	0.40
2:D:50:ASP:OD1	2:D:51:MET:HG3	2.21	0.40
2:D:76:MET:HE3	2:D:79:THR:CG2	2.48	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	479/510 (94%)	433 (90%)	42 (9%)	4 (1%)	16	50
1	B	457/510 (90%)	366 (80%)	67 (15%)	24 (5%)	1	9
1	C	499/510 (98%)	447 (90%)	42 (8%)	10 (2%)	6	28
2	D	141/148 (95%)	114 (81%)	19 (14%)	8 (6%)	1	8
2	E	141/148 (95%)	109 (77%)	24 (17%)	8 (6%)	1	8
2	F	141/148 (95%)	113 (80%)	21 (15%)	7 (5%)	1	10
All	All	1858/1974 (94%)	1582 (85%)	215 (12%)	61 (3%)	3	17

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	566	TYR
1	B	571	GLY
1	C	510	GLN
1	C	520	PRO
1	C	694	VAL
2	E	93	ASP
1	A	294	ASP

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Mol	Chain	Res	Type
1	A	298	GLY
1	A	787	THR
1	B	299	GLU
1	B	429	GLY
1	B	460	GLY
1	B	506	LYS
1	B	515	LYS
1	B	702	SER
1	B	704	TYR
1	B	734	ASN
1	B	735	VAL
1	C	663	PHE
1	B	428	ASN
1	B	526	GLN
1	B	527	LYS
1	C	521	ASN
2	D	73	ALA
2	D	76	MET
2	D	80	ASP
2	D	81	SER
2	E	73	ALA
2	E	76	MET
2	E	81	SER
2	E	114	GLU
2	F	76	MET
2	F	81	SER
2	F	93	ASP
1	C	298	GLY
1	C	692	GLU
1	C	741	ILE
2	D	50	ASP
2	D	93	ASP
2	D	114	GLU
2	E	27	ILE
2	E	50	ASP
2	F	27	ILE
2	F	50	ASP
2	F	114	GLU
1	A	740	GLN
1	B	298	GLY
1	B	323	ASN
1	B	694	VAL

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Mol	Chain	Res	Type
1	B	731	GLU
1	B	738	SER
1	C	677	GLY
2	D	27	ILE
2	F	80	ASP
1	C	438	ASN
2	E	80	ASP
1	B	537	GLY
1	B	649	ILE
1	B	547	GLY
1	B	519	THR
1	B	516	VAL

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	433/455 (95%)	398 (92%)	35 (8%)	11	38
1	B	414/455 (91%)	379 (92%)	35 (8%)	10	36
1	C	448/455 (98%)	417 (93%)	31 (7%)	14	45
2	D	121/126 (96%)	113 (93%)	8 (7%)	15	46
2	E	121/126 (96%)	113 (93%)	8 (7%)	15	46
2	F	121/126 (96%)	113 (93%)	8 (7%)	15	46
All	All	1658/1743 (95%)	1533 (92%)	125 (8%)	12	41

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	VAL
1	A	322	LEU
1	A	323	ASN
1	A	349	ASN
1	A	385	LEU
1	A	401	ILE

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Mol	Chain	Res	Type
1	A	406	ASP
1	A	438	ASN
1	A	445	ARG
1	A	447	SER
1	A	455	TYR
1	A	463	THR
1	A	479	LYS
1	A	485	LEU
1	A	510	GLN
1	A	511	LYS
1	A	515	LYS
1	A	531	ASN
1	A	540	ARG
1	A	549	LEU
1	A	557	LEU
1	A	559	ARG
1	A	574	VAL
1	A	622	LYS
1	A	629	ASN
1	A	631	SER
1	A	639	ASN
1	A	646	THR
1	A	662	GLU
1	A	670	ILE
1	A	710	HIS
1	A	737	LYS
1	A	775	LEU
1	A	780	LEU
1	A	782	PHE
1	B	320	ARG
1	B	322	LEU
1	B	336	THR
1	B	376	GLN
1	B	389	LYS
1	B	398	ILE
1	B	401	ILE
1	B	415	GLU
1	B	434	LEU
1	B	447	SER
1	B	463	THR
1	B	464	VAL
1	B	480	ASN

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Mol	Chain	Res	Type
1	B	485	LEU
1	B	508	ILE
1	B	510	GLN
1	B	526	GLN
1	B	536	TYR
1	B	544	SER
1	B	545	THR
1	B	551	ASN
1	B	552	TRP
1	B	557	LEU
1	B	570	THR
1	B	574	VAL
1	B	620	THR
1	B	629	ASN
1	B	631	SER
1	B	639	ASN
1	B	646	THR
1	B	711	ILE
1	B	712	PHE
1	B	731	GLU
1	B	752	LEU
1	B	784	GLU
1	C	295	VAL
1	C	320	ARG
1	C	323	ASN
1	C	349	ASN
1	C	385	LEU
1	C	401	ILE
1	C	406	ASP
1	C	438	ASN
1	C	455	TYR
1	C	463	THR
1	C	485	LEU
1	C	533	LEU
1	C	540	ARG
1	C	549	LEU
1	C	557	LEU
1	C	559	ARG
1	C	574	VAL
1	C	622	LYS
1	C	629	ASN
1	C	639	ASN

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Mol	Chain	Res	Type
1	C	646	THR
1	C	650	THR
1	C	659	THR
1	C	666	ASN
1	C	694	VAL
1	C	710	HIS
1	C	737	LYS
1	C	775	LEU
1	C	780	LEU
1	C	782	PHE
1	C	785	ASN
2	D	14	GLU
2	D	18	LEU
2	D	75	LYS
2	D	76	MET
2	D	82	GLU
2	D	94	LYS
2	D	115	LYS
2	D	135	GLN
2	E	14	GLU
2	E	18	LEU
2	E	75	LYS
2	E	76	MET
2	E	82	GLU
2	E	94	LYS
2	E	105	LEU
2	E	135	GLN
2	F	14	GLU
2	F	18	LEU
2	F	75	LYS
2	F	76	MET
2	F	82	GLU
2	F	94	LYS
2	F	105	LEU
2	F	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	ASN
1	A	349	ASN
1	A	351	HIS

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Mol	Chain	Res	Type
1	A	376	GLN
1	A	416	ASN
1	A	438	ASN
1	A	454	GLN
1	A	518	ASN
1	A	526	GLN
1	A	531	ASN
1	A	553	GLN
1	A	581	GLN
1	A	607	ASN
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	706	ASN
1	A	714	GLN
1	A	727	GLN
1	A	750	GLN
1	A	767	GLN
1	A	781	ASN
1	A	789	ASN
1	A	794	GLN
1	B	323	ASN
1	B	332	ASN
1	B	368	GLN
1	B	376	GLN
1	B	377	GLN
1	B	407	HIS
1	B	451	ASN
1	B	507	GLN
1	B	518	ASN
1	B	521	ASN
1	B	526	GLN
1	B	551	ASN
1	B	553	GLN
1	B	583	ASN
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	730	ASN
1	B	761	GLN
1	B	766	HIS
1	B	779	GLN

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Mol	Chain	Res	Type
1	C	323	ASN
1	C	337	ASN
1	C	349	ASN
1	C	351	HIS
1	C	376	GLN
1	C	377	GLN
1	C	416	ASN
1	C	438	ASN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	526	GLN
1	C	553	GLN
1	C	581	GLN
1	C	607	ASN
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	655	ASN
1	C	666	ASN
1	C	706	ASN
1	C	727	GLN
1	C	750	GLN
1	C	759	GLN
1	C	761	GLN
1	C	781	ASN
1	C	789	ASN
1	C	794	GLN
2	D	8	GLN
2	D	41	GLN
2	E	8	GLN
2	E	41	GLN
2	F	8	GLN
2	F	41	GLN
2	F	107	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](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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
4	APC	B	2139	-	29,33,33	1.89	7 (24%)	44,52,52	1.44	4 (9%)
4	APC	A	1139	3	29,33,33	1.99	8 (27%)	44,52,52	1.44	4 (9%)
4	APC	C	3139	-	29,33,33	1.73	8 (27%)	44,52,52	1.46	4 (9%)

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
4	APC	B	2139	-	-	10/19/38/38	0/3/3/3
4	APC	A	1139	3	-	10/19/38/38	0/3/3/3
4	APC	C	3139	-	-	11/19/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1139	APC	PB-O3B	5.97	1.65	1.58
4	B	2139	APC	PB-O3B	5.25	1.64	1.58
4	B	2139	APC	C6-N6	-4.66	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1139	APC	C6-N6	-4.64	1.22	1.34
4	C	3139	APC	C6-N6	-4.47	1.22	1.34
4	C	3139	APC	PB-O3B	3.40	1.62	1.58
4	A	1139	APC	C2-N1	2.94	1.39	1.33
4	C	3139	APC	C2-N1	2.86	1.39	1.33
4	B	2139	APC	C2-N1	2.85	1.39	1.33
4	C	3139	APC	PB-O2B	-2.82	1.49	1.56
4	B	2139	APC	PB-O2B	-2.80	1.49	1.56
4	A	1139	APC	PB-O2B	-2.73	1.49	1.56
4	A	1139	APC	PG-O2G	-2.44	1.45	1.54
4	B	2139	APC	C4-N9	2.42	1.42	1.37
4	A	1139	APC	C4-N3	2.38	1.38	1.34
4	C	3139	APC	C4-N9	2.33	1.42	1.37
4	B	2139	APC	C4-N3	2.19	1.38	1.34
4	C	3139	APC	PG-O2G	-2.14	1.46	1.54
4	B	2139	APC	PG-O2G	-2.10	1.47	1.54
4	C	3139	APC	C2-N3	-2.08	1.30	1.33
4	A	1139	APC	PA-O2A	-2.06	1.51	1.56
4	A	1139	APC	C2-N3	-2.03	1.30	1.33
4	C	3139	APC	C4-N3	2.01	1.38	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3139	APC	C2-N1-C6	5.52	127.79	118.73
4	B	2139	APC	C2-N1-C6	5.47	127.71	118.73
4	A	1139	APC	C2-N1-C6	5.45	127.69	118.73
4	A	1139	APC	N3-C2-N1	-4.29	122.08	128.58
4	B	2139	APC	N3-C2-N1	-4.25	122.15	128.58
4	C	3139	APC	N3-C2-N1	-4.12	122.34	128.58
4	B	2139	APC	C3'-C2'-C1'	3.04	107.20	101.46
4	C	3139	APC	C3'-C2'-C1'	3.00	107.14	101.46
4	A	1139	APC	C3'-C2'-C1'	2.96	107.06	101.46
4	C	3139	APC	C5-C6-N1	-2.63	110.84	117.51
4	B	2139	APC	C5-C6-N1	-2.57	110.99	117.51
4	A	1139	APC	C5-C6-N1	-2.52	111.11	117.51

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1139	APC	PA-C3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	A	1139	APC	PA-C3A-PB-O2B
4	A	1139	APC	PA-C3A-PB-O3B
4	A	1139	APC	PB-C3A-PA-O1A
4	A	1139	APC	PB-C3A-PA-O2A
4	A	1139	APC	PB-C3A-PA-O5'
4	B	2139	APC	PA-C3A-PB-O1B
4	B	2139	APC	PA-C3A-PB-O2B
4	B	2139	APC	PA-C3A-PB-O3B
4	B	2139	APC	PB-C3A-PA-O1A
4	B	2139	APC	PB-C3A-PA-O2A
4	B	2139	APC	PB-C3A-PA-O5'
4	C	3139	APC	PB-O3B-PG-O3G
4	C	3139	APC	PB-C3A-PA-O1A
4	C	3139	APC	PB-C3A-PA-O2A
4	C	3139	APC	PB-C3A-PA-O5'
4	C	3139	APC	C5'-O5'-PA-O1A
4	A	1139	APC	C3'-C4'-C5'-O5'
4	B	2139	APC	C3'-C4'-C5'-O5'
4	C	3139	APC	C3'-C4'-C5'-O5'
4	C	3139	APC	O4'-C4'-C5'-O5'
4	A	1139	APC	C4'-C5'-O5'-PA
4	A	1139	APC	O4'-C4'-C5'-O5'
4	B	2139	APC	O4'-C4'-C5'-O5'
4	B	2139	APC	C4'-C5'-O5'-PA
4	A	1139	APC	C5'-O5'-PA-O1A
4	B	2139	APC	C5'-O5'-PA-O1A
4	C	3139	APC	PA-C3A-PB-O2B
4	C	3139	APC	C4'-C5'-O5'-PA
4	C	3139	APC	PB-O3B-PG-O1G
4	C	3139	APC	PB-O3B-PG-O2G

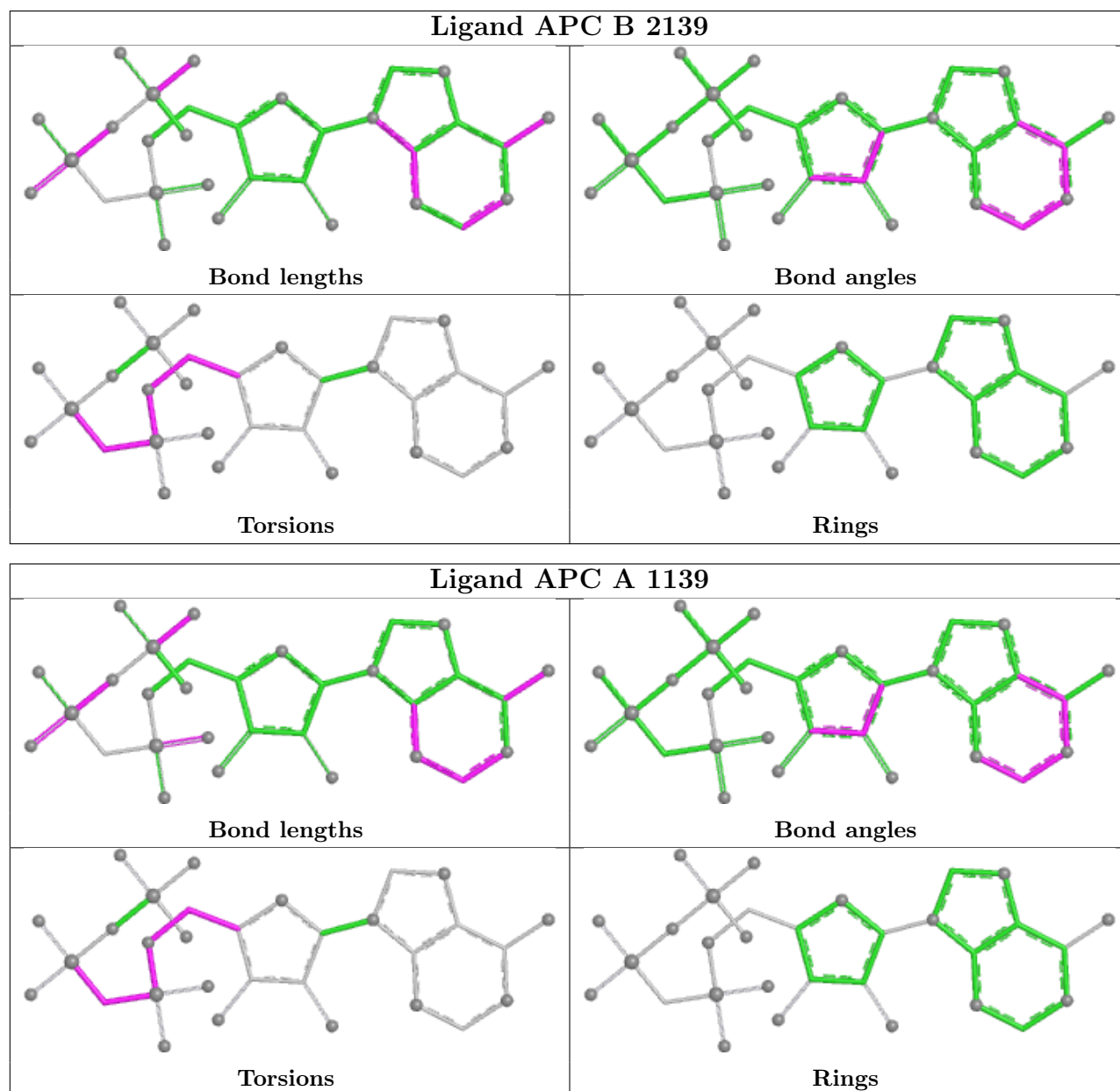
There are no ring outliers.

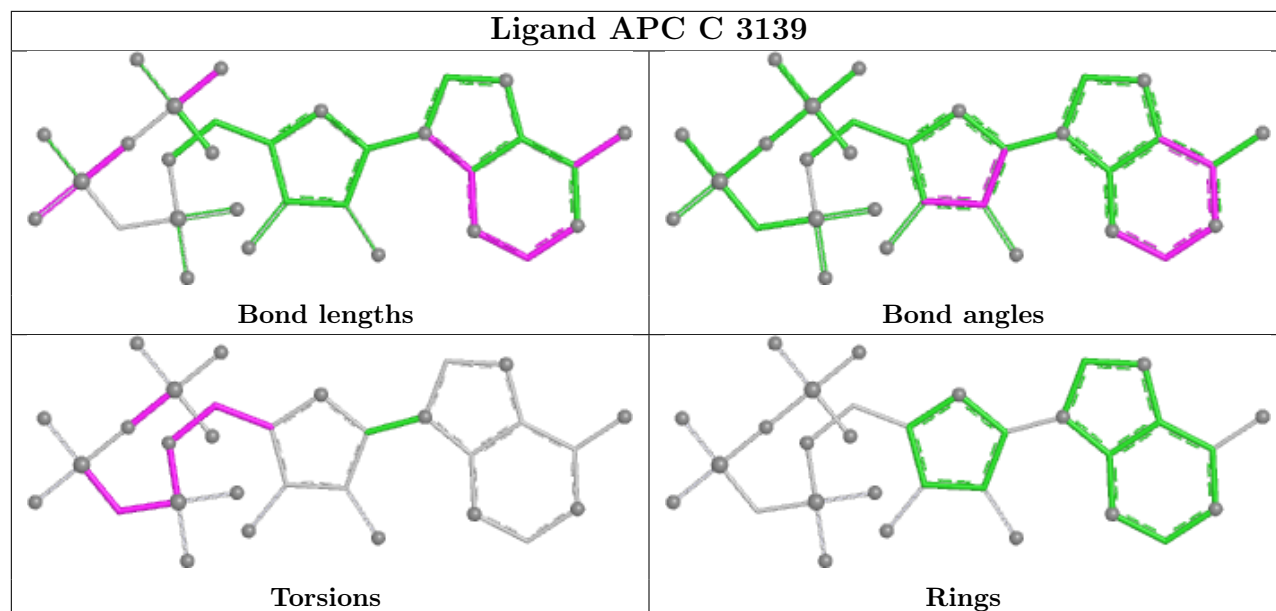
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2139	APC	3	0
4	A	1139	APC	2	0
4	C	3139	APC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

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	485/510 (95%)	0.11	20 (4%)	41 23	20, 56, 131, 158	16 (3%)
1	B	457/510 (89%)	0.52	39 (8%)	16 8	11, 67, 147, 154	12 (2%)
1	C	491/510 (96%)	0.23	22 (4%)	38 20	24, 59, 136, 160	19 (3%)
2	D	143/148 (96%)	1.01	28 (19%)	3 2	42, 122, 157, 165	0
2	E	143/148 (96%)	1.33	32 (22%)	2 1	59, 135, 161, 164	0
2	F	143/148 (96%)	0.87	18 (12%)	8 5	49, 129, 159, 164	0
All	All	1862/1974 (94%)	0.46	159 (8%)	16 8	11, 68, 153, 165	47 (2%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ILE	21.9
2	E	18	LEU	6.6
1	B	658	PRO	5.1
1	B	773	PHE	5.0
1	B	705	TYR	4.9
1	B	736	LEU	4.8
1	B	732	ILE	4.8
2	D	76	MET	4.6
2	E	69	LEU	4.5
1	B	759	GLN	4.5
2	F	38	SER	4.4
1	B	793	PHE	4.4
1	B	775	LEU	4.1
1	B	757	THR	4.0
1	B	777	TYR	4.0
2	D	5	THR	3.9
2	D	55	VAL	3.9
1	B	752	LEU	3.9
1	C	675	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	735	VAL	3.8
1	C	744	GLU	3.8
2	D	9	ILE	3.7
2	F	57	ALA	3.7
1	B	780	LEU	3.7
2	D	19	PHE	3.6
2	E	61	GLY	3.6
2	E	79	THR	3.6
2	E	130	ILE	3.6
2	D	48	LEU	3.5
2	D	57	ALA	3.5
2	D	39	LEU	3.5
1	C	788	ASP	3.5
1	C	422	GLY	3.4
1	C	741	ILE	3.4
2	F	55	VAL	3.4
1	A	779	GLN	3.4
2	E	5	THR	3.3
1	A	776	LEU	3.3
1	B	702	SER	3.3
1	B	748	TYR	3.3
2	E	12	PHE	3.3
2	E	19	PHE	3.3
1	A	792	VAL	3.2
1	B	654	ILE	3.2
2	E	66	PRO	3.2
2	F	9	ILE	3.1
1	A	694	VAL	3.1
1	B	792	VAL	3.0
2	E	80	ASP	3.0
1	A	793	PHE	3.0
2	D	56	ASP	3.0
2	D	24	ASP	2.9
2	D	43	PRO	2.9
1	C	775	LEU	2.9
1	A	747	ASN	2.9
2	D	15	ALA	2.9
2	D	65	PHE	2.9
1	B	656	THR	2.9
1	C	798	ASP	2.8
1	C	787	THR	2.8
1	C	694	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	9	ILE	2.8
1	A	674	SER	2.8
2	E	15	ALA	2.8
2	E	55	VAL	2.8
2	E	71	MET	2.8
1	C	523	LEU	2.8
1	A	775	LEU	2.7
1	B	657	ILE	2.7
2	F	34	THR	2.7
1	B	738	SER	2.7
1	C	739	LYS	2.7
2	D	12	PHE	2.7
1	B	704	TYR	2.6
1	B	737	LYS	2.6
1	C	691	LYS	2.6
2	F	63	ILE	2.6
2	F	19	PHE	2.6
1	B	734	ASN	2.6
1	B	762	LEU	2.6
2	E	35	VAL	2.5
2	F	66	PRO	2.5
2	E	32	LEU	2.5
1	A	735	VAL	2.5
1	B	756	ILE	2.5
2	D	79	THR	2.5
1	C	773	PHE	2.5
1	B	717	LYS	2.5
1	B	720	ILE	2.5
1	C	790	PHE	2.5
2	F	48	LEU	2.5
1	C	513	TRP	2.4
2	F	56	ASP	2.4
2	E	39	LEU	2.4
2	E	29	THR	2.4
2	F	62	THR	2.4
2	D	68	PHE	2.4
2	D	119	GLU	2.4
2	D	32	LEU	2.4
1	B	739	LYS	2.4
2	D	16	PHE	2.4
2	D	69	LEU	2.4
1	C	693	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	728	ALA	2.4
1	C	748	TYR	2.4
2	F	15	ALA	2.4
2	D	38	SER	2.4
1	B	766	HIS	2.3
1	B	715	GLU	2.3
2	F	29	THR	2.3
1	B	566	TYR	2.3
1	A	798	ASP	2.3
1	B	763	LEU	2.3
2	F	69	LEU	2.3
1	C	440	GLN	2.3
2	E	59	GLY	2.3
2	E	63	ILE	2.3
2	D	18	LEU	2.3
1	A	782	PHE	2.3
2	E	77	LYS	2.3
1	C	743	PRO	2.3
2	F	52	ILE	2.3
1	A	797	ILE	2.2
2	E	51	MET	2.2
2	D	35	VAL	2.2
2	E	131	ASP	2.2
2	F	24	ASP	2.2
1	A	773	PHE	2.2
1	B	520	PRO	2.2
1	B	716	LYS	2.2
1	A	744	GLU	2.2
2	D	53	ASN	2.2
2	E	76	MET	2.2
2	E	75	LYS	2.2
1	A	784	GLU	2.2
1	B	755	ARG	2.2
2	D	8	GLN	2.1
2	E	42	ASN	2.1
2	E	125	ILE	2.1
1	A	659	THR	2.1
1	A	695	LYS	2.1
1	C	701	LEU	2.1
2	E	41	GLN	2.1
2	D	31	GLU	2.1
2	E	38	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	75	LYS	2.1
2	E	62	THR	2.1
1	C	749	PHE	2.1
2	F	51	MET	2.1
1	A	729	TYR	2.1
1	C	767	GLN	2.1
2	E	8	GLN	2.1
2	E	136	VAL	2.0
1	A	783	THR	2.0
1	B	765	THR	2.0
2	D	22	ASP	2.0
1	B	790	PHE	2.0
1	A	739	LYS	2.0
2	D	13	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
4	APC	A	1139	31/31	0.85	0.17	53,103,118,119	0
4	APC	B	2139	31/31	0.86	0.17	65,109,118,118	0
4	APC	C	3139	31/31	0.87	0.18	65,110,118,118	0
5	CA	E	802	1/1	0.96	0.07	93,93,93,93	0
5	CA	E	803	1/1	0.96	0.05	84,84,84,84	0
5	CA	D	800	1/1	0.97	0.08	57,57,57,57	0
5	CA	F	804	1/1	0.97	0.04	58,58,58,58	0
5	CA	D	801	1/1	0.98	0.04	58,58,58,58	0
5	CA	F	805	1/1	0.98	0.05	66,66,66,66	0

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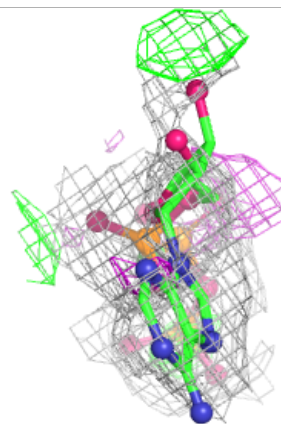
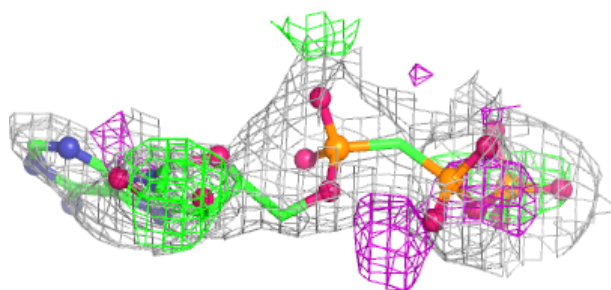
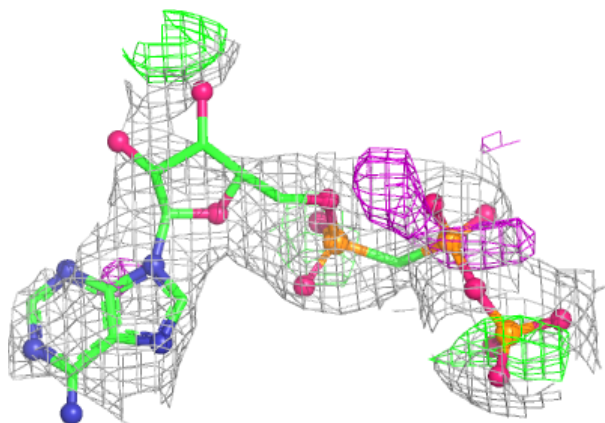
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YB	A	901	1/1	0.99	0.02	85,85,85,85	0
3	YB	B	902	1/1	0.99	0.06	101,101,101,101	0
3	YB	C	903	1/1	0.99	0.07	95,95,95,95	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

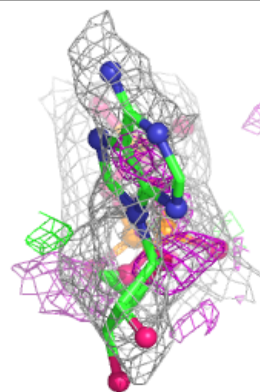
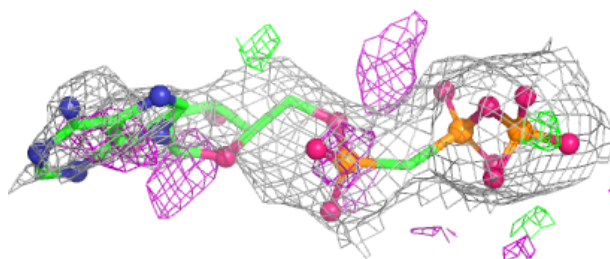
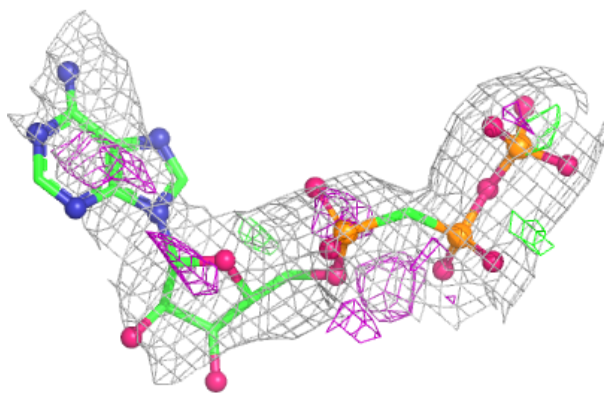
Electron density around APC A 1139:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

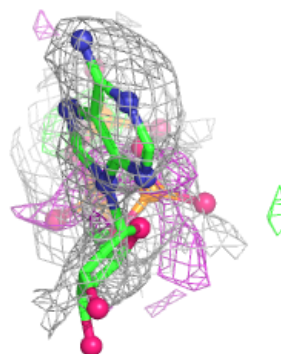
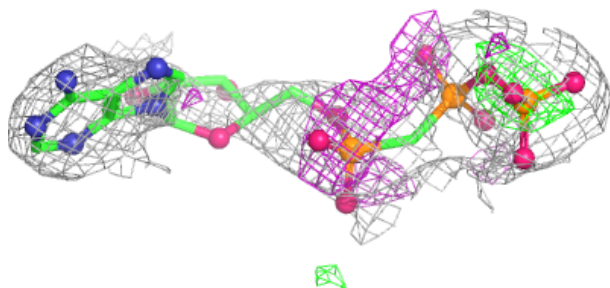
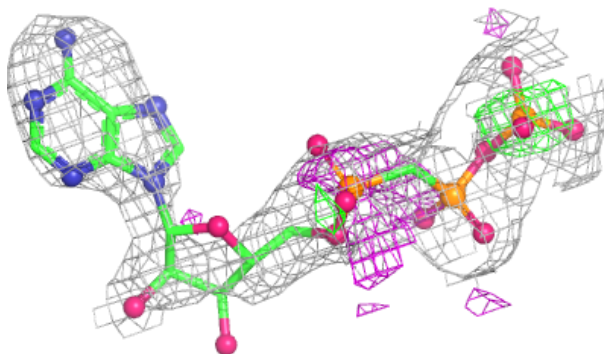


Electron density around APC B 2139:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around APC C 3139:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.