



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 1PK0 / pdb_00001pk0
Title : Crystal Structure of the EF3-CaM complexed with PMEApp
Authors : Shen, Y.; Tang, W.J.
Deposited on : 2003-06-04
Resolution : 3.30 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

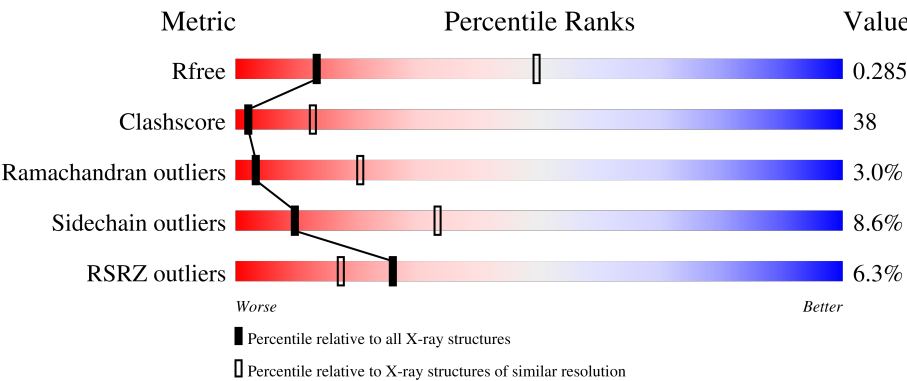
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	507	4% 41% 45% 10% 5%
1	B	507	8% 36% 45% 11% 7%
1	C	507	2% 44% 45% 10% .
2	D	147	12% 48% 47% . .
2	E	147	12% 48% 46% . .

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Mol	Chain	Length	Quality of chain
2	F	147	9% 48% 46%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15344 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 adenylylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	65	0	0
			3947	2525	672	747	3			
1	B	470	Total	C	N	O	S	113	0	0
			3820	2446	647	724	3			
1	C	503	Total	C	N	O	S	166	0	0
			4095	2616	696	780	3			

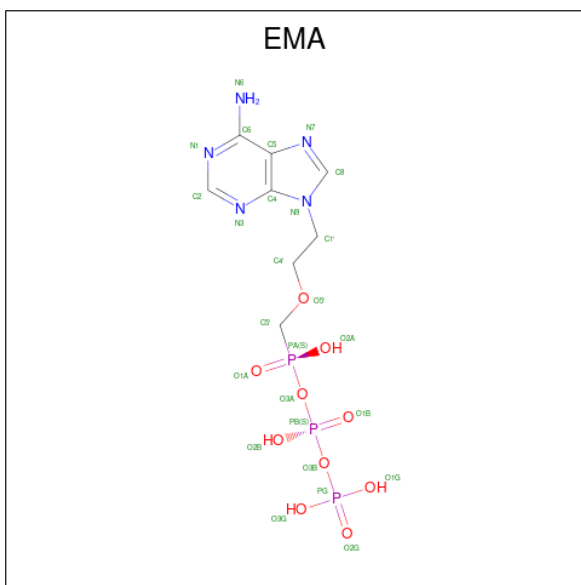
- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1126	690	181	246	9			
2	E	143	Total	C	N	O	S	0	0	0
			1126	690	181	246	9			
2	F	143	Total	C	N	O	S	0	0	0
			1126	690	181	246	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 (ADENIN-9-YL-ETHOXYMETHYL)-HYDROXYPHOSPHINYL-DIPHOSPHATE (CCD ID: EMA) (formula: C₈H₁₄N₅O₁₀P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			26	8	5	10	3		
4	B	1	Total	C	N	O	P	0	0
			26	8	5	10	3		
4	C	1	Total	C	N	O	P	0	0
			26	8	5	10	3		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	6	Total	O	0	0
			6	6		
6	C	4	Total	O	0	0
			4	4		

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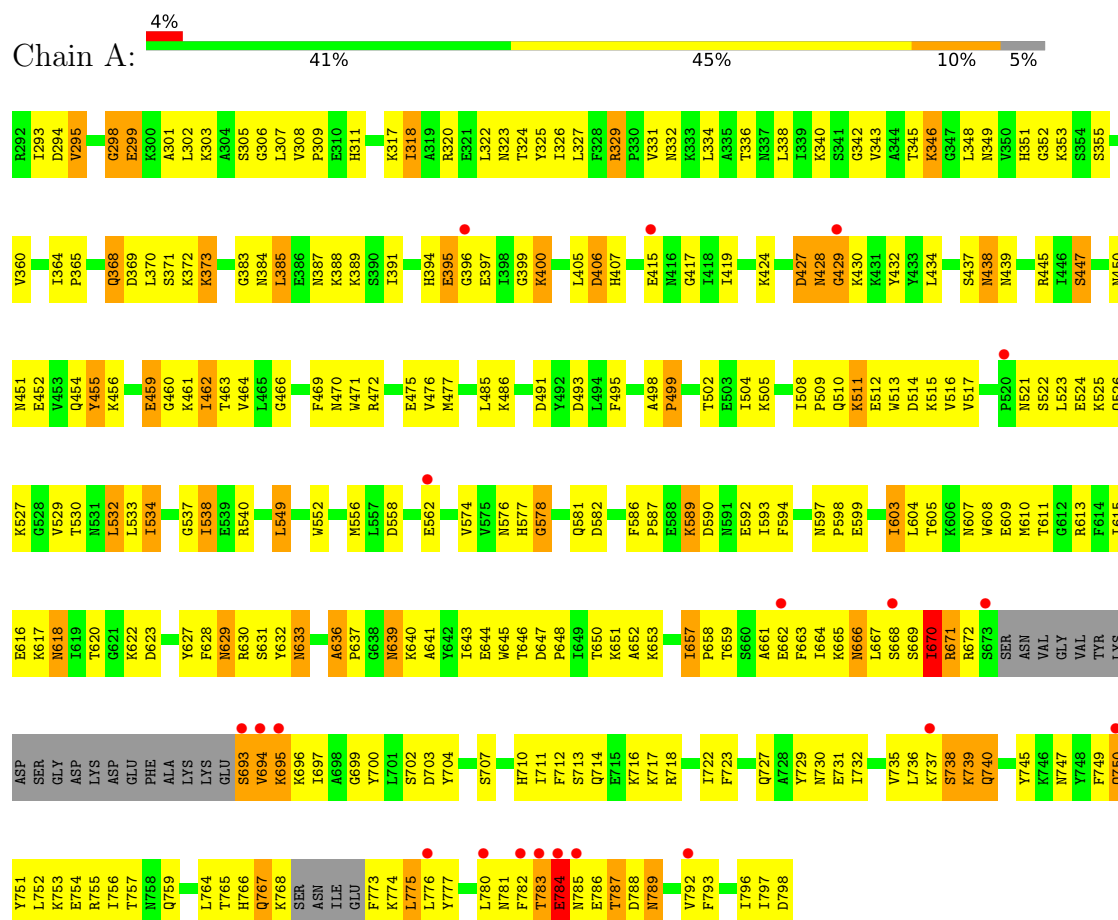
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	O	0	0
			1	1		

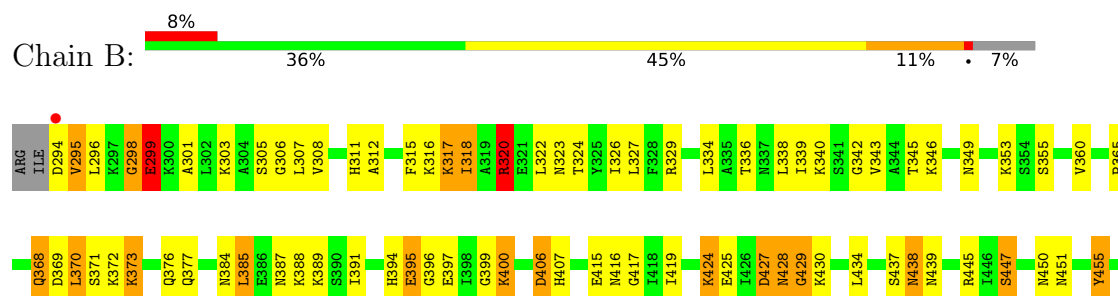
3 Residue-property plots

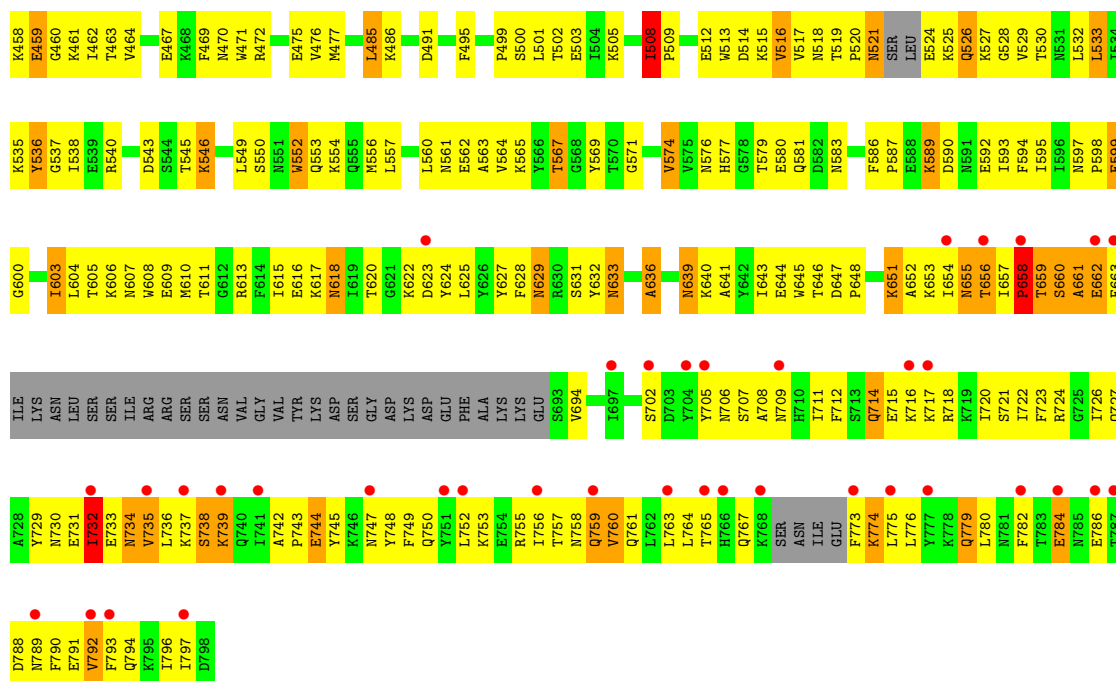
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

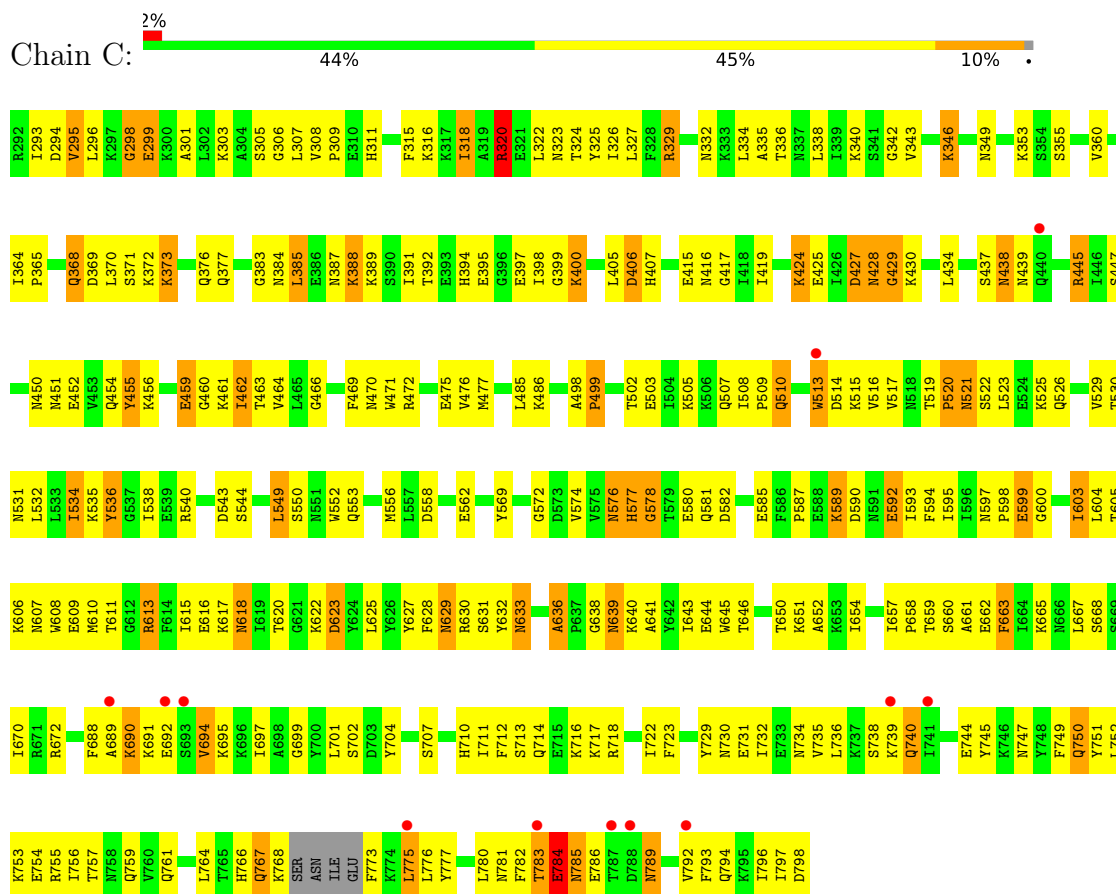


• Molecule 1: Calmodulin-sensitive adenylate cyclase

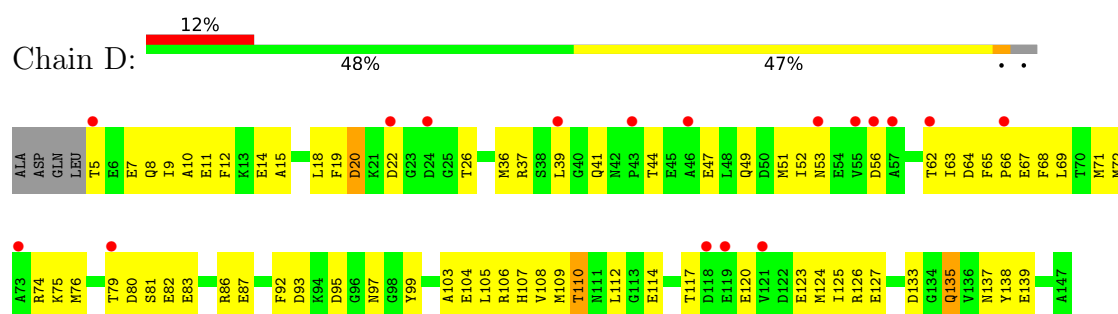




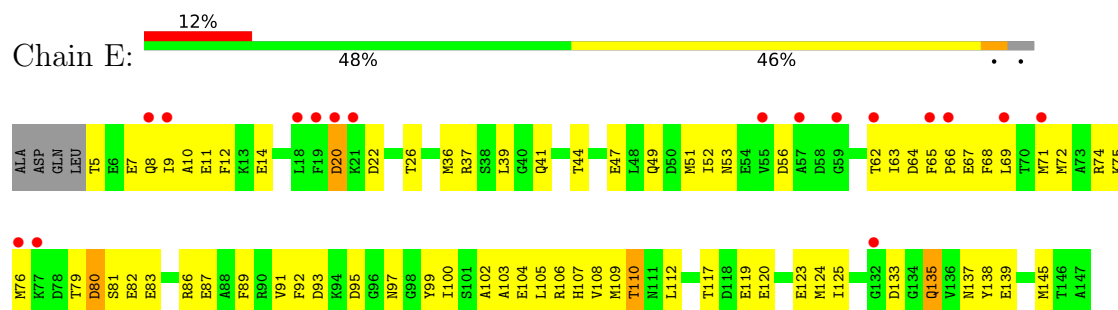
• Molecule 1: Calmodulin-sensitive adenylate cyclase



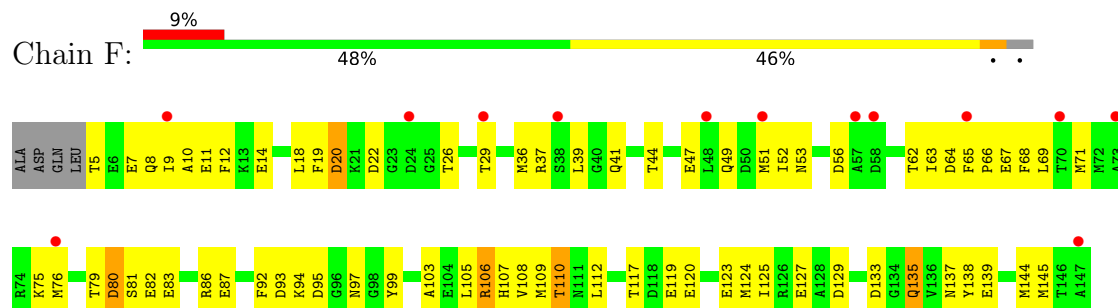
• Molecule 2: Calmodulin



• 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	116.26Å 165.76Å 342.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.30 14.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (14.98-3.30) 94.2 (14.98-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.264 , 0.302 0.255 , 0.285	Depositor DCC
R_{free} test set	4988 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15344	wwPDB-VP
Average B, all atoms (Å ²)	72.0	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: CA, EMA, 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	0.81	11/4022 (0.3%)	1.33	60/5411 (1.1%)
1	B	0.68	3/3893 (0.1%)	1.23	41/5239 (0.8%)
1	C	0.64	2/4173 (0.0%)	1.18	47/5613 (0.8%)
2	D	0.43	0/1138	0.77	0/1527
2	E	0.39	0/1138	0.77	0/1527
2	F	0.41	0/1138	0.87	3/1527 (0.2%)
All	All	0.66	16/15502 (0.1%)	1.17	151/20844 (0.7%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	694	VAL	N-CA	13.78	1.63	1.46
1	A	738	SER	C-N	-8.39	1.23	1.33
1	A	511	LYS	CA-C	8.04	1.63	1.52
1	A	511	LYS	C-N	7.92	1.44	1.33
1	A	785	ASN	N-CA	7.83	1.56	1.46
1	A	427	ASP	C-N	-7.29	1.24	1.33
1	B	427	ASP	C-N	-6.51	1.25	1.33
1	A	428	ASN	N-CA	-5.98	1.39	1.46
1	A	740	GLN	N-CA	-5.72	1.38	1.45
1	A	694	VAL	CA-C	5.64	1.59	1.52
1	B	702	SER	N-CA	5.52	1.52	1.46
1	A	783	THR	N-CA	5.47	1.53	1.46
1	A	511	LYS	N-CA	5.16	1.53	1.46
1	C	785	ASN	N-CA	5.13	1.52	1.46
1	B	655	ASN	C-N	5.09	1.40	1.33
1	C	740	GLN	CA-C	-5.07	1.46	1.52

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	785	ASN	N-CA-C	22.65	140.19	113.01
1	B	661	ALA	N-CA-C	-19.98	89.58	114.75
1	A	740	GLN	N-CA-C	-18.12	86.61	110.53
1	B	660	SER	N-CA-C	-15.87	90.95	111.90
1	A	783	THR	N-CA-C	15.62	132.65	112.34
1	B	428	ASN	N-CA-C	-14.51	84.53	108.32
1	C	785	ASN	N-CA-C	14.36	141.38	110.80
1	C	784	GLU	CB-CA-C	-12.81	95.55	111.43
1	A	695	LYS	N-CA-C	12.64	128.56	112.89
1	A	785	ASN	CA-CB-CG	-11.97	100.63	112.60
1	A	538	ILE	N-CA-C	11.76	121.44	110.74
1	A	428	ASN	N-CA-C	-11.49	87.61	107.61
1	C	783	THR	N-CA-C	11.44	135.17	110.80
2	F	106	ARG	NE-CZ-NH2	10.91	129.02	119.20
1	C	428	ASN	N-CA-C	-10.82	89.46	107.32
1	A	613	ARG	NE-CZ-NH1	-10.82	110.68	121.50
1	B	738	SER	N-CA-C	-10.82	93.05	109.60
1	A	613	ARG	NE-CZ-NH2	10.72	128.85	119.20
1	B	526	GLN	OE1-CD-NE2	-10.71	111.89	122.60
1	C	784	GLU	CA-C-N	10.70	141.98	121.54
1	C	784	GLU	C-N-CA	10.70	141.98	121.54
1	C	740	GLN	OE1-CD-NE2	-10.69	111.91	122.60
1	A	784	GLU	CB-CA-C	-10.43	97.59	110.94
2	F	106	ARG	NE-CZ-NH1	-10.16	111.34	121.50
1	A	427	ASP	N-CA-C	10.12	126.59	114.04
1	A	694	VAL	CB-CA-C	-9.90	93.23	110.65
1	A	767	GLN	OE1-CD-NE2	-9.90	112.70	122.60
1	B	427	ASP	N-CA-C	9.83	125.97	113.88
1	C	510	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	C	427	ASP	N-CA-C	9.63	125.98	114.04
1	B	546	LYS	N-CA-C	-9.58	96.28	110.46
1	A	740	GLN	OE1-CD-NE2	-9.27	113.33	122.60
1	C	767	GLN	OE1-CD-NE2	-9.21	113.39	122.60
1	C	740	GLN	N-CA-C	-9.08	94.52	108.96
1	B	767	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	B	458	LYS	CG-CD-CE	8.77	131.48	111.30
1	A	510	GLN	OE1-CD-NE2	-8.60	114.00	122.60
1	A	670	ILE	N-CA-C	-8.57	104.55	112.43
1	B	428	ASN	CA-CB-CG	8.24	120.84	112.60
2	F	106	ARG	CD-NE-CZ	8.10	135.74	124.40
1	C	785	ASN	CA-CB-CG	-7.91	104.69	112.60
1	B	543	ASP	N-CA-C	-7.89	94.00	110.80
1	B	662	GLU	N-CA-C	-7.75	103.71	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	GLN	O-C-N	-7.74	112.84	122.20
1	A	738	SER	N-CA-C	7.74	123.39	111.56
1	C	766	HIS	N-CA-C	-7.53	103.08	111.82
1	C	785	ASN	N-CA-CB	-7.44	97.92	110.49
1	A	613	ARG	CD-NE-CZ	7.37	134.71	124.40
1	C	740	GLN	CG-CD-NE2	7.32	127.38	116.40
1	B	656	THR	N-CA-C	7.13	120.10	108.55
1	A	740	GLN	CG-CD-NE2	7.05	126.98	116.40
1	C	428	ASN	CA-CB-CG	7.00	119.60	112.60
1	A	694	VAL	N-CA-C	6.77	117.55	108.27
1	A	510	GLN	CG-CD-NE2	6.76	126.55	116.40
1	B	739	LYS	N-CA-C	6.75	125.18	110.80
1	A	576	ASN	N-CA-C	6.75	121.58	112.88
1	B	427	ASP	CA-CB-CG	-6.72	105.88	112.60
1	C	580	GLU	N-CA-C	-6.63	103.88	112.23
1	A	510	GLN	CA-C-O	-6.61	113.29	121.02
1	A	320	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	A	486	LYS	CA-C-N	6.58	126.56	119.78
1	A	486	LYS	C-N-CA	6.58	126.56	119.78
1	A	428	ASN	CA-CB-CG	6.58	119.18	112.60
1	B	767	GLN	CG-CD-NE2	6.54	126.20	116.40
1	B	732	ILE	N-CA-C	-6.53	95.77	109.34
1	B	526	GLN	CG-CD-NE2	6.52	126.18	116.40
1	C	369	ASP	N-CA-C	-6.50	105.33	113.20
1	A	739	LYS	N-CA-C	-6.49	98.85	108.79
1	C	688	PHE	CA-C-N	-6.49	113.14	122.67
1	C	688	PHE	C-N-CA	-6.49	113.14	122.67
1	C	767	GLN	CG-CD-NE2	6.42	126.03	116.40
1	C	574	VAL	N-CA-C	-6.42	105.91	113.42
1	B	574	VAL	N-CA-C	-6.35	107.31	113.53
1	B	486	LYS	CA-C-N	6.29	126.26	119.78
1	B	486	LYS	C-N-CA	6.29	126.26	119.78
1	A	510	GLN	CA-C-N	-6.26	108.79	121.18
1	A	510	GLN	C-N-CA	-6.26	108.79	121.18
1	A	533	LEU	N-CA-C	-6.24	104.41	111.14
1	A	369	ASP	N-CA-C	-6.22	105.67	113.20
1	B	299	GLU	CA-CB-CG	6.14	126.38	114.10
1	A	293	ILE	CB-CA-C	6.13	119.95	111.19
1	A	574	VAL	N-CA-C	-6.09	106.29	113.42
1	C	510	GLN	CG-CD-NE2	6.09	125.53	116.40
1	C	486	LYS	CA-C-N	6.08	126.05	119.78
1	C	486	LYS	C-N-CA	6.08	126.05	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	658	PRO	O-C-N	6.07	130.83	122.64
1	A	784	GLU	CA-C-N	6.05	133.17	121.18
1	A	784	GLU	C-N-CA	6.05	133.17	121.18
1	A	767	GLN	CG-CD-NE2	6.04	125.45	116.40
1	A	636	ALA	CA-C-N	5.96	125.17	118.97
1	A	636	ALA	C-N-CA	5.96	125.17	118.97
1	A	693	SER	CA-CB-OG	5.95	123.00	111.10
1	C	688	PHE	N-CA-C	5.95	118.10	108.34
1	C	636	ALA	CA-C-N	5.92	125.13	118.97
1	C	636	ALA	C-N-CA	5.92	125.13	118.97
1	B	659	THR	N-CA-C	-5.92	98.19	110.80
1	A	711	ILE	N-CA-C	-5.90	107.54	113.20
1	B	369	ASP	N-CA-C	-5.90	106.06	113.20
1	C	750	GLN	N-CA-C	-5.87	105.38	112.54
1	B	532	LEU	N-CA-C	-5.87	106.10	113.20
1	A	766	HIS	N-CA-C	-5.84	105.41	112.54
1	A	785	ASN	CB-CA-C	-5.79	98.36	110.17
1	B	370	LEU	N-CA-C	-5.79	105.88	113.17
1	A	693	SER	N-CA-CB	-5.79	100.67	110.50
1	B	636	ALA	CA-C-N	5.77	124.97	118.97
1	B	636	ALA	C-N-CA	5.77	124.97	118.97
1	A	672	ARG	CB-CA-C	5.73	121.38	110.27
1	A	750	GLN	N-CA-C	-5.71	105.57	112.54
1	B	577	HIS	N-CA-C	5.67	116.75	108.14
1	B	579	THR	N-CA-C	5.66	118.00	110.53
1	C	320	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	B	658	PRO	CA-N-CD	-5.63	104.12	112.00
1	C	783	THR	CB-CA-C	-5.62	99.24	110.42
1	A	693	SER	N-CA-C	5.61	126.71	111.00
1	C	711	ILE	N-CA-C	-5.59	107.83	113.20
1	C	766	HIS	CB-CA-C	5.53	121.29	110.67
1	C	785	ASN	CB-CA-C	-5.53	99.42	110.42
1	C	694	VAL	N-CA-C	5.51	115.96	110.23
1	A	737	LYS	N-CA-C	-5.50	106.52	113.18
1	C	783	THR	CA-C-N	5.47	128.99	121.33
1	C	783	THR	C-N-CA	5.47	128.99	121.33
1	A	765	THR	N-CA-C	-5.46	106.46	113.01
1	B	320	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	B	533	LEU	N-CA-C	-5.41	106.81	113.41
1	C	577	HIS	N-CA-C	5.33	116.62	108.52
1	A	320	ARG	NE-CZ-NH1	5.32	126.81	121.50
1	C	320	ARG	NE-CZ-NH1	-5.30	116.19	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	666	ASN	N-CA-C	-5.27	106.70	113.23
1	B	508	ILE	N-CA-C	5.25	113.90	109.02
1	A	320	ARG	CD-NE-CZ	5.25	131.75	124.40
1	A	783	THR	CB-CA-C	-5.25	98.43	110.18
1	B	702	SER	N-CA-C	5.24	118.49	112.57
1	C	329	ARG	N-CA-C	-5.23	102.54	110.39
1	C	592	GLU	N-CA-C	5.21	117.23	108.73
1	C	513	TRP	N-CA-C	-5.21	106.19	112.54
1	B	779	GLN	N-CA-C	-5.20	107.45	112.97
1	C	536	TYR	N-CA-C	5.19	119.77	113.38
1	A	511	LYS	N-CA-C	5.19	119.23	113.01
1	A	671	ARG	N-CA-C	-5.18	106.54	112.92
1	B	660	SER	CA-C-N	5.18	130.53	121.52
1	B	660	SER	C-N-CA	5.18	130.53	121.52
1	B	576	ASN	N-CA-C	5.18	119.69	113.17
1	C	576	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	329	ARG	N-CA-C	-5.13	102.69	110.39
1	C	346	LYS	N-CA-C	5.09	117.86	109.76
1	C	738	SER	N-CA-C	5.09	119.35	111.56
1	C	613	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	A	592	GLU	N-CA-C	5.04	116.94	108.73
1	A	647	ASP	CA-C-N	5.01	126.10	119.84
1	A	647	ASP	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3947	0	3994	295	0
1	B	3820	0	3841	336	0
1	C	4095	0	4134	306	0
2	D	1126	0	1049	75	0
2	E	1126	0	1049	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1126	0	1049	80	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	26	0	9	1	0
4	B	26	0	9	4	0
4	C	26	0	9	7	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
6	A	6	0	0	2	0
6	B	6	0	0	0	0
6	C	4	0	0	0	0
6	D	1	0	0	0	0
All	All	15344	0	15143	1116	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 38.

All (1116) 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:731:GLU:HG3	1:B:732:ILE:H	1.03	1.19
1:B:428:ASN:O	1:B:430:LYS:N	1.77	1.17
1:C:577:HIS:O	1:C:578:GLY:O	1.60	1.16
1:B:427:ASP:OD1	1:B:427:ASP:O	1.72	1.08
1:C:690:LYS:HZ3	1:C:692:GLU:HA	1.18	1.08
1:B:726:ILE:HA	1:B:729:TYR:HB2	1.39	1.05
1:C:427:ASP:OD1	1:C:427:ASP:O	1.76	1.04
1:A:428:ASN:O	1:A:430:LYS:N	1.90	1.03
1:B:295:VAL:HG21	1:B:603:ILE:HG22	1.39	1.03
1:B:657:ILE:CD1	1:B:658:PRO:HD2	1.90	1.02
1:B:658:PRO:O	1:B:661:ALA:HB2	1.58	1.02
1:A:295:VAL:HG21	1:A:603:ILE:HG22	1.42	1.01
1:C:295:VAL:HG21	1:C:603:ILE:HG22	1.40	1.00
1:C:346:LYS:HE2	4:C:3999:EMA:O2G	1.60	0.99
1:B:629:ASN:ND2	1:B:631:SER:H	1.60	0.98
1:C:629:ASN:ND2	1:C:631:SER:H	1.60	0.98
1:A:629:ASN:ND2	1:A:631:SER:H	1.62	0.97
1:B:633:ASN:HD21	1:B:645:TRP:H	1.11	0.97
1:A:629:ASN:HD22	1:A:631:SER:H	1.11	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ASN:HD21	1:C:645:TRP:H	1.12	0.95
1:B:657:ILE:HG13	1:B:658:PRO:HD2	1.48	0.95
1:B:561:ASN:O	1:B:564:VAL:HG22	1.67	0.95
1:B:639:ASN:HD22	1:B:639:ASN:H	1.10	0.94
1:B:629:ASN:HD22	1:B:631:SER:H	1.09	0.94
1:B:295:VAL:CG2	1:B:603:ILE:HG22	1.96	0.93
1:B:657:ILE:CG1	1:B:658:PRO:HD2	1.98	0.93
1:C:629:ASN:HD22	1:C:631:SER:H	1.11	0.93
1:C:639:ASN:H	1:C:639:ASN:HD22	1.08	0.93
1:C:295:VAL:CG2	1:C:603:ILE:HG22	1.98	0.92
1:C:577:HIS:C	1:C:578:GLY:O	2.12	0.92
1:A:633:ASN:HD21	1:A:645:TRP:H	1.16	0.91
1:C:775:LEU:HD23	1:C:775:LEU:H	1.35	0.91
1:B:731:GLU:HG3	1:B:732:ILE:N	1.86	0.90
1:A:427:ASP:OD1	1:A:427:ASP:O	1.89	0.90
1:A:521:ASN:ND2	1:A:522:SER:H	1.70	0.89
1:A:639:ASN:H	1:A:639:ASN:HD22	1.16	0.89
1:A:295:VAL:CG2	1:A:603:ILE:HG22	2.02	0.89
1:A:445:ARG:HH22	1:A:456:LYS:HG2	1.36	0.89
1:A:775:LEU:HD23	1:A:775:LEU:H	1.38	0.89
1:A:427:ASP:O	6:A:5:HOH:O	1.91	0.88
1:C:385:LEU:HD11	1:C:389:LYS:HE3	1.55	0.88
1:B:731:GLU:CG	1:B:732:ILE:H	1.78	0.88
1:A:385:LEU:HD11	1:A:389:LYS:HE3	1.55	0.87
1:C:514:ASP:HA	1:C:517:VAL:HG12	1.57	0.86
1:A:739:LYS:HG3	1:A:740:GLN:O	1.74	0.86
1:C:659:THR:HG22	1:C:661:ALA:H	1.37	0.86
1:A:521:ASN:HD22	1:A:522:SER:H	1.17	0.86
1:B:318:ILE:HG21	1:B:556:MET:HE1	1.58	0.86
1:B:735:VAL:HG22	1:B:738:SER:HB2	1.57	0.85
1:C:346:LYS:CE	4:C:3999:EMA:O2G	2.25	0.85
1:B:385:LEU:HD11	1:B:389:LYS:HE3	1.58	0.83
1:C:577:HIS:CE1	4:C:3999:EMA:C8	2.62	0.81
1:C:633:ASN:HD21	1:C:645:TRP:N	1.78	0.81
1:A:523:LEU:HD13	2:D:127:GLU:HB3	1.61	0.81
1:B:427:ASP:OD1	1:B:427:ASP:C	2.22	0.81
1:B:518:ASN:C	1:B:520:PRO:HD3	2.04	0.81
1:B:633:ASN:HD21	1:B:645:TRP:N	1.77	0.81
1:C:400:LYS:HE2	1:C:475:GLU:OE2	1.80	0.80
1:A:617:LYS:HG2	1:A:618:ASN:ND2	1.95	0.80
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ASN:N	1:B:618:ASN:HD22	1.79	0.79
2:D:133:ASP:OD2	2:D:135:GLN:HG3	1.83	0.79
1:A:540:ARG:NH2	2:D:87:GLU:OE1	2.15	0.79
1:B:761:GLN:HA	1:B:764:LEU:HD12	1.65	0.79
1:B:400:LYS:HE2	1:B:475:GLU:OE2	1.82	0.79
1:C:427:ASP:OD1	1:C:427:ASP:C	2.25	0.78
1:B:323:ASN:OD1	1:B:500:SER:HB3	1.84	0.78
2:F:133:ASP:OD2	2:F:135:GLN:HG3	1.83	0.78
1:C:792:VAL:HG12	1:C:796:ILE:HD11	1.65	0.78
1:A:618:ASN:HD22	1:A:618:ASN:N	1.79	0.78
1:A:633:ASN:HD21	1:A:645:TRP:N	1.82	0.78
1:A:787:THR:O	1:A:787:THR:HG22	1.82	0.78
1:C:690:LYS:NZ	1:C:692:GLU:HA	1.99	0.78
2:E:65:PHE:HB2	2:E:66:PRO:HD3	1.65	0.78
1:C:581:GLN:HE21	1:C:628:PHE:HA	1.49	0.77
1:B:524:GLU:HB3	1:B:527:LYS:HG2	1.65	0.77
1:B:737:LYS:C	1:B:738:SER:O	2.23	0.77
1:C:577:HIS:O	1:C:578:GLY:C	2.24	0.77
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.65	0.77
1:B:564:VAL:O	1:B:567:THR:HG23	1.84	0.77
1:B:659:THR:C	1:B:661:ALA:N	2.29	0.77
1:B:745:TYR:HB3	1:B:749:PHE:HE1	1.49	0.77
2:E:133:ASP:OD2	2:E:135:GLN:HG3	1.84	0.77
1:C:618:ASN:N	1:C:618:ASN:HD22	1.82	0.76
1:A:781:ASN:ND2	1:A:782:PHE:H	1.84	0.76
1:C:633:ASN:HD22	1:C:633:ASN:N	1.83	0.76
1:A:400:LYS:HE2	1:A:475:GLU:OE2	1.86	0.76
1:A:792:VAL:HG12	1:A:796:ILE:HD11	1.66	0.76
1:C:617:LYS:HG2	1:C:618:ASN:ND2	2.00	0.76
1:B:629:ASN:ND2	1:B:631:SER:HB2	2.00	0.75
1:A:438:ASN:HD22	1:A:438:ASN:C	1.93	0.75
1:C:540:ARG:HD3	1:C:627:TYR:OH	1.86	0.75
1:A:581:GLN:HE21	1:A:628:PHE:HA	1.51	0.75
1:B:629:ASN:HD22	1:B:631:SER:N	1.84	0.75
1:B:722:ILE:O	1:B:726:ILE:HG13	1.85	0.75
1:C:629:ASN:ND2	1:C:631:SER:HB2	2.02	0.75
2:E:12:PHE:HD1	2:E:39:LEU:HD21	1.52	0.75
1:B:657:ILE:HG13	1:B:658:PRO:CD	2.17	0.74
1:B:639:ASN:HD22	1:B:639:ASN:N	1.84	0.74
1:B:537:GLY:O	1:B:625:LEU:HD21	1.88	0.74
1:A:324:THR:HG21	1:A:556:MET:HE1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:ASN:ND2	1:C:782:PHE:H	1.85	0.74
1:B:428:ASN:O	1:B:429:GLY:C	2.28	0.74
1:C:438:ASN:C	1:C:438:ASN:HD22	1.95	0.74
1:B:617:LYS:HG2	1:B:618:ASN:ND2	2.02	0.74
1:B:581:GLN:HE21	1:B:628:PHE:HA	1.53	0.74
1:B:633:ASN:N	1:B:633:ASN:HD22	1.86	0.74
2:F:12:PHE:HD1	2:F:39:LEU:HD21	1.52	0.74
1:A:428:ASN:O	1:A:429:GLY:C	2.31	0.73
1:B:438:ASN:C	1:B:438:ASN:HD22	1.97	0.73
1:B:718:ARG:HB2	1:B:763:LEU:HB3	1.69	0.73
1:A:318:ILE:HD12	1:A:318:ILE:H	1.52	0.73
1:A:633:ASN:N	1:A:633:ASN:HD22	1.81	0.73
1:C:617:LYS:C	1:C:618:ASN:HD22	1.97	0.73
1:C:629:ASN:HD22	1:C:631:SER:N	1.84	0.73
1:B:657:ILE:HD12	1:B:658:PRO:HD2	1.69	0.73
1:C:781:ASN:HD22	1:C:782:PHE:H	1.35	0.73
1:A:781:ASN:HD22	1:A:782:PHE:H	1.34	0.73
1:A:629:ASN:HD22	1:A:631:SER:N	1.86	0.73
1:A:427:ASP:OD1	1:A:427:ASP:C	2.30	0.73
1:A:318:ILE:HD12	1:A:318:ILE:N	2.03	0.72
1:C:692:GLU:O	1:C:735:VAL:HG22	1.88	0.72
1:A:617:LYS:C	1:A:618:ASN:HD22	1.96	0.72
1:C:318:ILE:HD12	1:C:318:ILE:N	2.04	0.72
1:B:516:VAL:HA	1:B:520:PRO:HG2	1.72	0.72
2:D:12:PHE:HD1	2:D:39:LEU:HD21	1.52	0.72
1:B:657:ILE:HD12	1:B:658:PRO:CD	2.20	0.72
1:C:320:ARG:HD2	1:C:599:GLU:O	1.88	0.72
1:A:513:TRP:HD1	1:A:532:LEU:HD12	1.54	0.71
1:B:629:ASN:HD21	1:B:631:SER:HB2	1.54	0.71
1:A:445:ARG:HG3	1:A:471:TRP:CH2	2.24	0.71
1:B:789:ASN:HD22	1:B:792:VAL:HB	1.55	0.71
1:C:400:LYS:HE2	1:C:475:GLU:CD	2.15	0.71
1:C:659:THR:HB	1:C:662:GLU:HB3	1.72	0.71
1:B:714:GLN:OE1	1:B:715:GLU:HG3	1.90	0.71
1:A:639:ASN:HD22	1:A:639:ASN:N	1.89	0.71
1:A:521:ASN:ND2	1:A:522:SER:N	2.38	0.71
1:A:695:LYS:HB2	2:D:18:LEU:HD22	1.72	0.71
1:B:757:THR:HG23	1:B:773:PHE:HB3	1.73	0.71
1:B:524:GLU:CB	1:B:527:LYS:HG2	2.20	0.70
1:A:735:VAL:O	1:A:738:SER:HB2	1.90	0.70
1:B:318:ILE:N	1:B:318:ILE:HD12	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:PRO:HA	1:B:651:LYS:HB2	1.73	0.70
1:C:318:ILE:HD12	1:C:318:ILE:H	1.54	0.70
1:A:324:THR:HG21	1:A:556:MET:CE	2.22	0.70
1:A:521:ASN:HD22	1:A:522:SER:N	1.87	0.70
1:A:629:ASN:ND2	1:A:631:SER:HB2	2.07	0.70
1:C:792:VAL:O	1:C:796:ILE:HG12	1.91	0.70
1:B:726:ILE:CA	1:B:729:TYR:HB2	2.19	0.69
1:B:784:GLU:OE1	1:B:788:ASP:HB3	1.91	0.69
1:A:493:ASP:OD1	6:A:7:HOH:O	2.10	0.69
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.55	0.69
1:A:666:ASN:O	1:A:670:ILE:HB	1.93	0.69
1:B:318:ILE:HD12	1:B:318:ILE:H	1.56	0.69
1:B:616:GLU:HA	1:B:620:THR:CG2	2.23	0.69
1:B:617:LYS:C	1:B:618:ASN:HD22	2.01	0.69
1:C:368:GLN:HB2	1:C:384:ASN:OD1	1.92	0.69
1:A:695:LYS:HD2	2:D:19:PHE:HB2	1.73	0.69
1:A:696:LYS:HD3	1:A:731:GLU:OE1	1.93	0.69
1:A:540:ARG:HD3	1:A:627:TYR:OH	1.92	0.69
1:A:577:HIS:O	1:A:578:GLY:O	2.10	0.68
1:B:318:ILE:CG2	1:B:556:MET:HE1	2.24	0.68
1:B:329:ARG:HD2	1:B:590:ASP:OD2	1.92	0.68
1:B:508:ILE:HG22	1:B:509:PRO:HD2	1.75	0.68
1:B:717:LYS:HA	1:B:720:ILE:HG12	1.75	0.68
1:B:720:ILE:HG13	1:B:721:SER:N	2.08	0.68
1:C:329:ARG:HD2	1:C:590:ASP:OD2	1.93	0.68
1:C:540:ARG:NH2	1:C:630:ARG:HH21	1.91	0.68
1:B:654:ILE:O	1:B:655:ASN:ND2	2.26	0.68
1:B:519:THR:N	1:B:520:PRO:HD3	2.08	0.68
1:B:538:ILE:O	1:B:540:ARG:HD3	1.94	0.68
1:A:792:VAL:O	1:A:796:ILE:HG12	1.93	0.68
1:B:308:VAL:HB	1:B:311:HIS:ND1	2.09	0.68
1:A:513:TRP:O	1:A:517:VAL:HG23	1.94	0.68
1:A:577:HIS:C	1:A:578:GLY:O	2.37	0.68
1:B:320:ARG:HD2	1:B:599:GLU:O	1.93	0.68
1:C:659:THR:HG22	1:C:661:ALA:N	2.08	0.68
1:C:327:LEU:N	1:C:327:LEU:HD12	2.10	0.67
1:C:639:ASN:HD22	1:C:639:ASN:N	1.84	0.67
1:B:720:ILE:HD12	1:B:724:ARG:NH2	2.10	0.67
1:C:747:ASN:O	1:C:750:GLN:HG2	1.95	0.67
1:A:360:VAL:HG22	1:A:360:VAL:O	1.95	0.67
1:C:526:GLN:HB2	2:F:124:MET:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:HD12	1:A:745:TYR:CE1	2.30	0.67
1:B:724:ARG:O	1:B:727:GLN:HB3	1.95	0.67
1:C:777:TYR:CD1	1:C:780:LEU:HD21	2.30	0.67
1:C:616:GLU:HA	1:C:620:THR:CG2	2.24	0.66
1:C:558:ASP:O	1:C:562:GLU:HG3	1.96	0.66
1:A:616:GLU:HA	1:A:620:THR:CG2	2.25	0.66
1:C:519:THR:OG1	1:C:520:PRO:HD2	1.95	0.66
1:A:323:ASN:HD22	1:A:598:PRO:HB2	1.61	0.66
1:A:777:TYR:CD1	1:A:780:LEU:HD21	2.31	0.66
1:B:360:VAL:O	1:B:360:VAL:HG22	1.95	0.66
1:B:540:ARG:HD2	1:B:627:TYR:CZ	2.31	0.66
1:B:605:THR:HG21	1:B:611:THR:HA	1.78	0.65
1:C:605:THR:HG21	1:C:611:THR:HA	1.77	0.65
1:B:659:THR:O	1:B:660:SER:C	2.33	0.65
1:B:327:LEU:HD12	1:B:327:LEU:N	2.11	0.65
1:B:735:VAL:CG2	1:B:738:SER:HB2	2.27	0.65
1:A:385:LEU:CD1	1:A:389:LYS:HE3	2.27	0.65
1:B:368:GLN:HB2	1:B:384:ASN:OD1	1.97	0.65
1:C:324:THR:HG21	1:C:556:MET:HE1	1.77	0.64
1:A:540:ARG:NH2	1:A:630:ARG:HH21	1.94	0.64
2:F:5:THR:OG1	2:F:8:GLN:HG2	1.97	0.64
1:B:346:LYS:HE2	4:B:2999:EMA:O2G	1.97	0.64
1:C:308:VAL:HB	1:C:311:HIS:ND1	2.12	0.64
1:A:400:LYS:HE2	1:A:475:GLU:CD	2.21	0.64
1:B:657:ILE:HD13	1:B:705:TYR:HD1	1.61	0.64
2:F:106:ARG:O	2:F:110:THR:HG23	1.96	0.64
1:B:556:MET:HE3	1:B:560:LEU:HG	1.80	0.64
1:C:629:ASN:HD21	1:C:631:SER:HB2	1.61	0.64
1:A:605:THR:HG21	1:A:611:THR:HA	1.79	0.64
1:B:400:LYS:HE2	1:B:475:GLU:CD	2.23	0.64
1:C:510:GLN:O	1:C:514:ASP:OD2	2.16	0.64
1:A:445:ARG:HG3	1:A:471:TRP:CZ2	2.32	0.64
1:B:654:ILE:HA	1:B:755:ARG:HD3	1.80	0.64
1:A:308:VAL:HB	1:A:311:HIS:ND1	2.13	0.64
1:B:346:LYS:HE3	4:B:2999:EMA:O1A	1.98	0.63
1:C:658:PRO:HG3	1:C:752:LEU:HD22	1.80	0.63
1:C:360:VAL:HG22	1:C:360:VAL:O	1.97	0.63
2:D:76:MET:HE3	2:D:79:THR:HG21	1.81	0.63
1:B:733:GLU:C	1:B:735:VAL:H	2.06	0.63
2:E:117:THR:OG1	2:E:120:GLU:HG3	1.98	0.63
1:A:368:GLN:HB2	1:A:384:ASN:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:MET:O	2:D:41:GLN:HB2	1.99	0.62
1:A:740:GLN:CD	1:A:740:GLN:H	2.07	0.62
1:B:385:LEU:CD1	1:B:389:LYS:HE3	2.29	0.62
1:B:789:ASN:ND2	1:B:792:VAL:HB	2.14	0.62
1:C:428:ASN:O	1:C:430:LYS:N	2.31	0.62
2:E:12:PHE:CD1	2:E:39:LEU:HD21	2.34	0.62
2:E:36:MET:O	2:E:41:GLN:HB2	1.98	0.62
1:A:747:ASN:O	1:A:750:GLN:HG2	1.99	0.62
2:F:12:PHE:CD1	2:F:39:LEU:HD21	2.35	0.62
1:B:720:ILE:O	1:B:723:PHE:HB3	2.00	0.62
1:B:372:LYS:HG3	1:B:373:LYS:HD3	1.81	0.62
2:E:106:ARG:O	2:E:110:THR:HG23	2.00	0.62
1:B:655:ASN:O	1:B:755:ARG:NH1	2.33	0.62
2:D:79:THR:C	2:D:81:SER:H	2.08	0.62
2:D:117:THR:OG1	2:D:120:GLU:HG3	1.99	0.62
1:A:505:LYS:HD3	2:D:112:LEU:O	1.98	0.62
1:B:589:LYS:HB2	1:B:643:ILE:HG12	1.82	0.61
1:B:706:ASN:O	1:B:709:ASN:HB2	1.99	0.61
1:B:731:GLU:HG3	1:B:733:GLU:H	1.63	0.61
1:A:786:GLU:O	1:A:788:ASP:N	2.31	0.61
1:B:657:ILE:CD1	1:B:658:PRO:CD	2.70	0.61
1:B:722:ILE:HG22	1:B:726:ILE:HD11	1.82	0.61
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.35	0.61
1:C:659:THR:H	1:C:662:GLU:HB3	1.64	0.61
1:A:327:LEU:N	1:A:327:LEU:HD12	2.15	0.61
2:F:26:THR:HA	2:F:63:ILE:O	2.01	0.61
2:F:36:MET:O	2:F:41:GLN:HB2	2.01	0.61
2:E:26:THR:HA	2:E:63:ILE:O	2.01	0.61
1:A:617:LYS:HG2	1:A:618:ASN:HD21	1.66	0.61
1:C:663:PHE:O	1:C:667:LEU:HG	2.00	0.61
1:C:781:ASN:ND2	1:C:782:PHE:N	2.49	0.61
1:A:629:ASN:HD21	1:A:631:SER:HB2	1.65	0.61
1:B:346:LYS:CE	4:B:2999:EMA:O1A	2.49	0.61
1:C:629:ASN:ND2	1:C:631:SER:N	2.42	0.61
2:F:76:MET:HE3	2:F:79:THR:HG21	1.82	0.60
2:F:79:THR:C	2:F:81:SER:H	2.09	0.60
1:A:534:ILE:HA	1:A:538:ILE:HB	1.83	0.60
1:B:659:THR:C	1:B:661:ALA:H	2.05	0.60
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.31	0.60
1:C:789:ASN:N	1:C:789:ASN:HD22	1.99	0.60
1:A:781:ASN:ND2	1:A:782:PHE:N	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:THR:HA	2:D:63:ILE:O	2.01	0.60
2:F:117:THR:OG1	2:F:120:GLU:HG3	2.00	0.60
1:B:323:ASN:OD1	1:B:500:SER:CB	2.48	0.60
1:B:516:VAL:CA	1:B:520:PRO:HG2	2.31	0.60
1:B:776:LEU:HD22	1:B:779:GLN:HG3	1.84	0.60
1:C:540:ARG:NH2	1:C:630:ARG:NH2	2.49	0.60
1:B:345:THR:HB	1:B:491:ASP:HB3	1.84	0.60
1:B:633:ASN:ND2	1:B:644:GLU:HA	2.17	0.60
1:B:639:ASN:H	1:B:639:ASN:ND2	1.91	0.60
1:C:650:THR:C	1:C:652:ALA:H	2.09	0.60
1:B:718:ARG:O	1:B:722:ILE:HG13	2.02	0.60
1:C:372:LYS:HG3	1:C:373:LYS:HD3	1.84	0.60
1:C:695:LYS:HD2	2:F:19:PHE:HB2	1.84	0.60
1:A:294:ASP:O	1:A:610:MET:HE1	2.02	0.59
1:C:514:ASP:C	1:C:516:VAL:H	2.09	0.59
1:A:789:ASN:N	1:A:789:ASN:HD22	1.99	0.59
1:C:455:TYR:HA	1:C:471:TRP:HZ3	1.66	0.59
2:E:79:THR:C	2:E:81:SER:H	2.09	0.59
1:B:731:GLU:HG3	1:B:733:GLU:N	2.17	0.59
1:A:558:ASP:O	1:A:562:GLU:HG3	2.02	0.59
1:B:776:LEU:HD13	1:B:779:GLN:OE1	2.03	0.59
1:C:324:THR:OG1	1:C:499:PRO:HA	2.03	0.59
1:C:469:PHE:CB	1:C:472:ARG:HH21	2.16	0.59
2:E:76:MET:HE3	2:E:79:THR:HG21	1.83	0.59
1:A:470:ASN:CG	1:A:471:TRP:H	2.11	0.59
1:B:509:PRO:HD3	1:B:536:TYR:HE1	1.68	0.59
1:C:657:ILE:HG13	1:C:759:GLN:HG2	1.84	0.59
1:C:665:LYS:HE3	2:F:11:GLU:OE2	2.02	0.59
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.37	0.59
1:A:469:PHE:CB	1:A:472:ARG:HH21	2.15	0.59
1:B:538:ILE:HD11	1:B:625:LEU:HD11	1.84	0.59
1:C:773:PHE:N	1:C:775:LEU:HD21	2.18	0.59
1:B:556:MET:CE	1:B:560:LEU:HG	2.33	0.59
1:B:657:ILE:HD13	1:B:705:TYR:CD1	2.38	0.59
1:B:745:TYR:O	1:B:749:PHE:HD1	1.85	0.59
1:C:296:LEU:CD2	1:C:606:LYS:HE3	2.33	0.59
1:A:540:ARG:HD3	1:A:627:TYR:CZ	2.38	0.58
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.32	0.58
2:D:68:PHE:HA	2:D:71:MET:HE3	1.85	0.58
2:F:68:PHE:HA	2:F:71:MET:HE3	1.85	0.58
1:A:372:LYS:HG3	1:A:373:LYS:HD3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:HG23	1:B:322:LEU:HD12	1.84	0.58
1:C:428:ASN:O	1:C:429:GLY:C	2.46	0.58
1:C:324:THR:HG21	1:C:556:MET:CE	2.33	0.58
2:D:106:ARG:O	2:D:110:THR:HG23	2.02	0.58
2:D:12:PHE:CD1	2:D:39:LEU:HD21	2.35	0.58
1:A:318:ILE:HG23	1:A:322:LEU:HD12	1.84	0.58
1:A:773:PHE:N	1:A:775:LEU:HD21	2.18	0.58
1:C:540:ARG:HD3	1:C:627:TYR:CZ	2.39	0.58
1:C:385:LEU:CD1	1:C:389:LYS:HE3	2.29	0.58
2:D:83:GLU:O	2:D:87:GLU:HG3	2.03	0.58
1:B:305:SER:HB3	1:B:594:PHE:CD1	2.39	0.58
1:B:752:LEU:CD2	1:B:756:ILE:HD11	2.33	0.58
2:D:137:ASN:OD1	2:D:139:GLU:HB2	2.04	0.58
1:B:773:PHE:O	1:B:775:LEU:N	2.34	0.58
1:C:526:GLN:OE1	2:F:144:MET:HE2	2.03	0.58
1:C:718:ARG:O	1:C:722:ILE:HG13	2.04	0.58
1:C:318:ILE:HG23	1:C:322:LEU:HD12	1.85	0.58
1:B:776:LEU:HD13	1:B:779:GLN:CD	2.28	0.57
1:C:529:VAL:CG1	2:F:112:LEU:HD13	2.34	0.57
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.86	0.57
1:C:509:PRO:HD2	1:C:536:TYR:CE2	2.40	0.57
1:A:633:ASN:ND2	1:A:644:GLU:HA	2.20	0.57
1:A:667:LEU:O	1:A:670:ILE:HG22	2.05	0.57
1:B:657:ILE:CG1	1:B:658:PRO:CD	2.76	0.57
1:A:589:LYS:HB2	1:A:643:ILE:HG12	1.87	0.57
1:B:655:ASN:O	1:B:755:ARG:HD2	2.05	0.57
1:B:744:GLU:OE1	1:C:397:GLU:OE1	2.22	0.57
1:B:709:ASN:OD1	1:B:717:LYS:HG2	2.04	0.57
1:B:758:ASN:C	1:B:760:VAL:H	2.12	0.57
1:B:514:ASP:HA	1:B:517:VAL:HG12	1.87	0.57
1:C:540:ARG:HD2	1:C:582:ASP:OD1	2.03	0.57
1:A:323:ASN:HD22	1:A:598:PRO:CB	2.17	0.57
1:A:668:SER:C	1:A:670:ILE:H	2.12	0.57
1:A:747:ASN:HA	1:A:750:GLN:HG2	1.87	0.57
1:B:629:ASN:ND2	1:B:631:SER:N	2.41	0.57
1:B:514:ASP:O	1:B:516:VAL:N	2.38	0.57
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.86	0.56
2:E:68:PHE:HA	2:E:71:MET:HE3	1.85	0.56
1:B:530:THR:HG22	2:E:92:PHE:CZ	2.41	0.56
1:B:794:GLN:NE2	1:B:797:ILE:HG21	2.20	0.56
1:C:318:ILE:H	1:C:318:ILE:CD1	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:ILE:HD13	1:C:732:ILE:HG12	1.87	0.56
1:A:697:ILE:HD11	1:A:731:GLU:O	2.05	0.56
1:C:549:LEU:HD12	1:C:549:LEU:H	1.69	0.56
2:E:137:ASN:OD1	2:E:139:GLU:HB2	2.05	0.56
1:A:329:ARG:HD2	1:A:590:ASP:OD2	2.06	0.56
1:B:731:GLU:CG	1:B:732:ILE:N	2.47	0.56
1:C:320:ARG:HG3	1:C:598:PRO:O	2.04	0.56
1:B:295:VAL:HG22	1:B:603:ILE:HG22	1.85	0.56
2:D:63:ILE:N	2:D:63:ILE:HD12	2.21	0.56
2:F:63:ILE:N	2:F:63:ILE:HD12	2.20	0.56
1:A:629:ASN:ND2	1:A:631:SER:N	2.44	0.56
1:B:470:ASN:CG	1:B:471:TRP:H	2.14	0.56
1:C:662:GLU:O	1:C:662:GLU:HG2	2.04	0.56
1:C:747:ASN:HA	1:C:750:GLN:HG2	1.86	0.56
1:A:697:ILE:HD12	1:A:697:ILE:N	2.21	0.56
1:A:718:ARG:O	1:A:722:ILE:HG13	2.04	0.56
1:A:739:LYS:CG	1:A:740:GLN:O	2.51	0.56
1:A:456:LYS:HD3	1:A:471:TRP:CD1	2.41	0.56
1:A:781:ASN:HD22	1:A:782:PHE:N	2.04	0.56
1:B:500:SER:HA	1:B:624:TYR:CD2	2.40	0.56
1:B:535:LYS:C	1:B:536:TYR:HD2	2.14	0.56
1:B:616:GLU:HA	1:B:620:THR:HG22	1.88	0.56
1:B:748:TYR:CZ	1:B:752:LEU:HD12	2.41	0.56
2:D:92:PHE:CD2	2:D:108:VAL:HG21	2.41	0.56
1:B:323:ASN:HD22	1:B:598:PRO:HB2	1.70	0.55
2:E:63:ILE:HD12	2:E:63:ILE:N	2.21	0.55
1:A:759:GLN:HE21	1:A:759:GLN:HA	1.72	0.55
2:D:105:LEU:HD23	2:D:105:LEU:O	2.06	0.55
1:B:307:LEU:HD12	1:B:307:LEU:H	1.71	0.55
1:B:505:LYS:O	1:B:508:ILE:HG13	2.07	0.55
1:B:538:ILE:N	1:B:538:ILE:HD12	2.21	0.55
1:A:540:ARG:NH2	1:A:630:ARG:NH2	2.55	0.55
1:C:722:ILE:HD13	1:C:764:LEU:HD23	1.88	0.55
2:E:95:ASP:OD2	2:E:97:ASN:HB3	2.06	0.55
2:E:5:THR:HG23	2:E:8:GLN:HG3	1.88	0.55
1:A:783:THR:O	1:A:784:GLU:OE1	2.23	0.55
1:A:540:ARG:NH2	2:D:87:GLU:CD	2.65	0.55
1:A:759:GLN:HA	1:A:759:GLN:NE2	2.21	0.55
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.89	0.55
1:B:731:GLU:CG	1:B:733:GLU:H	2.19	0.55
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:CZ	1:A:471:TRP:CD1	2.90	0.55
1:A:526:GLN:C	1:A:529:VAL:HG12	2.32	0.55
1:A:540:ARG:HH22	2:D:87:GLU:CD	2.15	0.55
1:A:740:GLN:CD	1:A:740:GLN:N	2.65	0.55
1:B:716:LYS:O	1:B:720:ILE:HG23	2.06	0.55
2:D:44:THR:HG22	2:D:47:GLU:OE1	2.07	0.55
1:C:759:GLN:NE2	1:C:759:GLN:HA	2.22	0.54
1:A:318:ILE:H	1:A:318:ILE:CD1	2.17	0.54
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.89	0.54
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.89	0.54
1:A:607:ASN:HD21	1:A:609:GLU:HB2	1.72	0.54
1:A:630:ARG:CZ	2:D:83:GLU:HB3	2.37	0.54
1:C:295:VAL:HG22	1:C:603:ILE:HG22	1.87	0.54
1:C:617:LYS:HG2	1:C:618:ASN:HD21	1.72	0.54
2:F:8:GLN:HE21	2:F:8:GLN:HA	1.73	0.54
2:F:41:GLN:NE2	2:F:76:MET:HE1	2.23	0.54
2:F:137:ASN:OD1	2:F:139:GLU:HB2	2.06	0.54
1:C:320:ARG:CD	1:C:599:GLU:O	2.56	0.54
1:C:323:ASN:HD22	1:C:598:PRO:HB2	1.73	0.54
1:C:520:PRO:HG2	1:C:521:ASN:H	1.72	0.54
1:C:589:LYS:HB2	1:C:643:ILE:HG12	1.89	0.54
1:A:549:LEU:HD12	1:A:549:LEU:H	1.72	0.54
1:A:633:ASN:N	1:A:633:ASN:ND2	2.52	0.54
1:A:695:LYS:CB	2:D:18:LEU:HD22	2.36	0.54
1:A:714:GLN:NE2	2:D:126:ARG:HG3	2.23	0.54
1:B:516:VAL:O	1:B:520:PRO:HD2	2.07	0.54
1:A:445:ARG:HH22	1:A:456:LYS:CG	2.15	0.54
1:A:616:GLU:HA	1:A:620:THR:HG22	1.90	0.54
1:B:530:THR:O	1:B:533:LEU:HB3	2.07	0.54
1:B:514:ASP:C	1:B:516:VAL:H	2.16	0.54
1:C:296:LEU:HD21	1:C:606:LYS:HE3	1.88	0.54
1:C:650:THR:C	1:C:652:ALA:N	2.66	0.54
1:C:718:ARG:HD2	1:C:767:GLN:OE1	2.07	0.54
2:F:105:LEU:HD23	2:F:105:LEU:O	2.07	0.54
1:C:759:GLN:HA	1:C:759:GLN:HE21	1.74	0.54
2:D:8:GLN:HA	2:D:8:GLN:HE21	1.73	0.54
2:D:20:ASP:C	2:D:22:ASP:H	2.16	0.54
1:B:663:PHE:CB	2:E:14:GLU:OE2	2.56	0.53
1:C:534:ILE:HA	1:C:538:ILE:HB	1.90	0.53
1:A:504:ILE:HD12	1:A:537:GLY:HA2	1.89	0.53
1:A:549:LEU:HB3	1:A:578:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ILE:CD1	1:A:731:GLU:HB3	2.38	0.53
1:B:529:VAL:HG21	2:E:109:MET:HE1	1.90	0.53
1:B:618:ASN:N	1:B:618:ASN:ND2	2.51	0.53
2:E:97:ASN:HD21	2:E:99:TYR:HB2	1.73	0.53
1:B:318:ILE:H	1:B:318:ILE:CD1	2.20	0.53
1:B:509:PRO:HG2	1:B:512:GLU:HB3	1.91	0.53
1:B:658:PRO:O	1:B:661:ALA:CB	2.47	0.53
1:C:581:GLN:NE2	1:C:628:PHE:HA	2.20	0.53
2:E:8:GLN:HE21	2:E:8:GLN:HA	1.73	0.53
2:F:44:THR:HG22	2:F:47:GLU:OE1	2.07	0.53
1:C:616:GLU:HA	1:C:620:THR:HG22	1.89	0.53
2:E:105:LEU:O	2:E:105:LEU:HD23	2.08	0.53
1:A:581:GLN:NE2	1:A:628:PHE:HA	2.22	0.53
1:B:536:TYR:N	1:B:536:TYR:CD2	2.77	0.53
1:B:633:ASN:ND2	1:B:645:TRP:H	1.95	0.53
1:B:438:ASN:C	1:B:438:ASN:ND2	2.67	0.53
1:B:715:GLU:O	1:B:718:ARG:HG2	2.08	0.53
1:B:730:ASN:CG	1:B:730:ASN:O	2.51	0.53
2:F:52:ILE:O	2:F:56:ASP:HB3	2.08	0.53
1:A:298:GLY:O	1:A:301:ALA:N	2.42	0.53
1:A:438:ASN:C	1:A:438:ASN:ND2	2.64	0.53
1:A:783:THR:HB	1:A:784:GLU:OE1	2.08	0.53
1:B:445:ARG:HD3	1:B:471:TRP:CZ2	2.44	0.53
1:C:697:ILE:HD11	1:C:731:GLU:O	2.08	0.53
2:E:20:ASP:C	2:E:22:ASP:H	2.16	0.53
1:C:305:SER:HB3	1:C:594:PHE:CD1	2.44	0.53
1:A:529:VAL:HG21	2:D:109:MET:SD	2.48	0.53
1:B:536:TYR:HD2	1:B:536:TYR:N	2.06	0.53
1:B:554:LYS:O	1:B:557:LEU:HB2	2.09	0.53
1:C:298:GLY:O	1:C:301:ALA:N	2.41	0.53
2:D:52:ILE:O	2:D:56:ASP:HB3	2.09	0.53
1:A:664:ILE:HD13	2:D:15:ALA:HB2	1.92	0.52
1:A:739:LYS:C	1:A:740:GLN:O	2.37	0.52
1:C:522:SER:O	1:C:525:LYS:HB3	2.08	0.52
2:E:44:THR:HG22	2:E:47:GLU:OE1	2.07	0.52
1:B:540:ARG:CZ	1:B:627:TYR:CE1	2.92	0.52
1:C:437:SER:C	1:C:439:ASN:H	2.18	0.52
1:B:327:LEU:HG	1:B:595:ILE:HG23	1.91	0.52
1:B:550:SER:H	1:B:553:GLN:HE21	1.56	0.52
1:C:607:ASN:HD21	1:C:609:GLU:HB2	1.73	0.52
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:ILE:HG23	2:E:69:LEU:HD22	1.91	0.52
2:F:52:ILE:O	2:F:52:ILE:HG13	2.10	0.52
1:B:502:THR:O	1:B:505:LYS:HB3	2.10	0.52
1:B:633:ASN:N	1:B:633:ASN:ND2	2.56	0.52
1:A:577:HIS:ND1	1:A:578:GLY:O	2.37	0.52
1:A:700:TYR:CE1	1:A:727:GLN:HB3	2.44	0.52
1:B:723:PHE:HB2	1:B:793:PHE:CE2	2.45	0.52
1:C:695:LYS:HZ2	2:F:18:LEU:HD13	1.74	0.52
1:C:755:ARG:O	1:C:756:ILE:C	2.53	0.52
1:B:295:VAL:HG21	1:B:603:ILE:CG2	2.28	0.52
1:C:346:LYS:HE3	4:C:3999:EMA:O1A	2.09	0.52
1:C:516:VAL:HG21	1:C:532:LEU:HD11	1.91	0.52
1:C:661:ALA:C	1:C:663:PHE:H	2.16	0.52
1:B:538:ILE:CD1	1:B:625:LEU:HD11	2.40	0.52
1:B:607:ASN:HD21	1:B:609:GLU:HB2	1.73	0.52
1:C:316:LYS:HD3	1:C:600:GLY:O	2.10	0.52
1:C:455:TYR:HA	1:C:471:TRP:CZ3	2.45	0.52
1:C:670:ILE:HD11	1:C:744:GLU:C	2.35	0.52
2:F:26:THR:HG21	2:F:62:THR:HB	1.92	0.52
1:A:577:HIS:O	1:A:578:GLY:C	2.51	0.52
1:B:617:LYS:HG2	1:B:618:ASN:HD21	1.75	0.52
1:C:657:ILE:HD12	1:C:704:TYR:CE1	2.45	0.52
2:E:26:THR:HG21	2:E:62:THR:HB	1.92	0.52
1:B:437:SER:C	1:B:439:ASN:H	2.17	0.52
1:C:593:ILE:HG13	1:C:611:THR:HG21	1.92	0.52
1:C:797:ILE:HD12	1:C:798:ASP:N	2.25	0.52
2:D:5:THR:OG1	2:D:8:GLN:HG2	2.10	0.52
2:E:41:GLN:NE2	2:E:76:MET:HE1	2.25	0.52
1:B:445:ARG:HD3	1:B:471:TRP:CE2	2.46	0.51
2:E:52:ILE:O	2:E:56:ASP:HB3	2.10	0.51
1:B:508:ILE:CG2	1:B:509:PRO:HD2	2.41	0.51
2:D:107:HIS:O	2:D:108:VAL:C	2.53	0.51
2:E:52:ILE:O	2:E:52:ILE:HG13	2.10	0.51
2:F:81:SER:O	2:F:82:GLU:C	2.54	0.51
2:F:92:PHE:CE2	2:F:108:VAL:HG11	2.45	0.51
2:F:20:ASP:C	2:F:22:ASP:H	2.16	0.51
1:A:657:ILE:HG23	1:A:759:GLN:HG2	1.91	0.51
1:B:320:ARG:CD	1:B:599:GLU:O	2.59	0.51
1:C:318:ILE:N	1:C:318:ILE:CD1	2.74	0.51
1:B:752:LEU:O	1:B:756:ILE:HG13	2.10	0.51
1:C:661:ALA:C	1:C:663:PHE:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:PHE:CD2	1:A:716:LYS:HG2	2.46	0.51
1:B:750:GLN:O	1:B:753:LYS:HB3	2.11	0.51
1:B:296:LEU:CD2	1:B:606:LYS:HE3	2.40	0.51
1:B:298:GLY:O	1:B:301:ALA:N	2.42	0.51
1:B:343:VAL:O	1:B:569:TYR:OH	2.22	0.51
1:B:561:ASN:O	1:B:562:GLU:C	2.54	0.51
1:C:459:GLU:C	1:C:461:LYS:H	2.18	0.51
2:D:9:ILE:HG23	2:D:69:LEU:HD22	1.91	0.51
2:D:52:ILE:O	2:D:52:ILE:HG13	2.11	0.51
1:A:508:ILE:HG21	1:A:532:LEU:HD13	1.91	0.51
1:B:733:GLU:C	1:B:735:VAL:N	2.69	0.51
2:D:26:THR:HG21	2:D:62:THR:HB	1.92	0.51
2:E:81:SER:O	2:E:82:GLU:C	2.53	0.51
2:F:9:ILE:HG23	2:F:69:LEU:HD22	1.93	0.51
1:A:695:LYS:HB2	2:D:18:LEU:CD2	2.40	0.51
1:C:505:LYS:HD2	1:C:508:ILE:HD12	1.93	0.51
1:C:659:THR:HB	1:C:662:GLU:CB	2.40	0.51
1:A:459:GLU:C	1:A:461:LYS:H	2.19	0.51
1:A:513:TRP:HD1	1:A:532:LEU:CD1	2.23	0.51
1:A:629:ASN:HB3	1:A:632:TYR:CE2	2.46	0.51
1:B:720:ILE:HD12	1:B:724:ARG:HH21	1.76	0.51
1:B:774:LYS:O	1:B:774:LYS:HG3	2.11	0.51
2:D:41:GLN:NE2	2:D:76:MET:HE1	2.26	0.51
1:A:587:PRO:HD2	1:A:639:ASN:HD21	1.75	0.50
1:C:294:ASP:O	1:C:610:MET:HE1	2.11	0.50
1:C:697:ILE:O	1:C:701:LEU:HG	2.11	0.50
1:A:797:ILE:HD12	1:A:798:ASP:N	2.25	0.50
1:B:329:ARG:HH11	1:B:590:ASP:CG	2.19	0.50
1:B:658:PRO:C	1:B:659:THR:O	2.53	0.50
1:C:668:SER:HB2	2:F:14:GLU:HG3	1.92	0.50
2:D:62:THR:C	2:D:63:ILE:HD12	2.37	0.50
2:E:103:ALA:O	2:E:106:ARG:HB3	2.11	0.50
1:A:469:PHE:HB3	1:A:472:ARG:HH21	1.76	0.50
1:B:734:ASN:C	1:B:736:LEU:H	2.18	0.50
1:B:727:GLN:HG3	1:B:786:GLU:OE1	2.11	0.50
1:C:633:ASN:ND2	1:C:644:GLU:HA	2.27	0.50
1:A:505:LYS:HD2	1:A:508:ILE:HD12	1.93	0.50
1:B:323:ASN:CG	1:B:500:SER:HB3	2.36	0.50
1:C:514:ASP:C	1:C:516:VAL:N	2.68	0.50
2:D:37:ARG:HA	2:D:41:GLN:O	2.11	0.50
2:F:62:THR:C	2:F:63:ILE:HD12	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:HIS:CE1	4:C:3999:EMA:H8	2.44	0.50
1:B:756:ILE:O	1:B:760:VAL:HG23	2.11	0.50
1:C:296:LEU:HD21	1:C:606:LYS:CE	2.42	0.50
1:A:618:ASN:ND2	1:A:618:ASN:N	2.51	0.50
1:B:384:ASN:O	1:B:385:LEU:C	2.55	0.50
1:B:743:PRO:O	1:B:747:ASN:HB2	2.12	0.50
1:A:593:ILE:HG13	1:A:611:THR:HG21	1.94	0.50
1:B:320:ARG:HG3	1:B:598:PRO:O	2.12	0.50
1:B:459:GLU:C	1:B:461:LYS:H	2.19	0.50
1:B:505:LYS:HA	1:B:508:ILE:CD1	2.42	0.50
1:B:521:ASN:C	1:B:521:ASN:HD22	2.19	0.50
1:C:307:LEU:H	1:C:307:LEU:HD12	1.77	0.50
1:C:712:PHE:CD2	1:C:716:LYS:HG2	2.47	0.50
1:A:456:LYS:HD3	1:A:471:TRP:HD1	1.77	0.49
1:B:629:ASN:HD21	1:B:631:SER:CB	2.24	0.49
1:B:653:LYS:O	1:B:653:LYS:HG3	2.10	0.49
1:C:325:TYR:HB2	1:C:498:ALA:HB3	1.93	0.49
1:C:525:LYS:HB3	2:F:124:MET:HE3	1.94	0.49
1:A:697:ILE:HD11	1:A:731:GLU:HB3	1.95	0.49
1:B:322:LEU:HD23	1:B:503:GLU:OE1	2.12	0.49
1:B:780:LEU:HB3	1:B:782:PHE:CE1	2.47	0.49
1:C:349:ASN:H	1:C:349:ASN:ND2	2.11	0.49
1:C:730:ASN:C	1:C:732:ILE:H	2.20	0.49
1:C:754:GLU:O	1:C:757:THR:HB	2.12	0.49
1:C:623:ASP:H	2:F:94:LYS:HD2	1.75	0.49
1:B:525:LYS:C	1:B:528:GLY:H	2.20	0.49
1:B:581:GLN:NE2	1:B:628:PHE:HA	2.22	0.49
1:C:650:THR:O	1:C:652:ALA:N	2.45	0.49
2:D:51:MET:C	2:D:53:ASN:H	2.21	0.49
2:D:81:SER:O	2:D:82:GLU:C	2.55	0.49
2:E:37:ARG:HA	2:E:41:GLN:O	2.11	0.49
1:B:318:ILE:N	1:B:318:ILE:CD1	2.76	0.49
1:B:525:LYS:O	1:B:528:GLY:N	2.46	0.49
1:B:580:GLU:CD	1:B:583:ASN:HD22	2.20	0.49
1:B:745:TYR:HB3	1:B:749:PHE:CE1	2.38	0.49
1:B:717:LYS:CA	1:B:720:ILE:HG12	2.41	0.49
1:B:761:GLN:NE2	1:B:773:PHE:N	2.61	0.49
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.47	0.49
2:D:7:GLU:HA	2:D:10:ALA:HB3	1.95	0.49
2:E:5:THR:HG22	2:E:5:THR:O	2.12	0.49
1:B:306:GLY:O	1:B:336:THR:OG1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:C	1:B:397:GLU:H	2.21	0.49
1:B:415:GLU:C	1:B:417:GLY:H	2.21	0.49
1:B:455:TYR:HA	1:B:471:TRP:HZ3	1.77	0.49
1:C:540:ARG:CZ	1:C:627:TYR:CE1	2.96	0.49
1:C:549:LEU:HD12	1:C:549:LEU:N	2.27	0.49
1:A:437:SER:C	1:A:439:ASN:H	2.20	0.49
1:B:298:GLY:O	1:B:299:GLU:C	2.56	0.49
1:B:648:PRO:O	1:B:651:LYS:CB	2.61	0.49
2:D:117:THR:HG23	2:D:120:GLU:OE2	2.13	0.49
1:A:617:LYS:HG2	1:A:618:ASN:HD22	1.76	0.49
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.94	0.49
1:C:777:TYR:HD1	1:C:780:LEU:HD21	1.76	0.49
1:A:522:SER:OG	2:D:127:GLU:HG3	2.13	0.48
1:A:755:ARG:O	1:A:756:ILE:C	2.53	0.48
1:B:463:THR:HG22	1:B:464:VAL:N	2.28	0.48
1:B:722:ILE:HG12	1:B:760:VAL:HG13	1.95	0.48
1:C:387:ASN:OD1	1:C:477:MET:HE2	2.13	0.48
2:E:51:MET:C	2:E:53:ASN:H	2.20	0.48
2:F:107:HIS:O	2:F:108:VAL:C	2.56	0.48
1:C:505:LYS:HD3	2:F:112:LEU:O	2.13	0.48
2:D:76:MET:HE3	2:D:79:THR:CG2	2.43	0.48
2:D:92:PHE:CE2	2:D:108:VAL:HG11	2.48	0.48
2:F:95:ASP:OD2	2:F:97:ASN:HB3	2.13	0.48
1:A:525:LYS:C	1:A:527:LYS:N	2.71	0.48
1:B:537:GLY:C	1:B:538:ILE:HD12	2.38	0.48
1:C:628:PHE:CD1	1:C:628:PHE:C	2.91	0.48
1:A:307:LEU:HD12	1:A:307:LEU:H	1.78	0.48
1:A:395:GLU:C	1:A:397:GLU:H	2.21	0.48
1:B:345:THR:HB	1:B:491:ASP:CB	2.44	0.48
1:C:360:VAL:HG21	1:C:365:PRO:HB3	1.95	0.48
1:C:617:LYS:HG2	1:C:618:ASN:HD22	1.77	0.48
1:A:306:GLY:O	1:A:336:THR:OG1	2.31	0.48
1:A:325:TYR:HB2	1:A:498:ALA:HB3	1.95	0.48
1:A:395:GLU:HG3	1:A:396:GLY:N	2.28	0.48
1:A:415:GLU:C	1:A:417:GLY:H	2.21	0.48
1:A:445:ARG:NE	1:A:471:TRP:CE2	2.81	0.48
1:A:502:THR:O	1:A:505:LYS:HB3	2.14	0.48
1:A:529:VAL:HG13	1:A:530:THR:N	2.28	0.48
1:B:307:LEU:HD12	1:B:307:LEU:N	2.28	0.48
1:B:323:ASN:HD22	1:B:598:PRO:CB	2.26	0.48
1:B:744:GLU:CD	1:C:397:GLU:HG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLU:C	1:C:397:GLU:H	2.21	0.48
1:C:415:GLU:C	1:C:417:GLY:H	2.21	0.48
1:C:652:ALA:C	1:C:654:ILE:H	2.22	0.48
2:E:107:HIS:O	2:E:108:VAL:C	2.56	0.48
2:F:37:ARG:HA	2:F:41:GLN:O	2.13	0.48
2:F:103:ALA:O	2:F:106:ARG:HB3	2.13	0.48
1:A:615:ILE:O	1:A:620:THR:HG22	2.14	0.48
1:B:296:LEU:HD21	1:B:606:LYS:HE3	1.95	0.48
2:D:103:ALA:O	2:D:106:ARG:HB3	2.14	0.48
2:E:117:THR:HG23	2:E:120:GLU:OE2	2.13	0.48
1:A:415:GLU:C	1:A:417:GLY:N	2.72	0.48
1:A:730:ASN:C	1:A:732:ILE:H	2.20	0.48
1:B:355:SER:HB2	1:B:371:SER:HA	1.95	0.48
1:B:745:TYR:O	1:B:749:PHE:CD1	2.67	0.48
1:C:523:LEU:HD13	2:F:127:GLU:HB3	1.94	0.48
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.49	0.48
1:A:327:LEU:O	1:A:495:PHE:N	2.44	0.48
1:B:469:PHE:CB	1:B:472:ARG:HH21	2.26	0.48
2:E:62:THR:C	2:E:63:ILE:HD12	2.38	0.48
1:A:540:ARG:CZ	1:A:627:TYR:CE1	2.97	0.48
2:E:7:GLU:HA	2:E:10:ALA:HB3	1.95	0.48
2:F:97:ASN:HD21	2:F:99:TYR:HB2	1.79	0.48
1:A:513:TRP:HH2	2:D:114:GLU:N	2.12	0.48
1:B:395:GLU:HG3	1:B:396:GLY:N	2.27	0.48
2:F:51:MET:C	2:F:53:ASN:H	2.21	0.48
1:A:628:PHE:CD1	1:A:628:PHE:C	2.92	0.47
1:A:783:THR:C	1:A:784:GLU:OE1	2.57	0.47
1:B:549:LEU:HG	1:B:550:SER:N	2.28	0.47
1:B:655:ASN:N	1:B:755:ARG:HD2	2.29	0.47
1:C:294:ASP:O	1:C:606:LYS:HG3	2.14	0.47
1:C:629:ASN:HD21	1:C:631:SER:CB	2.27	0.47
2:F:7:GLU:HA	2:F:10:ALA:HB3	1.96	0.47
1:A:777:TYR:O	1:A:780:LEU:HG	2.14	0.47
1:B:586:PHE:HA	1:B:639:ASN:ND2	2.28	0.47
1:B:659:THR:HA	1:B:661:ALA:HB3	1.95	0.47
1:B:780:LEU:HB3	1:B:782:PHE:HE1	1.78	0.47
1:A:639:ASN:H	1:A:639:ASN:ND2	1.96	0.47
1:A:768:LYS:HD2	1:A:797:ILE:O	2.14	0.47
1:C:346:LYS:CE	4:C:3999:EMA:O1A	2.62	0.47
1:B:794:GLN:NE2	1:B:797:ILE:HD13	2.29	0.47
1:C:415:GLU:C	1:C:417:GLY:N	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:ASN:C	1:C:438:ASN:ND2	2.65	0.47
2:E:83:GLU:O	2:E:87:GLU:HG3	2.14	0.47
1:C:306:GLY:O	1:C:336:THR:OG1	2.28	0.47
1:C:338:LEU:O	1:C:343:VAL:HG23	2.14	0.47
1:C:502:THR:O	1:C:505:LYS:HB3	2.14	0.47
1:C:540:ARG:NH2	2:F:87:GLU:OE1	2.48	0.47
2:E:5:THR:O	2:E:8:GLN:HB2	2.15	0.47
1:A:349:ASN:ND2	1:A:349:ASN:H	2.12	0.47
1:A:650:THR:O	1:A:651:LYS:C	2.57	0.47
1:B:387:ASN:OD1	1:B:477:MET:HE2	2.14	0.47
1:C:530:THR:O	1:C:534:ILE:HG13	2.14	0.47
1:C:761:GLN:HA	1:C:761:GLN:NE2	2.30	0.47
2:F:137:ASN:OD1	2:F:137:ASN:C	2.58	0.47
1:A:353:LYS:N	1:A:368:GLN:HE22	2.12	0.47
1:A:394:HIS:O	1:A:395:GLU:C	2.57	0.47
1:A:514:ASP:C	1:A:516:VAL:H	2.21	0.47
1:A:515:LYS:HG2	1:A:515:LYS:O	2.14	0.47
1:A:516:VAL:O	1:A:517:VAL:C	2.58	0.47
1:A:759:GLN:HE21	1:A:759:GLN:CA	2.27	0.47
1:B:349:ASN:ND2	1:B:349:ASN:H	2.13	0.47
2:E:120:GLU:O	2:E:123:GLU:HB2	2.14	0.47
1:B:360:VAL:HG21	1:B:365:PRO:HB3	1.95	0.47
2:E:8:GLN:HA	2:E:8:GLN:NE2	2.30	0.47
1:B:655:ASN:HA	1:B:759:GLN:NE2	2.30	0.47
1:B:660:SER:N	1:B:662:GLU:H	2.11	0.47
1:B:794:GLN:HE21	1:B:797:ILE:HD13	1.78	0.47
1:C:636:ALA:O	1:C:640:LYS:HA	2.14	0.47
2:D:49:GLN:HA	2:D:52:ILE:HG22	1.97	0.47
2:D:86:ARG:HA	2:D:138:TYR:HE1	1.79	0.47
1:A:670:ILE:O	1:A:670:ILE:HG23	2.15	0.47
1:C:633:ASN:ND2	1:C:645:TRP:H	1.94	0.47
1:C:714:GLN:HE22	1:C:717:LYS:NZ	2.13	0.47
1:A:364:ILE:HB	1:A:477:MET:HB2	1.98	0.46
1:B:587:PRO:HD2	1:B:639:ASN:HD21	1.79	0.46
1:C:695:LYS:NZ	2:F:18:LEU:HD13	2.30	0.46
1:C:768:LYS:HD2	1:C:797:ILE:O	2.15	0.46
2:E:49:GLN:HA	2:E:52:ILE:HG22	1.97	0.46
2:F:65:PHE:N	2:F:65:PHE:CD1	2.83	0.46
1:A:298:GLY:O	1:A:299:GLU:C	2.58	0.46
1:B:647:ASP:O	1:B:648:PRO:C	2.58	0.46
1:C:323:ASN:HD22	1:C:598:PRO:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:PHE:HB3	1:C:472:ARG:HH21	1.79	0.46
1:C:694:VAL:HG23	1:C:695:LYS:H	1.80	0.46
1:C:777:TYR:O	1:C:780:LEU:HG	2.15	0.46
1:A:463:THR:HG22	1:A:464:VAL:N	2.30	0.46
1:B:663:PHE:CB	2:E:14:GLU:HG3	2.45	0.46
1:C:730:ASN:C	1:C:732:ILE:N	2.73	0.46
1:C:740:GLN:H	1:C:740:GLN:CD	2.23	0.46
1:C:740:GLN:CD	1:C:740:GLN:N	2.74	0.46
2:F:49:GLN:HA	2:F:52:ILE:HG22	1.97	0.46
1:B:324:THR:OG1	1:B:499:PRO:HA	2.16	0.46
1:B:712:PHE:HB3	1:B:716:LYS:HD3	1.98	0.46
1:C:340:LYS:C	1:C:342:GLY:H	2.23	0.46
1:C:470:ASN:CG	1:C:471:TRP:H	2.24	0.46
2:F:65:PHE:HB2	2:F:66:PRO:CD	2.42	0.46
1:A:340:LYS:C	1:A:342:GLY:H	2.23	0.46
1:B:415:GLU:C	1:B:417:GLY:N	2.72	0.46
1:B:720:ILE:HB	1:B:724:ARG:HE	1.81	0.46
1:C:322:LEU:O	1:C:323:ASN:C	2.59	0.46
1:C:629:ASN:ND2	1:C:631:SER:CB	2.75	0.46
2:D:97:ASN:HD21	2:D:99:TYR:HB2	1.80	0.46
2:E:65:PHE:HB2	2:E:66:PRO:CD	2.42	0.46
2:F:8:GLN:HA	2:F:8:GLN:NE2	2.31	0.46
2:F:120:GLU:O	2:F:123:GLU:HB2	2.16	0.46
1:A:338:LEU:O	1:A:343:VAL:HG23	2.16	0.46
1:A:346:LYS:NZ	1:A:352:GLY:O	2.49	0.46
1:A:700:TYR:O	1:A:703:ASP:HB2	2.16	0.46
1:A:730:ASN:C	1:A:732:ILE:N	2.74	0.46
1:A:754:GLU:O	1:A:757:THR:HB	2.15	0.46
1:B:593:ILE:HG13	1:B:611:THR:HG21	1.98	0.46
1:B:628:PHE:CD1	1:B:628:PHE:C	2.93	0.46
1:C:665:LYS:HG2	2:F:11:GLU:CD	2.41	0.46
1:C:752:LEU:O	1:C:753:LYS:C	2.58	0.46
2:F:76:MET:HE3	2:F:79:THR:CG2	2.45	0.46
1:A:526:GLN:OE1	2:D:124:MET:HB3	2.15	0.46
1:A:723:PHE:HB2	1:A:793:PHE:CE2	2.50	0.46
1:B:629:ASN:ND2	1:B:631:SER:CB	2.75	0.46
1:B:654:ILE:C	1:B:655:ASN:ND2	2.74	0.46
1:C:657:ILE:HG12	1:C:756:ILE:HD13	1.96	0.46
1:A:639:ASN:OD1	1:A:641:ALA:HB2	2.15	0.46
1:A:657:ILE:HD11	1:A:704:TYR:CG	2.51	0.46
1:B:353:LYS:N	1:B:368:GLN:HE22	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LYS:HG3	1:B:425:GLU:N	2.30	0.46
1:B:608:TRP:CZ2	1:B:643:ILE:HG21	2.50	0.46
1:C:633:ASN:N	1:C:633:ASN:ND2	2.55	0.46
1:C:759:GLN:HE21	1:C:759:GLN:CA	2.28	0.46
2:D:65:PHE:CD1	2:D:65:PHE:N	2.84	0.46
1:C:639:ASN:OD1	1:C:641:ALA:HB2	2.16	0.46
2:D:8:GLN:HA	2:D:8:GLN:NE2	2.31	0.46
1:A:322:LEU:O	1:A:323:ASN:C	2.58	0.45
1:A:713:SER:O	1:A:714:GLN:C	2.58	0.45
1:B:784:GLU:HG2	1:B:788:ASP:OD2	2.16	0.45
2:E:65:PHE:N	2:E:65:PHE:CD1	2.83	0.45
1:A:718:ARG:HD2	1:A:767:GLN:OE1	2.15	0.45
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.29	0.45
1:C:631:SER:O	1:C:632:TYR:C	2.59	0.45
1:A:586:PHE:HA	1:A:639:ASN:ND2	2.30	0.45
1:B:322:LEU:O	1:B:323:ASN:C	2.60	0.45
1:C:450:ASN:OD1	1:C:452:GLU:HG3	2.16	0.45
1:C:514:ASP:O	1:C:516:VAL:N	2.49	0.45
1:C:615:ILE:O	1:C:620:THR:HG22	2.16	0.45
2:F:133:ASP:CG	2:F:135:GLN:HG3	2.41	0.45
1:B:537:GLY:C	1:B:625:LEU:HD21	2.40	0.45
1:C:450:ASN:CG	1:C:452:GLU:HG3	2.42	0.45
1:C:462:ILE:HG12	1:C:466:GLY:HA2	1.97	0.45
2:D:95:ASP:OD1	2:D:104:GLU:OE2	2.35	0.45
2:D:120:GLU:O	2:D:123:GLU:HB2	2.16	0.45
1:A:307:LEU:HD12	1:A:307:LEU:N	2.31	0.45
1:C:353:LYS:N	1:C:368:GLN:HE22	2.14	0.45
1:C:499:PRO:HD3	1:C:552:TRP:CH2	2.51	0.45
2:D:79:THR:O	2:D:81:SER:N	2.49	0.45
2:D:86:ARG:HA	2:D:138:TYR:CE1	2.51	0.45
2:E:76:MET:HE3	2:E:79:THR:CG2	2.45	0.45
2:F:117:THR:HG23	2:F:120:GLU:OE2	2.16	0.45
1:A:462:ILE:HG12	1:A:466:GLY:HA2	1.98	0.45
1:C:327:LEU:HG	1:C:595:ILE:HG23	1.99	0.45
1:C:713:SER:O	1:C:716:LYS:HB3	2.16	0.45
1:C:783:THR:O	1:C:784:GLU:OE1	2.35	0.45
2:E:137:ASN:OD1	2:E:137:ASN:C	2.59	0.45
1:A:549:LEU:HD12	1:A:549:LEU:N	2.30	0.45
1:A:633:ASN:HD22	1:A:633:ASN:H	1.64	0.45
1:A:657:ILE:HB	1:A:756:ILE:HD13	1.98	0.45
1:A:752:LEU:O	1:A:753:LYS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:TYR:HD1	1:A:780:LEU:HD21	1.76	0.45
1:B:513:TRP:CZ2	2:E:112:LEU:O	2.69	0.45
2:E:79:THR:C	2:E:81:SER:N	2.75	0.45
1:B:360:VAL:O	1:B:360:VAL:CG2	2.64	0.45
1:B:445:ARG:NH1	1:B:471:TRP:CD1	2.85	0.45
1:C:499:PRO:HG2	1:C:625:LEU:HB3	1.98	0.45
1:C:781:ASN:HD22	1:C:782:PHE:N	2.05	0.45
2:D:79:THR:C	2:D:81:SER:N	2.74	0.45
2:D:137:ASN:OD1	2:D:137:ASN:C	2.60	0.45
2:F:79:THR:O	2:F:81:SER:N	2.50	0.45
1:A:607:ASN:O	1:A:610:MET:N	2.50	0.45
1:B:316:LYS:HD3	1:B:600:GLY:O	2.17	0.45
1:B:538:ILE:N	1:B:538:ILE:CD1	2.80	0.45
1:B:656:THR:O	1:B:705:TYR:HE1	2.00	0.45
1:B:735:VAL:HG13	1:B:735:VAL:O	2.16	0.45
2:F:105:LEU:HD12	2:F:125:ILE:HD13	1.99	0.45
1:A:324:THR:OG1	1:A:499:PRO:HA	2.16	0.45
1:B:294:ASP:CG	1:B:294:ASP:O	2.60	0.45
1:B:509:PRO:HD3	1:B:536:TYR:CE1	2.49	0.45
1:C:657:ILE:HG23	1:C:658:PRO:HD2	1.98	0.45
2:E:133:ASP:CG	2:E:135:GLN:HG3	2.42	0.45
1:A:295:VAL:HG22	1:A:603:ILE:HG22	1.91	0.44
1:A:324:THR:HG21	1:A:556:MET:HE3	1.99	0.44
1:B:742:ALA:C	1:B:744:GLU:H	2.25	0.44
1:A:384:ASN:O	1:A:385:LEU:C	2.57	0.44
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.52	0.44
1:A:540:ARG:HD2	1:A:582:ASP:OD1	2.17	0.44
1:B:556:MET:HE3	1:B:556:MET:O	2.16	0.44
1:B:651:LYS:HB3	1:B:652:ALA:H	1.69	0.44
1:B:657:ILE:O	1:B:659:THR:N	2.51	0.44
2:F:79:THR:C	2:F:81:SER:N	2.75	0.44
1:A:670:ILE:HG23	1:A:745:TYR:CZ	2.53	0.44
1:A:700:TYR:CD1	1:A:727:GLN:HB3	2.52	0.44
1:C:540:ARG:CD	1:C:582:ASP:OD1	2.65	0.44
1:C:689:ALA:O	1:C:690:LYS:HB2	2.17	0.44
1:C:761:GLN:HA	1:C:761:GLN:HE21	1.81	0.44
2:E:89:PHE:CE1	2:E:100:ILE:HG13	2.53	0.44
1:A:360:VAL:HG21	1:A:365:PRO:HB3	1.99	0.44
1:A:630:ARG:HH21	2:D:87:GLU:CD	2.26	0.44
1:B:526:GLN:HG3	2:E:124:MET:CE	2.47	0.44
1:C:307:LEU:HD12	1:C:307:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:THR:O	2:E:81:SER:N	2.50	0.44
1:B:340:LYS:C	1:B:342:GLY:H	2.26	0.44
1:B:505:LYS:HA	1:B:508:ILE:HD11	2.00	0.44
1:C:445:ARG:HD3	1:C:454:GLN:HB2	1.99	0.44
1:C:450:ASN:O	1:C:451:ASN:HB2	2.18	0.44
1:A:317:LYS:HE2	1:A:317:LYS:HB2	1.88	0.44
1:A:432:TYR:CE1	1:A:471:TRP:HZ3	2.35	0.44
1:B:519:THR:C	1:B:521:ASN:H	2.26	0.44
1:B:717:LYS:O	1:B:720:ILE:HG12	2.18	0.44
1:C:628:PHE:CD1	1:C:628:PHE:O	2.71	0.44
1:A:345:THR:HB	1:A:491:ASP:HB3	1.99	0.44
1:A:348:LEU:O	1:A:351:HIS:CE1	2.71	0.44
1:B:447:SER:O	1:B:451:ASN:HA	2.18	0.44
1:B:607:ASN:O	1:B:610:MET:N	2.51	0.44
1:C:523:LEU:C	1:C:525:LYS:H	2.25	0.44
1:C:576:ASN:O	1:C:577:HIS:HB3	2.18	0.44
1:C:739:LYS:HG3	1:C:740:GLN:N	2.33	0.44
1:B:326:ILE:C	1:B:327:LEU:HD12	2.43	0.44
1:C:695:LYS:HZ2	2:F:18:LEU:HB3	1.82	0.44
1:C:789:ASN:N	1:C:789:ASN:ND2	2.63	0.44
2:F:86:ARG:HA	2:F:138:TYR:CE1	2.53	0.44
1:A:295:VAL:HG23	1:A:604:LEU:C	2.43	0.43
1:A:305:SER:HB3	1:A:594:PHE:CD1	2.53	0.43
1:A:447:SER:O	1:A:451:ASN:HA	2.18	0.43
1:C:326:ILE:C	1:C:327:LEU:HD12	2.43	0.43
1:C:424:LYS:HG3	1:C:425:GLU:N	2.32	0.43
1:C:618:ASN:N	1:C:618:ASN:ND2	2.54	0.43
1:C:672:ARG:NE	1:C:672:ARG:HA	2.33	0.43
1:C:690:LYS:HZ3	1:C:692:GLU:CA	2.09	0.43
1:C:751:TYR:O	1:C:752:LEU:C	2.60	0.43
1:C:786:GLU:HA	1:C:786:GLU:OE1	2.18	0.43
2:F:117:THR:C	2:F:119:GLU:N	2.76	0.43
1:B:717:LYS:HA	1:B:720:ILE:CG1	2.45	0.43
1:C:320:ARG:HA	1:C:598:PRO:O	2.17	0.43
1:C:463:THR:HG22	1:C:464:VAL:N	2.32	0.43
1:C:550:SER:H	1:C:553:GLN:NE2	2.16	0.43
1:C:695:LYS:HG3	2:F:18:LEU:HD22	2.00	0.43
2:E:95:ASP:OD1	2:E:104:GLU:OE2	2.36	0.43
1:B:296:LEU:HD21	1:B:606:LYS:CE	2.49	0.43
1:C:322:LEU:HD23	1:C:503:GLU:CD	2.44	0.43
1:C:324:THR:OG1	1:C:499:PRO:CA	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:THR:HG21	2:F:145:MET:SD	2.58	0.43
1:A:631:SER:O	1:A:632:TYR:C	2.60	0.43
1:B:657:ILE:HG13	1:B:658:PRO:N	2.33	0.43
1:C:384:ASN:O	1:C:385:LEU:C	2.60	0.43
1:C:394:HIS:O	1:C:395:GLU:C	2.61	0.43
2:E:86:ARG:HA	2:E:138:TYR:CE1	2.52	0.43
1:A:663:PHE:CE1	1:A:752:LEU:HD11	2.53	0.43
1:C:415:GLU:O	1:C:417:GLY:N	2.51	0.43
2:D:133:ASP:CG	2:D:135:GLN:HG3	2.42	0.43
2:E:80:ASP:C	2:E:82:GLU:H	2.27	0.43
2:E:105:LEU:HD12	2:E:125:ILE:HD13	1.99	0.43
1:A:450:ASN:O	1:A:451:ASN:HB2	2.19	0.43
1:B:712:PHE:HB3	1:B:716:LYS:HB3	1.99	0.43
1:B:796:ILE:O	1:B:796:ILE:HG22	2.18	0.43
1:C:639:ASN:H	1:C:639:ASN:ND2	1.90	0.43
1:C:660:SER:O	1:C:663:PHE:HB3	2.18	0.43
1:A:445:ARG:NH2	1:A:471:TRP:NE1	2.66	0.43
1:A:653:LYS:O	1:A:755:ARG:HD2	2.19	0.43
1:B:437:SER:C	1:B:439:ASN:N	2.77	0.43
1:C:792:VAL:CG1	1:C:796:ILE:HD11	2.42	0.43
1:A:509:PRO:HG2	1:A:512:GLU:OE1	2.19	0.43
1:B:327:LEU:O	1:B:495:PHE:N	2.49	0.43
1:B:794:GLN:O	1:B:797:ILE:HG23	2.19	0.43
2:E:86:ARG:HA	2:E:138:TYR:HE1	1.84	0.43
1:A:661:ALA:O	1:A:662:GLU:C	2.61	0.43
1:A:714:GLN:HE22	1:A:717:LYS:NZ	2.17	0.43
1:A:759:GLN:NE2	1:A:759:GLN:CA	2.82	0.43
1:A:787:THR:O	1:A:787:THR:CG2	2.55	0.43
1:B:317:LYS:HE2	1:B:317:LYS:HB2	1.88	0.43
1:B:415:GLU:O	1:B:417:GLY:N	2.52	0.43
1:C:293:ILE:HD12	1:C:293:ILE:N	2.34	0.43
1:C:298:GLY:O	1:C:299:GLU:C	2.61	0.43
1:A:294:ASP:O	1:A:610:MET:CE	2.66	0.43
1:B:654:ILE:O	1:B:654:ILE:HG13	2.19	0.43
2:D:65:PHE:HB2	2:D:66:PRO:CD	2.42	0.43
2:E:87:GLU:O	2:E:91:VAL:HG23	2.19	0.43
1:A:636:ALA:HA	1:A:637:PRO:HD3	1.89	0.42
1:B:463:THR:HB	1:B:467:GLU:H	1.83	0.42
1:B:552:TRP:CD1	1:B:552:TRP:C	2.94	0.42
1:B:714:GLN:HA	1:B:717:LYS:CE	2.49	0.42
1:C:608:TRP:O	1:C:609:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ILE:CG2	1:A:756:ILE:HD13	2.49	0.42
1:B:752:LEU:O	1:B:755:ARG:HB2	2.19	0.42
1:B:761:GLN:O	1:B:765:THR:HG23	2.19	0.42
1:C:712:PHE:HB3	1:C:716:LYS:HG2	2.01	0.42
2:D:95:ASP:OD2	2:D:97:ASN:HB3	2.19	0.42
2:E:117:THR:C	2:E:119:GLU:N	2.75	0.42
1:A:751:TYR:O	1:A:752:LEU:C	2.60	0.42
1:B:597:ASN:C	1:B:599:GLU:H	2.28	0.42
1:C:329:ARG:HH11	1:C:590:ASP:CG	2.24	0.42
1:C:505:LYS:HE3	1:C:513:TRP:CE2	2.54	0.42
1:A:360:VAL:O	1:A:360:VAL:CG2	2.65	0.42
1:A:628:PHE:CD1	1:A:628:PHE:O	2.72	0.42
1:A:644:GLU:OE2	1:B:400:LYS:NZ	2.53	0.42
1:A:776:LEU:HD12	1:A:776:LEU:N	2.35	0.42
1:B:450:ASN:O	1:B:451:ASN:HB2	2.18	0.42
1:B:529:VAL:O	1:B:530:THR:C	2.63	0.42
1:B:731:GLU:H	1:B:731:GLU:HG2	1.35	0.42
1:C:710:HIS:O	1:C:710:HIS:CG	2.73	0.42
1:C:776:LEU:N	1:C:776:LEU:HD12	2.35	0.42
2:E:64:ASP:OD1	2:E:67:GLU:HG3	2.19	0.42
2:E:97:ASN:ND2	2:E:99:TYR:HB2	2.34	0.42
2:E:145:MET:HE2	2:E:145:MET:HB2	1.85	0.42
1:A:295:VAL:HG23	1:A:604:LEU:O	2.20	0.42
1:A:346:LYS:HE3	4:A:1999:EMA:O2G	2.18	0.42
1:A:355:SER:HB2	1:A:371:SER:HA	2.01	0.42
1:A:526:GLN:O	1:A:529:VAL:HG12	2.19	0.42
1:B:406:ASP:OD2	1:B:407:HIS:N	2.51	0.42
1:B:615:ILE:O	1:B:620:THR:HG22	2.20	0.42
1:B:629:ASN:HB3	1:B:632:TYR:CE2	2.54	0.42
1:B:657:ILE:HD12	1:B:658:PRO:HD3	1.99	0.42
1:C:629:ASN:HB3	1:C:632:TYR:CD2	2.55	0.42
1:C:661:ALA:O	1:C:663:PHE:N	2.38	0.42
1:C:775:LEU:HD12	1:C:776:LEU:CD1	2.50	0.42
2:D:64:ASP:OD1	2:D:67:GLU:HG3	2.20	0.42
1:A:326:ILE:C	1:A:327:LEU:HD12	2.45	0.42
1:A:370:LEU:HD11	1:A:455:TYR:CE1	2.55	0.42
1:A:648:PRO:O	1:A:651:LYS:HB2	2.19	0.42
1:A:710:HIS:O	1:A:710:HIS:CG	2.73	0.42
1:B:742:ALA:C	1:B:744:GLU:N	2.77	0.42
1:C:670:ILE:CD1	1:C:745:TYR:HA	2.50	0.42
2:F:64:ASP:OD1	2:F:67:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:O	1:B:315:PHE:HB2	2.19	0.42
1:B:370:LEU:HD23	1:B:370:LEU:HA	1.87	0.42
1:B:394:HIS:O	1:B:395:GLU:C	2.62	0.42
1:B:731:GLU:HG2	1:B:733:GLU:HB2	2.02	0.42
2:F:7:GLU:O	2:F:11:GLU:HG3	2.19	0.42
1:A:323:ASN:ND2	1:A:598:PRO:CB	2.82	0.42
1:B:611:THR:O	1:B:615:ILE:HG13	2.19	0.42
1:B:720:ILE:CG1	1:B:721:SER:N	2.79	0.42
1:C:332:ASN:O	1:C:335:ALA:HB3	2.19	0.42
1:C:349:ASN:H	1:C:349:ASN:HD22	1.68	0.42
1:A:323:ASN:ND2	1:A:598:PRO:HB2	2.30	0.42
1:A:713:SER:O	1:A:716:LYS:HB3	2.19	0.42
1:B:346:LYS:NZ	4:B:2999:EMA:O1A	2.52	0.42
1:B:636:ALA:O	1:B:640:LYS:HA	2.20	0.42
1:B:653:LYS:O	1:B:755:ARG:HD3	2.20	0.42
1:B:790:PHE:C	1:B:790:PHE:CD2	2.97	0.42
1:B:338:LEU:O	1:B:339:ILE:C	2.62	0.42
1:C:691:LYS:O	1:C:694:VAL:HG13	2.20	0.42
2:F:14:GLU:OE1	2:F:14:GLU:HA	2.20	0.42
2:F:86:ARG:HA	2:F:138:TYR:HE1	1.84	0.42
1:A:387:ASN:OD1	1:A:477:MET:HE2	2.20	0.41
1:A:513:TRP:CE3	1:A:517:VAL:HG21	2.55	0.41
1:A:629:ASN:HB3	1:A:632:TYR:CD2	2.55	0.41
1:A:792:VAL:CG1	1:A:796:ILE:HD11	2.42	0.41
1:B:514:ASP:C	1:B:516:VAL:N	2.78	0.41
1:C:670:ILE:HG23	1:C:745:TYR:CE1	2.55	0.41
1:C:736:LEU:HD21	1:C:749:PHE:HB2	2.02	0.41
2:E:7:GLU:O	2:E:11:GLU:HG3	2.20	0.41
2:E:108:VAL:O	2:E:112:LEU:HG	2.20	0.41
2:F:108:VAL:O	2:F:112:LEU:HG	2.19	0.41
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.78	0.41
1:A:636:ALA:O	1:A:640:LYS:HA	2.20	0.41
1:A:665:LYS:HG2	2:D:11:GLU:CD	2.45	0.41
1:B:485:LEU:HD12	1:B:485:LEU:HA	1.90	0.41
1:B:580:GLU:OE1	1:B:587:PRO:HA	2.20	0.41
1:C:346:LYS:NZ	4:C:3999:EMA:PG	2.93	0.41
1:C:592:GLU:HG2	1:C:604:LEU:HD21	2.02	0.41
1:C:663:PHE:CE2	1:C:667:LEU:HD11	2.56	0.41
2:E:5:THR:CG2	2:E:8:GLN:HB2	2.50	0.41
2:F:5:THR:O	2:F:9:ILE:HG13	2.20	0.41
1:A:331:VAL:O	1:A:332:ASN:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:NH1	1:A:627:TYR:CE1	2.88	0.41
1:B:376:GLN:O	1:B:377:GLN:C	2.63	0.41
1:B:385:LEU:HD13	1:B:385:LEU:O	2.20	0.41
1:B:445:ARG:CZ	1:B:471:TRP:CD1	3.03	0.41
1:B:608:TRP:CZ2	1:B:643:ILE:CG2	3.03	0.41
1:C:355:SER:HB2	1:C:371:SER:HA	2.03	0.41
1:C:581:GLN:O	1:C:629:ASN:HA	2.20	0.41
1:C:695:LYS:CG	2:F:18:LEU:HD22	2.50	0.41
1:A:505:LYS:HE3	1:A:513:TRP:CD2	2.55	0.41
1:B:726:ILE:C	1:B:729:TYR:H	2.28	0.41
1:C:388:LYS:O	1:C:392:THR:HG23	2.19	0.41
1:C:505:LYS:HE3	1:C:513:TRP:CD2	2.55	0.41
1:C:658:PRO:HB3	1:C:755:ARG:NH2	2.34	0.41
1:C:759:GLN:NE2	1:C:759:GLN:CA	2.83	0.41
2:D:105:LEU:HD12	2:D:125:ILE:HD13	2.02	0.41
1:A:664:ILE:O	1:A:667:LEU:N	2.43	0.41
1:B:394:HIS:O	1:B:397:GLU:CB	2.69	0.41
1:C:308:VAL:O	1:C:311:HIS:HB2	2.21	0.41
1:C:437:SER:C	1:C:439:ASN:N	2.77	0.41
1:C:734:ASN:OD1	1:C:734:ASN:C	2.63	0.41
2:F:80:ASP:C	2:F:82:GLU:H	2.28	0.41
1:A:450:ASN:CG	1:A:452:GLU:HG3	2.45	0.41
1:A:628:PHE:O	1:A:629:ASN:C	2.64	0.41
1:A:699:GLY:O	1:A:702:SER:N	2.52	0.41
1:B:745:TYR:O	1:B:748:TYR:HB3	2.20	0.41
1:C:406:ASP:OD2	1:C:407:HIS:N	2.53	0.41
1:C:510:GLN:O	1:C:510:GLN:HG3	2.20	0.41
1:C:569:TYR:CE2	1:C:572:GLY:O	2.73	0.41
2:D:108:VAL:O	2:D:112:LEU:HG	2.20	0.41
2:E:105:LEU:O	2:E:109:MET:HG2	2.21	0.41
1:A:368:GLN:HG3	1:A:383:GLY:C	2.46	0.41
1:A:406:ASP:OD2	1:A:407:HIS:N	2.54	0.41
1:A:629:ASN:HD21	1:A:631:SER:CB	2.33	0.41
1:A:658:PRO:HB3	1:A:755:ARG:NH2	2.35	0.41
1:A:713:SER:O	1:A:716:LYS:N	2.53	0.41
1:A:736:LEU:HD21	1:A:749:PHE:HB2	2.01	0.41
1:A:775:LEU:HD12	1:A:776:LEU:CD1	2.50	0.41
1:A:789:ASN:N	1:A:789:ASN:ND2	2.63	0.41
1:C:370:LEU:HD11	1:C:455:TYR:CE1	2.56	0.41
1:C:391:ILE:HD13	1:C:399:GLY:HA2	2.02	0.41
1:C:398:ILE:HG22	1:C:399:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:GLU:O	1:C:638:GLY:HA3	2.21	0.41
1:C:608:TRP:CZ2	1:C:643:ILE:HG21	2.55	0.41
1:A:454:GLN:OE1	1:A:471:TRP:CE3	2.73	0.41
1:A:663:PHE:HE1	1:A:752:LEU:HD11	1.85	0.41
2:E:72:MET:C	2:E:74:ARG:H	2.29	0.41
2:F:83:GLU:O	2:F:87:GLU:HG3	2.21	0.41
1:A:349:ASN:H	1:A:349:ASN:HD22	1.69	0.41
1:A:437:SER:C	1:A:439:ASN:N	2.79	0.41
1:A:581:GLN:O	1:A:629:ASN:HA	2.21	0.41
1:B:597:ASN:C	1:B:599:GLU:N	2.78	0.41
1:B:639:ASN:OD1	1:B:641:ALA:HB2	2.21	0.41
1:C:364:ILE:HB	1:C:477:MET:HB2	2.02	0.41
1:C:456:LYS:HD3	1:C:471:TRP:CE2	2.56	0.41
1:C:543:ASP:CG	1:C:544:SER:N	2.79	0.41
1:C:587:PRO:HD2	1:C:639:ASN:HD21	1.86	0.41
1:C:713:SER:O	1:C:714:GLN:C	2.63	0.41
1:C:793:PHE:O	1:C:794:GLN:C	2.64	0.41
1:A:391:ILE:HD13	1:A:399:GLY:HA2	2.03	0.41
1:B:459:GLU:C	1:B:461:LYS:N	2.79	0.41
1:B:524:GLU:HB2	1:B:527:LYS:HG2	2.02	0.41
1:B:733:GLU:O	1:B:735:VAL:N	2.53	0.41
1:C:459:GLU:C	1:C:461:LYS:N	2.79	0.41
1:C:534:ILE:HG22	1:C:535:LYS:N	2.35	0.41
1:C:783:THR:HB	1:C:784:GLU:OE1	2.20	0.41
2:D:7:GLU:O	2:D:8:GLN:C	2.64	0.41
2:E:102:ALA:HB2	2:E:125:ILE:HG13	2.03	0.41
2:F:39:LEU:HG	2:F:39:LEU:O	2.21	0.41
2:F:144:MET:SD	2:F:144:MET:C	3.04	0.41
1:B:391:ILE:HD13	1:B:399:GLY:HA2	2.03	0.40
1:B:792:VAL:O	1:B:796:ILE:HG12	2.20	0.40
1:C:797:ILE:HD12	1:C:798:ASP:CG	2.47	0.40
2:F:29:THR:O	2:F:29:THR:HG22	2.21	0.40
1:A:459:GLU:C	1:A:461:LYS:N	2.79	0.40
1:A:509:PRO:HG2	1:A:512:GLU:HB3	2.04	0.40
1:A:608:TRP:CZ2	1:A:643:ILE:HG21	2.56	0.40
1:B:502:THR:OG1	1:B:503:GLU:N	2.54	0.40
1:B:628:PHE:CD1	1:B:628:PHE:O	2.74	0.40
1:B:659:THR:O	1:B:660:SER:CB	2.63	0.40
1:C:315:PHE:O	1:C:316:LYS:C	2.65	0.40
1:C:368:GLN:HG3	1:C:383:GLY:C	2.46	0.40
2:D:14:GLU:OE1	2:D:14:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:MET:C	2:D:74:ARG:H	2.29	0.40
1:A:400:LYS:NZ	1:C:644:GLU:OE2	2.53	0.40
1:A:415:GLU:O	1:A:417:GLY:N	2.54	0.40
1:A:668:SER:O	1:A:671:ARG:HB3	2.21	0.40
1:A:773:PHE:N	1:A:775:LEU:CD2	2.84	0.40
1:A:797:ILE:HD12	1:A:798:ASP:CG	2.47	0.40
1:B:791:GLU:HG3	1:B:792:VAL:N	2.36	0.40
1:C:597:ASN:C	1:C:599:GLU:N	2.79	0.40
2:F:137:ASN:OD1	2:F:139:GLU:N	2.55	0.40
1:A:346:LYS:HE2	1:A:364:ILE:HD12	2.03	0.40
1:A:652:ALA:O	1:A:653:LYS:C	2.65	0.40
1:A:695:LYS:N	2:D:18:LEU:HD21	2.36	0.40
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.56	0.40
1:C:376:GLN:O	1:C:377:GLN:C	2.64	0.40
1:C:387:ASN:CG	1:C:477:MET:HE2	2.47	0.40
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.80	0.40
1:C:699:GLY:O	1:C:702:SER:N	2.54	0.40
2:F:105:LEU:O	2:F:109:MET:HG2	2.21	0.40
2:F:129:ASP:OD1	2:F:129:ASP:C	2.64	0.40
1:A:428:ASN:C	1:A:430:LYS:N	2.72	0.40
1:A:774:LYS:O	1:A:775:LEU:C	2.64	0.40
1:B:562:GLU:HA	1:B:565:LYS:HG3	2.03	0.40
1:B:592:GLU:HG2	1:B:604:LEU:HD21	2.03	0.40
1:B:654:ILE:HA	1:B:755:ARG:CD	2.48	0.40
1:B:706:ASN:O	1:B:707:SER:C	2.65	0.40
1:B:761:GLN:O	1:B:764:LEU:HB2	2.22	0.40
1:C:406:ASP:OD2	1:C:406:ASP:C	2.64	0.40
1:C:520:PRO:O	1:C:521:ASN:C	2.64	0.40
1:C:549:LEU:HB3	1:C:578:GLY:HA2	2.03	0.40
1:C:773:PHE:N	1:C:775:LEU:CD2	2.84	0.40
2:D:5:THR:N	2:D:8:GLN:HG3	2.37	0.40

There are no symmetry-related clashes.

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	478/507 (94%)	399 (84%)	69 (14%)	10 (2%)	5	26
1	B	462/507 (91%)	372 (80%)	69 (15%)	21 (4%)	2	13
1	C	499/507 (98%)	416 (83%)	68 (14%)	15 (3%)	3	20
2	D	141/147 (96%)	112 (79%)	26 (18%)	3 (2%)	5	26
2	E	141/147 (96%)	113 (80%)	25 (18%)	3 (2%)	5	26
2	F	141/147 (96%)	112 (79%)	26 (18%)	3 (2%)	5	26
All	All	1862/1962 (95%)	1524 (82%)	283 (15%)	55 (3%)	3	20

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLU
1	A	429	GLY
1	B	299	GLU
1	B	429	GLY
1	B	515	LYS
1	C	299	GLU
1	C	578	GLY
1	A	578	GLY
1	A	669	SER
1	A	787	THR
1	B	571	GLY
1	B	651	LYS
1	B	774	LYS
1	C	429	GLY
1	C	520	PRO
1	C	521	ASN
2	D	80	ASP
2	E	80	ASP
2	F	80	ASP
1	B	563	ALA
1	B	658	PRO
1	B	735	VAL
1	B	760	VAL
1	C	515	LYS
1	C	651	LYS
1	C	663	PHE
1	C	785	ASN

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Mol	Chain	Res	Type
2	E	93	ASP
1	B	734	ASN
1	C	368	GLN
2	D	20	ASP
2	D	93	ASP
2	E	20	ASP
2	F	20	ASP
2	F	93	ASP
1	A	395	GLU
1	B	368	GLN
1	B	694	VAL
1	B	708	ALA
1	B	759	GLN
1	C	690	LYS
1	A	368	GLN
1	A	534	ILE
1	B	395	GLU
1	B	416	ASN
1	B	460	GLY
1	C	416	ASN
1	B	516	VAL
1	C	298	GLY
1	C	460	GLY
1	A	460	GLY
1	A	298	GLY
1	B	298	GLY
1	C	534	ILE
1	B	792	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	432/452 (96%)	386 (89%)	46 (11%)	6	24
1	B	414/452 (92%)	367 (89%)	47 (11%)	5	21
1	C	448/452 (99%)	407 (91%)	41 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	121/125 (97%)	118 (98%)	3 (2%)	42	64
2	E	121/125 (97%)	118 (98%)	3 (2%)	42	64
2	F	121/125 (97%)	118 (98%)	3 (2%)	42	64
All	All	1657/1731 (96%)	1514 (91%)	143 (9%)	10	33

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	VAL
1	A	302	LEU
1	A	303	LYS
1	A	309	PRO
1	A	318	ILE
1	A	334	LEU
1	A	346	LYS
1	A	373	LYS
1	A	385	LEU
1	A	388	LYS
1	A	400	LYS
1	A	406	ASP
1	A	419	ILE
1	A	424	LYS
1	A	434	LEU
1	A	438	ASN
1	A	447	SER
1	A	455	TYR
1	A	459	GLU
1	A	462	ILE
1	A	476	VAL
1	A	485	LEU
1	A	499	PRO
1	A	511	LYS
1	A	524	GLU
1	A	532	LEU
1	A	549	LEU
1	A	589	LYS
1	A	599	GLU
1	A	603	ILE
1	A	618	ASN
1	A	622	LYS
1	A	623	ASP

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Mol	Chain	Res	Type
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	646	THR
1	A	657	ILE
1	A	659	THR
1	A	670	ILE
1	A	693	SER
1	A	694	VAL
1	A	707	SER
1	A	775	LEU
1	A	784	GLU
1	A	789	ASN
1	B	295	VAL
1	B	299	GLU
1	B	303	LYS
1	B	317	LYS
1	B	318	ILE
1	B	320	ARG
1	B	334	LEU
1	B	373	LYS
1	B	385	LEU
1	B	388	LYS
1	B	400	LYS
1	B	406	ASP
1	B	419	ILE
1	B	424	LYS
1	B	434	LEU
1	B	438	ASN
1	B	447	SER
1	B	455	TYR
1	B	459	GLU
1	B	462	ILE
1	B	476	VAL
1	B	485	LEU
1	B	501	LEU
1	B	508	ILE
1	B	521	ASN
1	B	536	TYR
1	B	545	THR
1	B	546	LYS
1	B	552	TRP

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Mol	Chain	Res	Type
1	B	567	THR
1	B	574	VAL
1	B	589	LYS
1	B	599	GLU
1	B	603	ILE
1	B	613	ARG
1	B	618	ASN
1	B	622	LYS
1	B	623	ASP
1	B	629	ASN
1	B	633	ASN
1	B	639	ASN
1	B	646	THR
1	B	714	GLN
1	B	732	ILE
1	B	739	LYS
1	B	744	GLU
1	B	784	GLU
1	C	295	VAL
1	C	303	LYS
1	C	309	PRO
1	C	318	ILE
1	C	320	ARG
1	C	334	LEU
1	C	373	LYS
1	C	385	LEU
1	C	388	LYS
1	C	400	LYS
1	C	406	ASP
1	C	419	ILE
1	C	424	LYS
1	C	434	LEU
1	C	438	ASN
1	C	445	ARG
1	C	447	SER
1	C	455	TYR
1	C	459	GLU
1	C	462	ILE
1	C	476	VAL
1	C	485	LEU
1	C	499	PRO
1	C	507	GLN

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Mol	Chain	Res	Type
1	C	531	ASN
1	C	549	LEU
1	C	589	LYS
1	C	599	GLU
1	C	603	ILE
1	C	613	ARG
1	C	618	ASN
1	C	622	LYS
1	C	623	ASP
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	646	THR
1	C	707	SER
1	C	775	LEU
1	C	784	GLU
1	C	789	ASN
2	D	75	LYS
2	D	110	THR
2	D	135	GLN
2	E	75	LYS
2	E	110	THR
2	E	135	GLN
2	F	75	LYS
2	F	110	THR
2	F	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	351	HIS
1	A	368	GLN
1	A	438	ASN
1	A	454	GLN
1	A	507	GLN
1	A	510	GLN
1	A	518	ASN
1	A	521	ASN
1	A	531	ASN
1	A	553	GLN
1	A	581	GLN

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Mol	Chain	Res	Type
1	A	607	ASN
1	A	618	ASN
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	666	ASN
1	A	714	GLN
1	A	727	GLN
1	A	740	GLN
1	A	759	GLN
1	A	781	ASN
1	A	789	ASN
1	A	794	GLN
1	B	323	ASN
1	B	351	HIS
1	B	368	GLN
1	B	376	GLN
1	B	377	GLN
1	B	407	HIS
1	B	438	ASN
1	B	507	GLN
1	B	521	ASN
1	B	531	ASN
1	B	551	ASN
1	B	553	GLN
1	B	577	HIS
1	B	581	GLN
1	B	583	ASN
1	B	607	ASN
1	B	618	ASN
1	B	629	ASN
1	B	633	ASN
1	B	639	ASN
1	B	655	ASN
1	B	730	ASN
1	B	747	ASN
1	B	758	ASN
1	B	759	GLN
1	B	761	GLN
1	B	789	ASN
1	B	794	GLN
1	C	323	ASN

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Mol	Chain	Res	Type
1	C	351	HIS
1	C	368	GLN
1	C	377	GLN
1	C	407	HIS
1	C	438	ASN
1	C	518	ASN
1	C	553	GLN
1	C	581	GLN
1	C	607	ASN
1	C	618	ASN
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	655	ASN
1	C	714	GLN
1	C	727	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	42	ASN
2	E	8	GLN
2	F	8	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

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	EMA	A	1999	3	26,27,27	2.54	6 (23%)	35,41,41	1.57	8 (22%)
4	EMA	B	2999	3	26,27,27	2.75	9 (34%)	35,41,41	1.51	6 (17%)
4	EMA	C	3999	3	26,27,27	3.07	12 (46%)	35,41,41	2.28	11 (31%)

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	EMA	A	1999	3	-	3/17/20/20	0/2/2/2
4	EMA	B	2999	3	-	4/17/20/20	0/2/2/2
4	EMA	C	3999	3	-	4/17/20/20	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3999	EMA	PA-C5'	-7.91	1.60	1.80
4	A	1999	EMA	PA-C5'	-7.89	1.61	1.80
4	B	2999	EMA	PB-O3B	7.65	1.67	1.59
4	B	2999	EMA	PA-C5'	-7.23	1.62	1.80
4	A	1999	EMA	PB-O3B	6.97	1.67	1.59
4	C	3999	EMA	C1'-N9	5.08	1.57	1.47
4	C	3999	EMA	O5'-C5'	5.04	1.49	1.42
4	B	2999	EMA	O5'-C5'	4.96	1.49	1.42
4	C	3999	EMA	C8-N9	4.66	1.44	1.36
4	C	3999	EMA	PB-O3B	4.52	1.64	1.59
4	C	3999	EMA	C4-N3	4.12	1.42	1.34
4	C	3999	EMA	C1'-C4'	3.39	1.61	1.50
4	B	2999	EMA	C1'-N9	3.19	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3999	EMA	C8-N7	3.11	1.37	1.31
4	C	3999	EMA	PA-O2A	-3.00	1.49	1.56
4	A	1999	EMA	PB-O3A	-2.95	1.56	1.59
4	A	1999	EMA	PA-O2A	-2.88	1.49	1.56
4	B	2999	EMA	C4-N3	2.86	1.39	1.34
4	C	3999	EMA	O5'-C4'	2.66	1.53	1.42
4	B	2999	EMA	PB-O3A	-2.37	1.56	1.59
4	B	2999	EMA	C1'-C4'	2.30	1.57	1.50
4	C	3999	EMA	C4-N9	-2.29	1.34	1.37
4	B	2999	EMA	PA-O2A	-2.28	1.50	1.56
4	C	3999	EMA	PG-O1G	-2.17	1.46	1.54
4	A	1999	EMA	PG-O1G	-2.11	1.47	1.54
4	A	1999	EMA	O5'-C5'	2.11	1.45	1.42
4	B	2999	EMA	PG-O1G	-2.02	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3999	EMA	C1'-N9-C8	5.60	138.69	127.05
4	C	3999	EMA	C1'-N9-C4	-5.34	117.91	126.63
4	C	3999	EMA	C5-C4-N9	4.66	110.75	105.98
4	C	3999	EMA	C4'-C1'-N9	4.62	128.28	112.30
4	B	2999	EMA	C4'-C1'-N9	3.87	125.69	112.30
4	C	3999	EMA	N9-C8-N7	-3.83	110.62	114.16
4	C	3999	EMA	C4-N9-C8	-3.31	103.36	105.75
4	A	1999	EMA	C5'-O5'-C4'	-3.31	104.82	112.90
4	A	1999	EMA	C4'-C1'-N9	3.24	123.52	112.30
4	C	3999	EMA	N3-C4-N9	-3.04	123.11	126.87
4	B	2999	EMA	O5'-C4'-C1'	3.02	119.78	109.46
4	A	1999	EMA	O5'-C4'-C1'	2.98	119.65	109.46
4	C	3999	EMA	O2A-PA-O1A	2.78	119.01	109.95
4	B	2999	EMA	C1'-N9-C8	2.59	132.43	127.05
4	A	1999	EMA	O2A-PA-O1A	2.43	117.86	109.95
4	C	3999	EMA	O1A-PA-C5'	-2.37	104.66	112.86
4	C	3999	EMA	O3B-PG-O2G	-2.26	99.16	111.04
4	B	2999	EMA	C4-N9-C8	-2.22	104.15	105.75
4	A	1999	EMA	O3B-PG-O2G	-2.22	99.36	111.04
4	A	1999	EMA	C4-C5-N7	2.20	113.09	110.58
4	A	1999	EMA	N6-C6-N1	2.19	123.25	118.38
4	B	2999	EMA	O2A-PA-O1A	2.17	117.01	109.95
4	C	3999	EMA	O2B-PB-O3A	2.15	113.08	107.27
4	B	2999	EMA	O3B-PG-O2G	-2.15	99.75	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1999	EMA	O1A-PA-C5'	-2.02	105.87	112.86

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1999	EMA	PA-C5'-O5'-C4'
4	B	2999	EMA	PA-C5'-O5'-C4'
4	C	3999	EMA	PA-C5'-O5'-C4'
4	A	1999	EMA	N9-C1'-C4'-O5'
4	B	2999	EMA	N9-C1'-C4'-O5'
4	C	3999	EMA	N9-C1'-C4'-O5'
4	C	3999	EMA	C4'-C1'-N9-C4
4	C	3999	EMA	C4'-C1'-N9-C8
4	A	1999	EMA	C4'-C1'-N9-C4
4	B	2999	EMA	C4'-C1'-N9-C8
4	B	2999	EMA	C4'-C1'-N9-C4

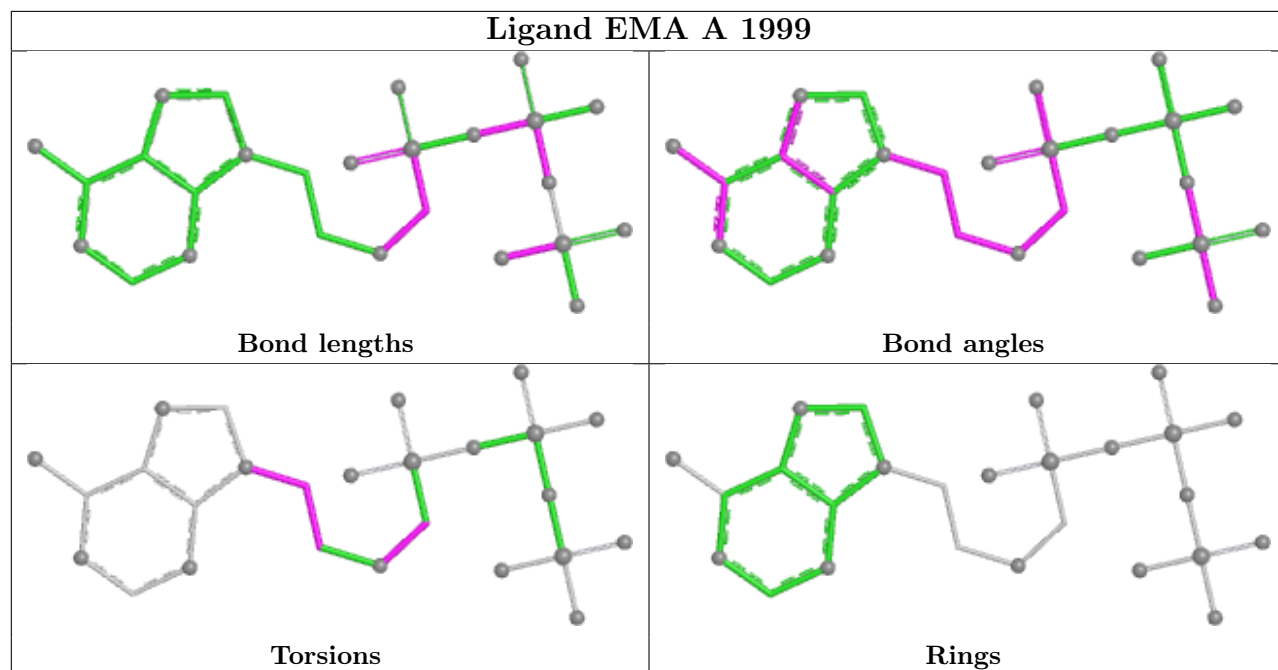
There are no ring outliers.

3 monomers are involved in 12 short contacts:

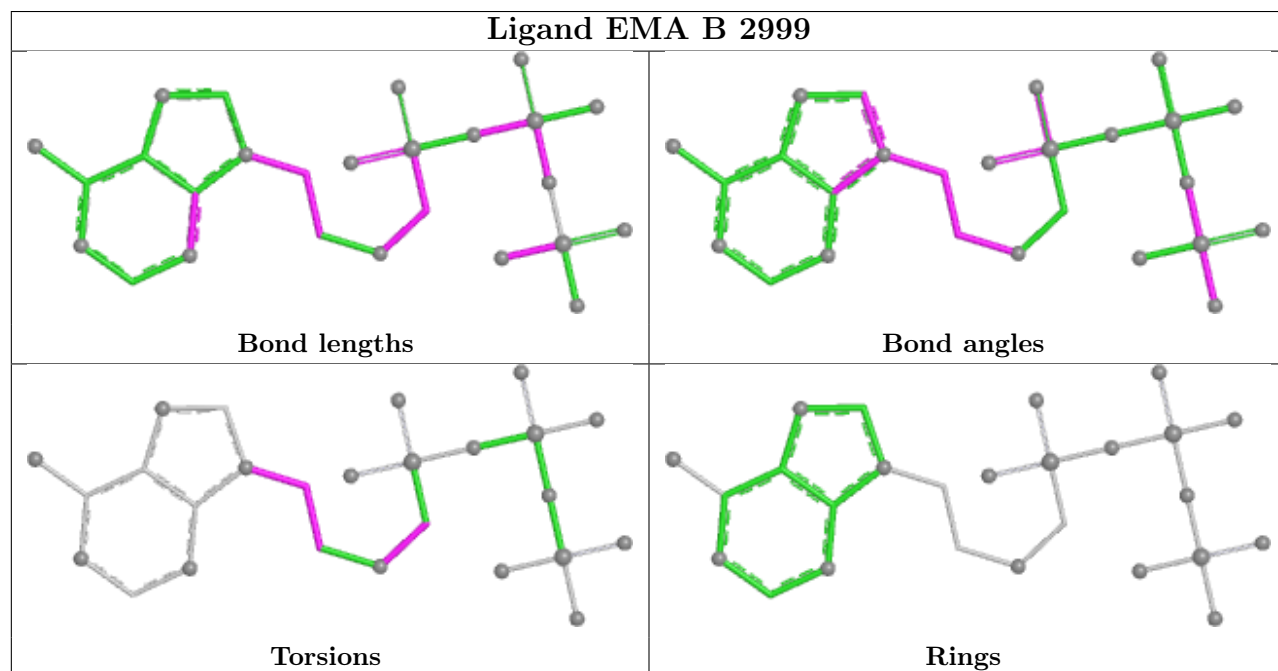
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1999	EMA	1	0
4	B	2999	EMA	4	0
4	C	3999	EMA	7	0

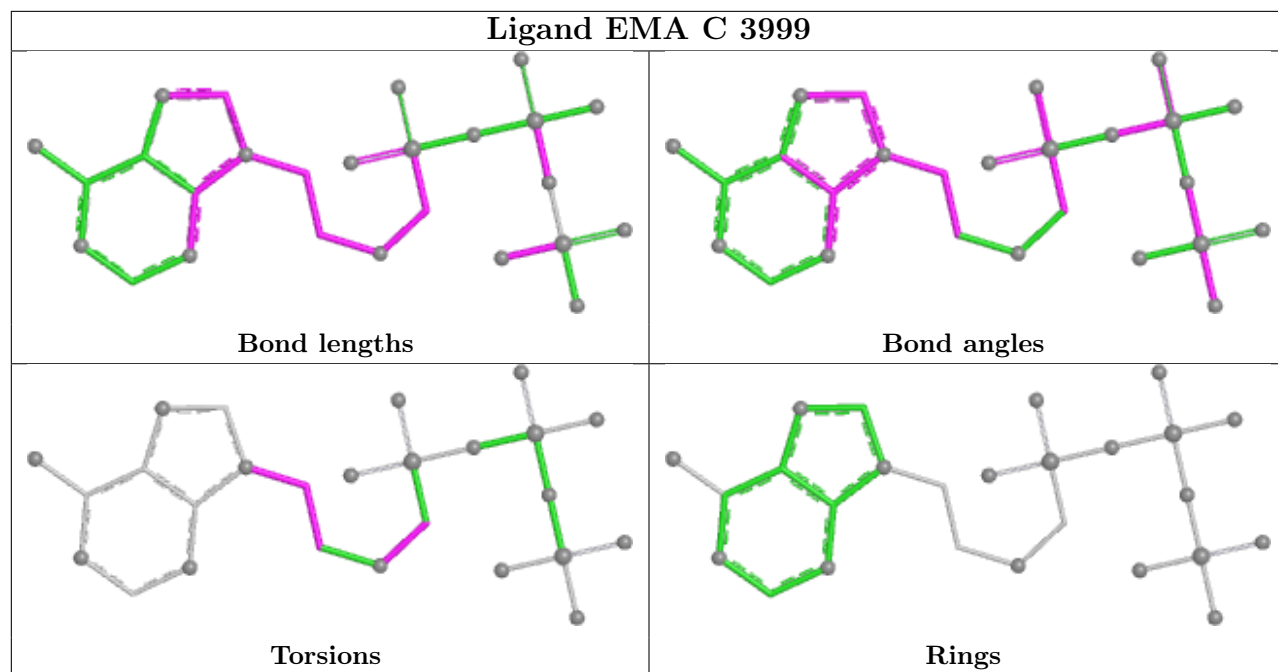
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand EMA A 1999



Ligand EMA B 2999





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	484/507 (95%)	0.13	20 (4%)	41	27	11, 50, 126, 154	16 (3%)
1	B	462/507 (91%)	0.36	39 (8%)	17	13	9, 53, 141, 149	12 (2%)
1	C	491/507 (96%)	0.06	12 (2%)	59	40	12, 52, 129, 152	19 (3%)
2	D	143/147 (97%)	0.90	17 (11%)	9	7	34, 123, 158, 160	0
2	E	143/147 (97%)	0.91	17 (11%)	9	7	36, 130, 158, 160	0
2	F	143/147 (97%)	0.69	13 (9%)	15	11	37, 128, 157, 159	0
All	All	1866/1962 (95%)	0.33	118 (6%)	26	17	9, 58, 150, 160	47 (2%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ILE	10.6
1	A	693	SER	7.7
1	B	732	ILE	4.8
2	D	24	ASP	4.6
1	A	694	VAL	4.5
1	B	663	PHE	4.4
1	B	747	ASN	4.4
1	A	784	GLU	4.2
2	F	48	LEU	4.2
2	E	59	GLY	4.0
2	F	73	ALA	3.9
1	B	705	TYR	3.9
1	A	737	LYS	3.6
1	C	692	GLU	3.6
1	C	783	THR	3.6
2	F	57	ALA	3.6
1	B	759	GLN	3.6
1	B	702	SER	3.5
2	D	62	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	57	ALA	3.5
1	A	562	GLU	3.4
2	E	55	VAL	3.4
2	D	43	PRO	3.3
1	B	784	GLU	3.2
1	B	765	THR	3.2
2	D	79	THR	3.2
1	B	751	TYR	3.1
1	B	773	PHE	3.1
2	E	69	LEU	3.1
1	A	673	SER	3.1
2	D	66	PRO	2.9
1	A	396	GLY	2.9
1	B	717	LYS	2.9
1	B	662	GLU	2.9
1	B	654	ILE	2.9
2	E	9	ILE	2.9
1	B	782	PHE	2.9
1	B	752	LEU	2.9
1	C	775	LEU	2.8
1	C	787	THR	2.8
2	F	29	THR	2.8
1	C	689	ALA	2.8
1	B	775	LEU	2.8
2	E	19	PHE	2.7
1	C	693	SER	2.7
2	F	38	SER	2.7
1	C	741	ILE	2.7
2	E	20	ASP	2.7
1	B	704	TYR	2.7
2	E	18	LEU	2.7
2	E	66	PRO	2.6
2	D	121	VAL	2.6
1	A	785	ASN	2.6
1	B	737	LYS	2.6
1	B	768	LYS	2.6
1	B	789	ASN	2.6
1	A	792	VAL	2.6
1	B	735	VAL	2.6
1	B	656	THR	2.6
2	E	76	MET	2.6
1	B	786	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	792	VAL	2.6
2	D	73	ALA	2.5
1	A	695	LYS	2.5
2	D	39	LEU	2.5
2	F	147	ALA	2.5
1	A	783	THR	2.5
2	E	62	THR	2.5
1	B	739	LYS	2.5
1	B	777	TYR	2.5
2	D	119	GLU	2.5
1	B	793	PHE	2.5
2	F	70	THR	2.5
1	B	658	PRO	2.5
2	F	65	PHE	2.4
1	B	787	THR	2.4
2	D	57	ALA	2.4
1	B	741	ILE	2.4
1	A	750	GLN	2.4
1	B	716	LYS	2.3
1	B	756	ILE	2.3
2	F	24	ASP	2.3
2	F	58	ASP	2.3
1	C	788	ASP	2.3
2	D	5	THR	2.3
1	A	415	GLU	2.3
1	B	792	VAL	2.3
1	A	780	LEU	2.3
2	E	8	GLN	2.3
2	E	21	LYS	2.3
1	A	429	GLY	2.2
1	A	662	GLU	2.2
1	B	763	LEU	2.2
2	D	118	ASP	2.2
1	A	668	SER	2.2
1	C	440	GLN	2.2
1	B	709	ASN	2.2
2	D	22	ASP	2.2
2	F	9	ILE	2.2
2	F	76	MET	2.2
2	E	132	GLY	2.1
2	D	53	ASN	2.1
1	A	782	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	623	ASP	2.1
2	F	51	MET	2.1
2	E	65	PHE	2.1
2	E	71	MET	2.1
1	B	766	HIS	2.1
1	C	739	LYS	2.1
1	A	520	PRO	2.1
2	E	77	LYS	2.0
2	D	46	ALA	2.0
2	D	56	ASP	2.0
2	D	55	VAL	2.0
1	A	776	LEU	2.0
1	C	513	TRP	2.0
1	B	294	ASP	2.0
1	B	797	ILE	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	EMA	B	2999	26/26	0.89	0.12	43,55,60,63	0
4	EMA	C	3999	26/26	0.91	0.15	46,63,71,72	0
4	EMA	A	1999	26/26	0.93	0.09	29,37,41,41	0
5	CA	F	804	1/1	0.94	0.06	44,44,44,44	0
3	YB	B	902	1/1	0.97	0.08	82,82,82,82	0
5	CA	E	803	1/1	0.98	0.04	47,47,47,47	0
5	CA	E	802	1/1	0.98	0.04	83,83,83,83	0
5	CA	F	805	1/1	0.98	0.06	48,48,48,48	0

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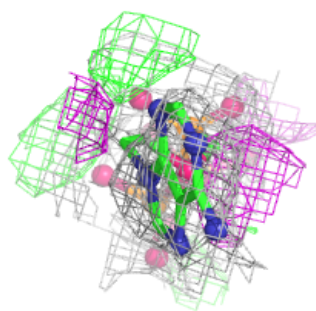
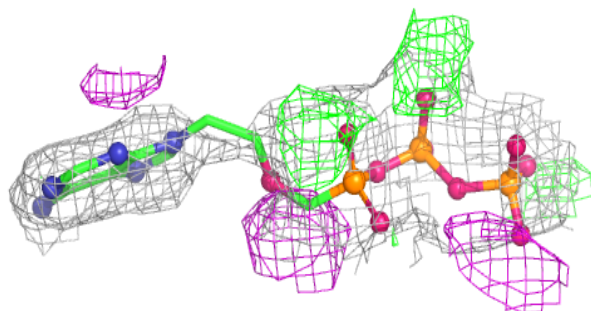
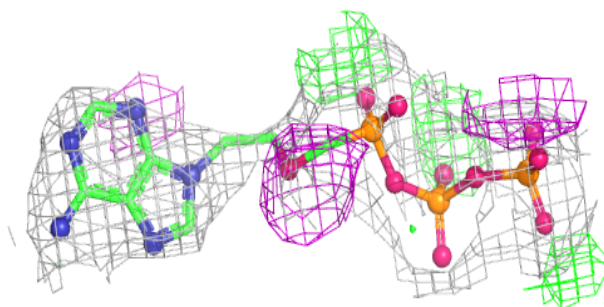
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YB	C	903	1/1	0.99	0.06	86,86,86,86	0
3	YB	A	901	1/1	0.99	0.04	77,77,77,77	0
5	CA	D	800	1/1	0.99	0.03	30,30,30,30	0
5	CA	D	801	1/1	0.99	0.04	37,37,37,37	0

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.

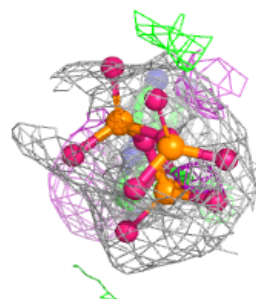
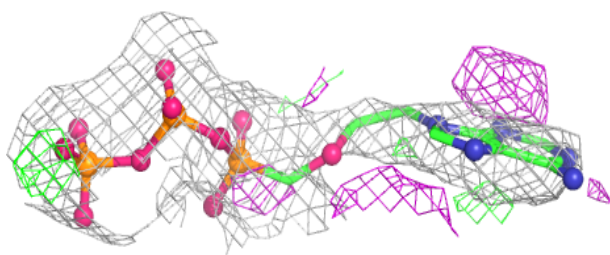
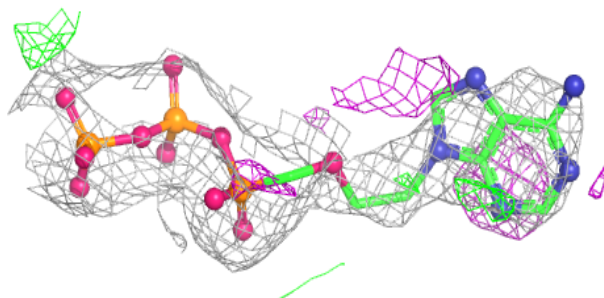
Electron density around EMA B 2999:

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

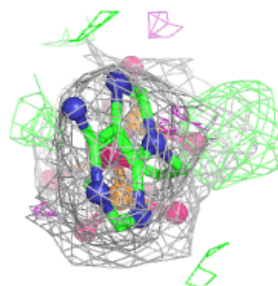
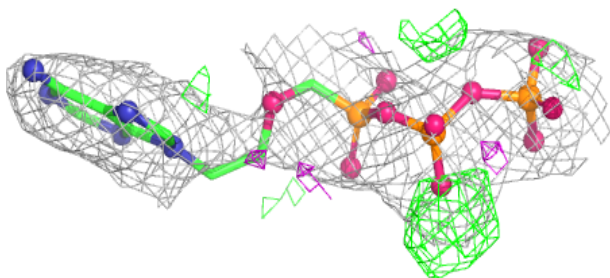
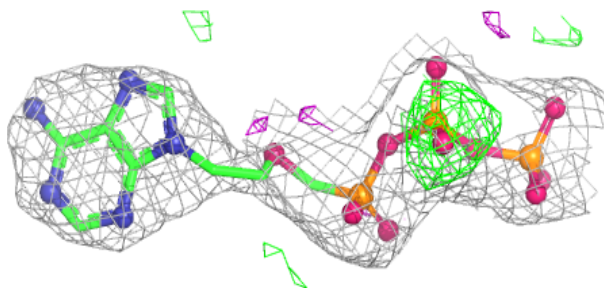


Electron density around EMA C 3999:

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

**Electron density around EMA A 1999:**

$2mF_o-DF_c$ (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.