



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:47 pm BST

PDB ID : 1PK0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

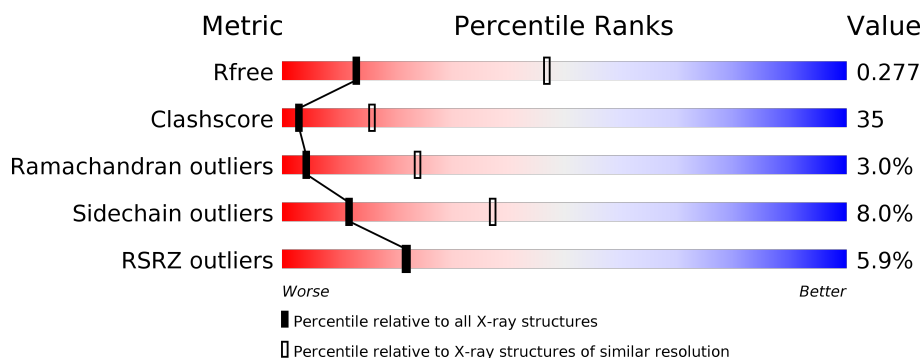
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	<div> <div>2%</div> <div> <div>47%</div> <div>41%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	507	<div> <div>3%</div> <div> <div>41%</div> <div>41%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	507	<div> <div>3%</div> <div> <div>48%</div> <div>43%</div> <div>8%</div> </div> </div>
2	D	147	<div> <div>16%</div> <div> <div>51%</div> <div>44%</div> </div> </div>
2	E	147	<div> <div>15%</div> <div> <div>51%</div> <div>44%</div> </div> </div>
2	F	147	<div> <div>15%</div> <div> <div>51%</div> <div>44%</div> </div> </div>

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 adenylate 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			

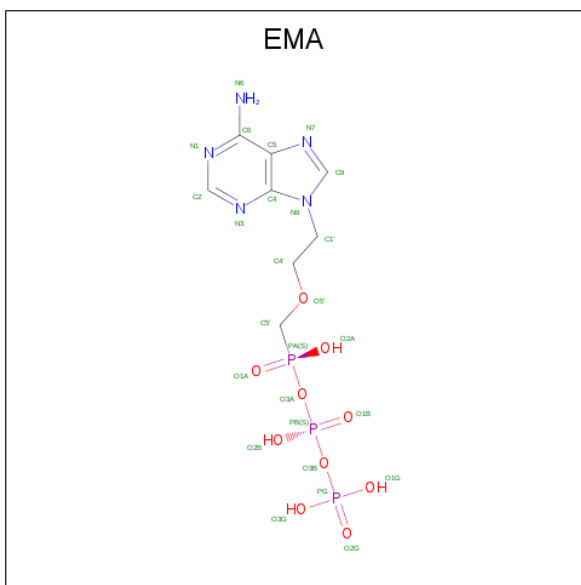
- Molecule 2 is a protein called Calmodulin.

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 (three-letter code: YB) (formula: Yb).

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

- Molecule 4 is (ADENIN-9-YL-ETHOXYMETHYL)-HYDROXYPHOSPHINYLDIPHOSPHATE (three-letter code: 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 (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Ca	0	0
			2	2		
5	F	2	Total	Ca	0	0
			2	2		
5	E	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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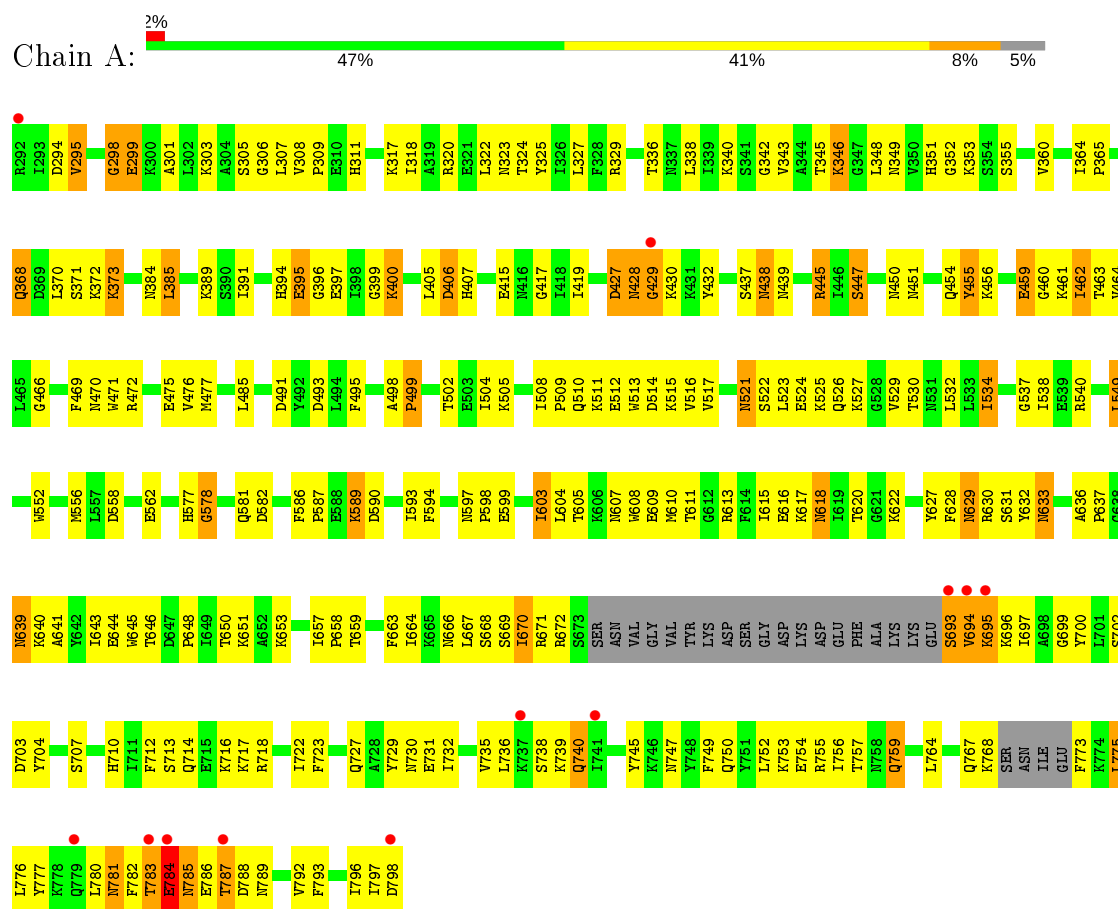
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	O	0	0
			1	1		

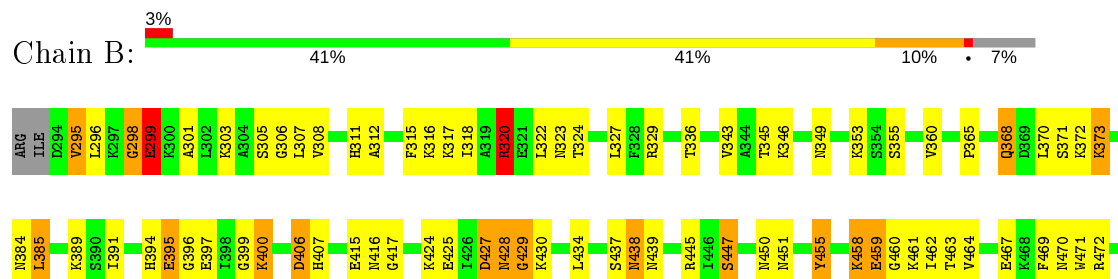
3 Residue-property plots

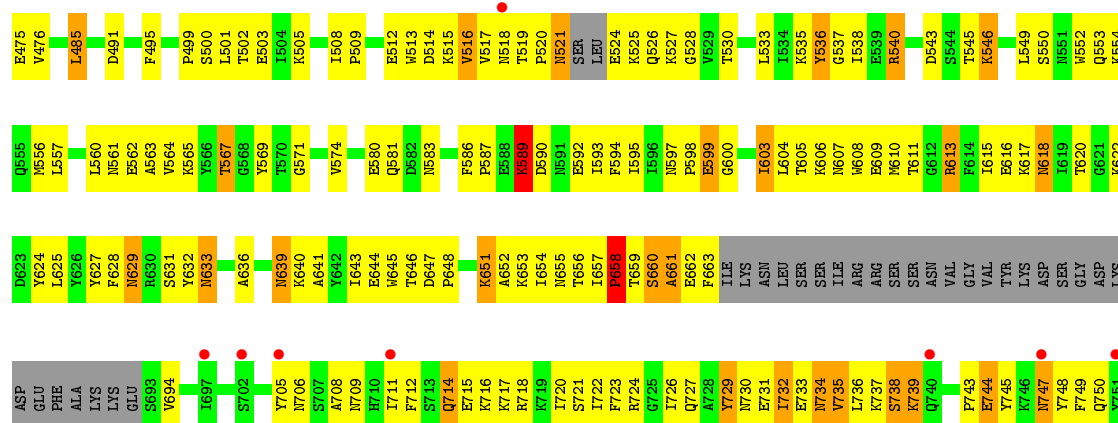
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

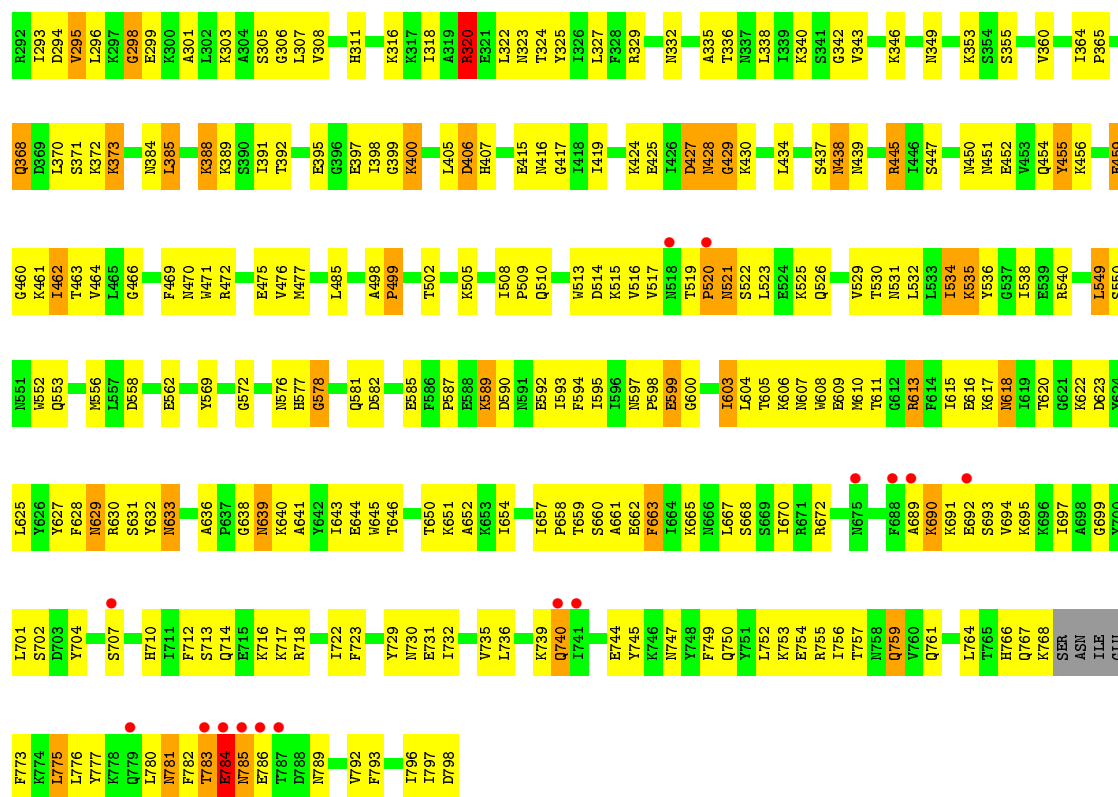


• Molecule 1: Calmodulin-sensitive adenylate cyclase



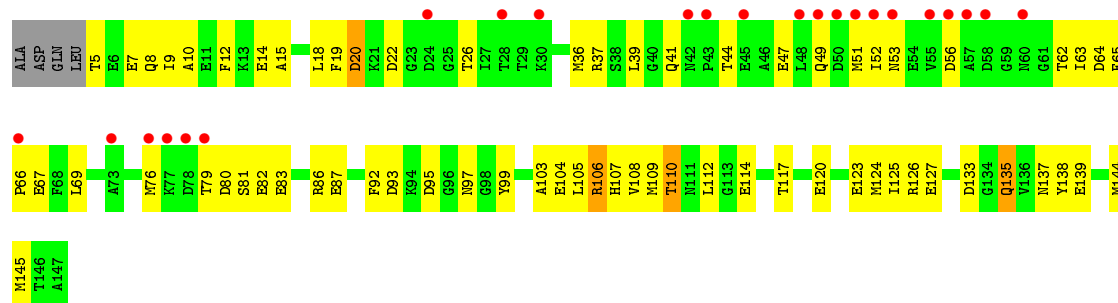


• Molecule 1: Calmodulin-sensitive adenylate cyclase

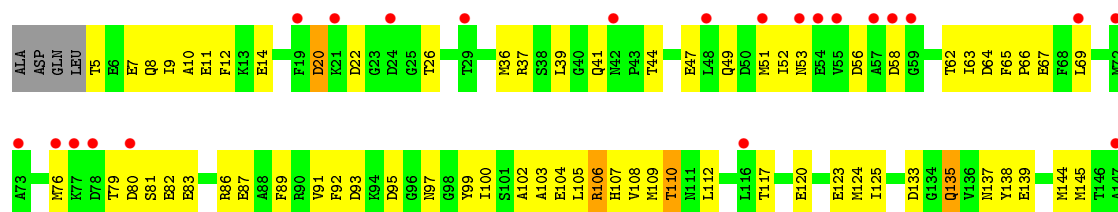


• Molecule 2: Calmodulin

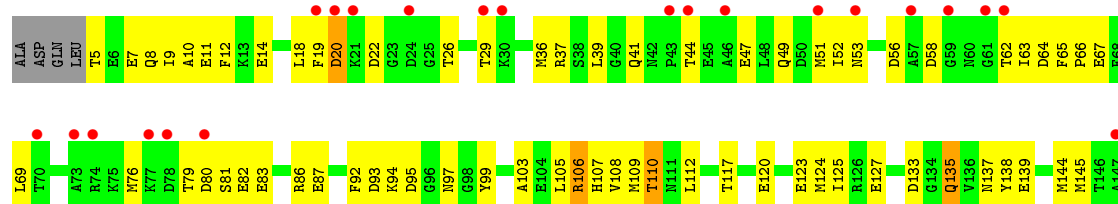




• Molecule 2: Calmodulin



• 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	116.26 Å 165.76 Å 342.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.30 29.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (14.98-3.30) 95.1 (29.88-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 3.31 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.264 , 0.302 0.245 , 0.277	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)	0.30 , 72.0	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	0.88	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, YB, EMA

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	0.60	2/4022 (0.0%)	0.98	22/5411 (0.4%)
1	B	0.54	0/3893	0.87	19/5239 (0.4%)
1	C	0.51	0/4173	0.83	15/5613 (0.3%)
2	D	0.36	0/1138	0.58	2/1527 (0.1%)
2	E	0.37	0/1138	0.58	2/1527 (0.1%)
2	F	0.36	0/1138	0.83	3/1527 (0.2%)
All	All	0.52	2/15502 (0.0%)	0.85	63/20844 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	694	VAL	N-CA	8.49	1.63	1.46
1	A	785	ASN	N-CA	5.19	1.56	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ARG	NE-CZ-NH1	-19.24	110.68	120.30
2	F	106	ARG	NE-CZ-NH1	-17.92	111.34	120.30
2	F	106	ARG	NE-CZ-NH2	17.43	129.02	120.30
1	A	613	ARG	NE-CZ-NH2	17.10	128.85	120.30
1	A	320	ARG	NE-CZ-NH2	-14.05	113.27	120.30
1	A	320	ARG	NE-CZ-NH1	13.03	126.81	120.30
1	C	613	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	C	785	ASN	N-CA-C	11.25	141.38	111.00
1	A	785	ASN	N-CA-C	10.81	140.19	111.00
1	B	613	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	C	613	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	428	ASN	N-CA-C	-9.80	84.53	111.00
1	A	694	VAL	CB-CA-C	-9.56	93.23	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	GLN	N-CA-C	-9.03	86.61	111.00
2	E	106	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	783	THR	N-CA-C	8.95	135.17	111.00
1	B	613	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	F	106	ARG	CD-NE-CZ	8.67	135.74	123.60
1	A	428	ASN	N-CA-C	-8.66	87.61	111.00
2	E	106	ARG	NE-CZ-NH1	8.63	124.62	120.30
2	D	106	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	D	106	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	320	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	B	320	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	C	784	GLU	C-N-CA	8.11	141.98	121.70
1	A	783	THR	N-CA-C	8.02	132.65	111.00
1	C	428	ASN	N-CA-C	-7.98	89.46	111.00
1	C	320	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	A	613	ARG	CD-NE-CZ	7.94	134.71	123.60
1	B	661	ALA	N-CA-C	-7.93	89.58	111.00
1	B	320	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	A	510	GLN	CA-C-N	7.54	133.78	117.20
1	B	660	SER	N-CA-C	-7.43	90.95	111.00
1	C	784	GLU	CB-CA-C	-7.42	95.55	110.40
1	C	785	ASN	N-CA-CB	-7.04	97.92	110.60
1	B	658	PRO	CA-C-N	-6.90	102.02	117.20
1	B	738	SER	N-CA-C	-6.65	93.05	111.00
1	A	693	SER	N-CA-CB	-6.56	100.67	110.50
1	B	458	LYS	CG-CD-CE	6.53	131.48	111.90
1	A	695	LYS	N-CA-C	6.50	128.56	111.00
1	A	784	GLU	CB-CA-C	-6.40	97.59	110.40
1	B	543	ASP	N-CA-C	-6.30	94.00	111.00
1	B	589	LYS	CD-CE-NZ	6.27	126.12	111.70
1	A	510	GLN	O-C-N	-6.16	112.84	122.70
1	C	740	GLN	N-CA-C	-6.11	94.52	111.00
1	A	785	ASN	CB-CA-C	-6.02	98.36	110.40
1	B	299	GLU	CA-CB-CG	5.90	126.38	113.40
1	A	693	SER	N-CA-C	5.82	126.71	111.00
1	A	320	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	785	ASN	CA-CB-CG	-5.81	100.63	113.40
1	A	427	ASP	N-CA-C	5.77	126.59	111.00
1	B	732	ILE	N-CA-C	-5.64	95.77	111.00
1	C	427	ASP	N-CA-C	5.55	125.98	111.00
1	B	427	ASP	N-CA-C	5.54	125.97	111.00
1	C	785	ASN	CB-CA-C	-5.49	99.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	ARG	CB-CA-C	5.49	121.38	110.40
1	B	546	LYS	N-CA-C	-5.45	96.28	111.00
1	C	766	HIS	CB-CA-C	5.45	121.29	110.40
1	B	658	PRO	CA-N-CD	-5.27	104.12	111.50
1	B	739	LYS	N-CA-C	5.25	125.18	111.00
1	A	510	GLN	C-N-CA	-5.16	108.79	121.70
1	B	658	PRO	O-C-N	5.08	130.83	122.70
1	C	613	ARG	CG-CD-NE	-5.02	101.25	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3947	0	3994	277	0
1	B	3820	0	3841	315	0
1	C	4095	0	4133	280	0
2	D	1126	0	1049	66	0
2	E	1126	0	1049	63	0
2	F	1126	0	1049	69	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	5	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	15142	1027	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 (1027) 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:B:726:ILE:HA	1:B:729:TYR:HB2	1.39	1.05
1:C:427:ASP:O	1:C:427:ASP:OD1	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
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:H	1:B:639:ASN:HD22	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:HD22	1:C:639:ASN:H	1.08	0.93
1:C:295:VAL:CG2	1:C:603:ILE:HG22	1.98	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:O	1:A:427:ASP:OD1	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:445:ARG:HH22	1:A:456:LYS:HG2	1.36	0.89
1:A:295:VAL:CG2	1:A:603:ILE:HG22	2.02	0.89
1:A:775:LEU:HD23	1:A:775:LEU:H	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:577:HIS:C	1:C:578:GLY:O	2.12	0.87
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: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:A:324:THR:HG21	1:A:556:MET:HE1	1.62	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
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: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:N	1:A:618:ASN:HD22	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
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:745:TYR:HB3	1:B:749:PHE:HE1	1.49	0.77
1:B:518:ASN:C	1:B:520:PRO:HD3	2.04	0.77
2:E:133:ASP:OD2	2:E:135:GLN:HG3	1.84	0.77
1:B:427:ASP:OD1	1:B:427:ASP:C	2.22	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:633:ASN:HD22	1.83	0.76
1:A:400:LYS:HE2	1:A:475:GLU:OE2	1.86	0.76
1:B:659:THR:C	1:B:661:ALA:N	2.29	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: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:C:781:ASN:ND2	1:C:782:PHE:H	1.85	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:C:427:ASP:C	1:C:427:ASP:OD1	2.25	0.74
1:B:633:ASN:HD22	1:B:633:ASN:N	1.86	0.74
2:F:12:PHE:HD1	2:F:39:LEU:HD21	1.52	0.74
1:B:718:ARG:HB2	1:B:763:LEU:HB3	1.69	0.73
1:A:318:ILE:H	1:A:318:ILE:HD12	1.52	0.73
1:A:633:ASN:HD22	1:A:633:ASN:N	1.81	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:318:ILE:N	1:A:318:ILE:HD12	2.03	0.72
1:B:737:LYS:C	1:B:738:SER:O	2.23	0.72
1:C:692:GLU:O	1:C:735:VAL:HG22	1.88	0.72
1:C:318:ILE:N	1:C:318:ILE:HD12	2.04	0.72
1:C:577:HIS:O	1:C:578:GLY:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:438:ASN:HD22	1:A:438:ASN:C	1.93	0.70
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
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: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:690:LYS:HZ3	1:C:693:SER:H	1.39	0.70
1:C:792:VAL:O	1:C:796:ILE:HG12	1.91	0.70
1:C:438:ASN:C	1:C:438:ASN:HD22	1.95	0.69
1:C:690:LYS:HZ2	1:C:692:GLU:HA	1.57	0.69
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:B:519:THR:N	1:B:520:PRO:HD3	2.08	0.69
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.55	0.69
1:A:324:THR:HG21	1:A:556:MET:CE	2.22	0.69
1:B:616:GLU:HA	1:B:620:THR:CG2	2.23	0.69
1:C:368:GLN:HB2	1:C:384:ASN:OD1	1.92	0.69
1:A:428:ASN:O	1:A:429:GLY:C	2.31	0.69
1:A:666:ASN:O	1:A:670:ILE:HB	1.93	0.69
1:B:318:ILE:H	1:B:318:ILE:HD12	1.56	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:329:ARG:HD2	1:B:590:ASP:OD2	1.92	0.68
1:C:617:LYS:C	1:C:618:ASN:HD22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ARG:HD2	1:C:590:ASP:OD2	1.93	0.68
1:B:438:ASN:HD22	1:B:438:ASN:C	1.97	0.68
1:C:540:ARG:NH2	1:C:630:ARG:HH21	1.91	0.68
1:A:427:ASP:C	1:A:427:ASP:OD1	2.30	0.68
1:B:654:ILE:O	1:B:655:ASN:ND2	2.26	0.68
1:B:538:ILE:O	1:B:540:ARG:HD3	1.94	0.68
1:A:617:LYS:C	1:A:618:ASN:HD22	1.96	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: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:HD12	1:C:327:LEU:N	2.10	0.67
1:C:639:ASN:N	1:C:639:ASN:HD22	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:O	1:A:360:VAL:HG22	1.95	0.67
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:B:360:VAL:HG22	1:B:360:VAL:O	1.95	0.67
1:C:616:GLU:HA	1:C:620:THR:CG2	2.24	0.66
1:C:400:LYS:HE2	1:C:475:GLU:CD	2.15	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:B:428:ASN:O	1:B:429:GLY:C	2.28	0.66
1:A:777:TYR:CD1	1:A:780:LEU:HD21	2.31	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:327:LEU:N	1:B:327:LEU:HD12	2.11	0.65
1:B:735:VAL:CG2	1:B:738:SER:HB2	2.27	0.65
1:C:360:VAL:HG22	1:C:360:VAL:O	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:617:LYS:C	1:B:618:ASN:HD22	2.01	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: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
2:E:117:THR:OG1	2:E:120:GLU:HG3	1.98	0.63
1:A:577:HIS:C	1:A:578:GLY:O	2.37	0.63
1:A:368:GLN:HB2	1:A:384:ASN:OD1	1.99	0.62
2:D:36:MET:O	2:D:41:GLN:HB2	1.99	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:36:MET:O	2:E:41:GLN:HB2	1.98	0.62
2:E:12:PHE:CD1	2:E:39:LEU:HD21	2.34	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: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:HD12	1:A:327:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:534:ILE:HA	1:A:538:ILE:HB	1.83	0.60
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.31	0.60
1:B:659:THR:O	1:B:660:SER:C	2.33	0.60
1:C:324:THR:HG21	1:C:556:MET:HE1	1.82	0.60
1:C:789:ASN:HD22	1:C:789:ASN:N	1.99	0.60
1:A:781:ASN:ND2	1:A:782:PHE:N	2.49	0.60
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: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:400:LYS:HE2	1:A:475:GLU:CD	2.21	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
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
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
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.37	0.59
1:C:665:LYS:HE3	2:F:11:GLU:OE2	2.02	0.59
1:A:469:PHE:CB	1:A:472:ARG:HH21	2.15	0.59
1:B:400:LYS:HE2	1:B:475:GLU:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:372:LYS:HG3	1:A:373:LYS:HD3	1.83	0.58
1:B:318:ILE:HG23	1:B:322:LEU:HD12	1.84	0.58
1:B:733:GLU:C	1:B:735:VAL:H	2.06	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
1:C:346:LYS:HZ1	4:C:3999:EMA:PG	2.26	0.58
2:D:137:ASN:OD1	2:D:139:GLU:HB2	2.04	0.58
1:A:740:GLN:H	1:A:740:GLN:CD	2.07	0.58
1:B:773:PHE:O	1:B:775:LEU:N	2.34	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: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
2:D:79:THR:C	2:D:81:SER:H	2.08	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:C:318:ILE:H	2.18	0.56
1:C:697:ILE:HD13	1:C:732:ILE:HG12	1.87	0.56
1:A:639:ASN:H	1:A:639:ASN:ND2	1.96	0.56
1:C:549:LEU:H	1:C:549:LEU:HD12	1.69	0.56
1:A:697:ILE:HD11	1:A:731:GLU:O	2.05	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:E:79:THR:C	2:E:81:SER:H	2.09	0.56
2:F:63:ILE:N	2:F:63:ILE:HD12	2.20	0.56
2:F:79:THR:C	2:F:81:SER:H	2.09	0.56
1:A:629:ASN:ND2	1:A:631:SER:N	2.44	0.56
1:A:633:ASN:ND2	1:A:633:ASN:N	2.52	0.56
1:C:662:GLU:HG2	1:C:662:GLU:O	2.04	0.56
1:C:747:ASN:HA	1:C:750:GLN:HG2	1.86	0.56
1:A:697:ILE:N	1:A:697:ILE:HD12	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:616:GLU:HA	1:B:620:THR:HG22	1.88	0.56
1:B:500:SER:HA	1:B:624:TYR:CD2	2.40	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:N	2:E:63:ILE:HD12	2.21	0.55
1:A:759:GLN:HA	1:A:759:GLN:HE21	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:HD12	1:B:538:ILE:N	2.21	0.55
1:C:650:THR:C	1:C:652:ALA:H	2.09	0.55
1:A:540:ARG:NH2	1:A:630:ARG:NH2	2.55	0.55
1:C:514:ASP:C	1:C:516:VAL:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:445:ARG:CZ	1:A:471:TRP:CD1	2.90	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:B:659:THR:C	1:B:661:ALA:H	2.05	0.54
1:C:759:GLN:HA	1:C:759:GLN:NE2	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:137:ASN:OD1	2:F:139:GLU:HB2	2.06	0.54
2:F:8:GLN:HA	2:F:8:GLN:HE21	1.73	0.54
1:A:470:ASN:CG	1:A:471:TRP:H	2.11	0.54
1:C:320:ARG:CD	1:C:599:GLU:O	2.56	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:C:323:ASN:HD22	1:C:598:PRO:HB2	1.73	0.54
1:C:618:ASN:N	1:C:618:ASN:ND2	2.54	0.54
1:A:549:LEU:H	1:A:549:LEU:HD12	1.72	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:695:LYS:CB	2:D:18:LEU:HD22	2.36	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:C:428:ASN:O	1:C:429:GLY:C	2.46	0.54
1:A:294:ASP:O	1:A:610:MET:HE1	2.08	0.54
1:A:739:LYS:C	1:A:740:GLN:O	2.37	0.54
1:C:296:LEU:HD21	1:C:606:LYS:HE3	1.88	0.54
1:C:718:ARG:HD2	1:C:767:GLN:OE1	2.07	0.54
2:F:105:LEU:O	2:F:105:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:PHE:CB	2:E:14:GLU:OE2	2.56	0.53
1:B:776:LEU:HD13	1:B:779:GLN:CD	2.28	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
1:A:697:ILE:CD1	1:A:731:GLU:HB3	2.38	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:C:695:LYS:HZ2	2:F:18:LEU:HD13	1.72	0.53
1:B:318:ILE:CD1	1:B:318:ILE:H	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:HD23	2:E:105:LEU:O	2.08	0.53
1:A:581:GLN:NE2	1:A:628:PHE:HA	2.22	0.53
1:B:536:TYR:CD2	1:B:536:TYR:N	2.77	0.53
1:B:633:ASN:ND2	1:B:645:TRP:H	1.95	0.53
1:B:715:GLU:O	1:B:718:ARG:HG2	2.08	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: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
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:N	1:B:536:TYR:HD2	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:C:522:SER:O	1:C:525:LYS:HB3	2.08	0.52
1:A:664:ILE:HD13	2:D:15:ALA:HB2	1.92	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: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
2:E:9:ILE:HG23	2:E:69:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:ILE:O	2:F:52:ILE:HG13	2.10	0.52
1:A:668:SER:C	1:A:670:ILE:H	2.12	0.52
1:B:502:THR:O	1:B:505:LYS:HB3	2.10	0.52
1:B:556:MET:HE2	1:B:560:LEU:HG	1.90	0.52
1:B:633:ASN:ND2	1:B:633:ASN:N	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:639:ASN:ND2	1:C:639:ASN:H	1.90	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: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
2:F:26:THR:HG21	2:F:62:THR:HB	1.92	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:758:ASN:C	1:B:760:VAL:H	2.12	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
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:E:52:ILE:HG13	2:E:52:ILE:O	2.10	0.51
2:F:92:PHE:CE2	2:F:108:VAL:HG11	2.45	0.51
1:B:470:ASN:CG	1:B:471:TRP:H	2.14	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:A:712:PHE:CD2	1:A:716:LYS:HG2	2.46	0.51
1:B:535:LYS:C	1:B:536:TYR:HD2	2.14	0.51
1:B:750:GLN:O	1:B:753:LYS:HB3	2.11	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:296:LEU:CD2	1:B:606:LYS:HE3	2.40	0.51
2:D:52:ILE:O	2:D:52:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:ILE:HG23	2:D:69:LEU:HD22	1.91	0.51
1:A:508:ILE:HG21	1:A:532:LEU:HD13	1.91	0.51
2:D:26:THR:HG21	2:D:62:THR:HB	1.92	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
2:F:144:MET:SD	2:F:145:MET:HE2	2.51	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:HG3	1:B:774:LYS:O	2.11	0.51
1:A:587:PRO:HD2	1:A:639:ASN:HD21	1.75	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
2:E:103:ALA:O	2:E:106:ARG:HB3	2.11	0.50
1:C:668:SER:HB2	2:F:14:GLU:HG3	1.92	0.50
1:A:469:PHE:HB3	1:A:472:ARG:HH21	1.76	0.50
1:B:653:LYS:O	1:B:653:LYS:HG3	2.10	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
2:D:37:ARG:HA	2:D:41:GLN:O	2.11	0.50
1:C:577:HIS:CE1	4:C:3999:EMA:H8	2.44	0.50
1:A:540:ARG:NH2	2:D:87:GLU:CD	2.65	0.50
1:A:740:GLN:N	1:A:740:GLN:CD	2.65	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:743:PRO:O	1:B:747:ASN:HB2	2.12	0.50
2:D:144:MET:SD	2:D:145:MET:HE2	2.52	0.50
1:A:540:ARG:HH22	2:D:87:GLU:CD	2.15	0.50
2:E:5:THR:O	2:E:5:THR:HG22	2.12	0.50
1:A:593:ILE:HG13	1:A:611:THR:HG21	1.94	0.50
1:B:505:LYS:HA	1:B:508:ILE:CD1	2.42	0.50
1:B:320:ARG:HG3	1:B:598:PRO:O	2.12	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:C:325:TYR:HB2	1:C:498:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASN:ND2	1:A:438:ASN:C	2.64	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:ND2	1:C:349:ASN:H	2.11	0.49
1:A:526:GLN:C	1:A:529:VAL:HG12	2.32	0.49
1:C:754:GLU:O	1:C:757:THR:HB	2.12	0.49
1:B:395:GLU:HG3	1:B:396:GLY:N	2.27	0.49
1:C:623:ASP:H	2:F:94:LYS:HD2	1.75	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:E:37:ARG:HA	2:E:41:GLN:O	2.11	0.49
1:B:318:ILE:CD1	1:B:318:ILE:N	2.76	0.49
1:B:525:LYS:O	1:B:528:GLY:N	2.46	0.49
1:B:745:TYR:HB3	1:B:749:PHE:CE1	2.38	0.49
1:B:514:ASP:C	1:B:516:VAL:H	2.16	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:D:20:ASP:C	2:D:22:ASP:H	2.16	0.49
1:B:306:GLY:O	1:B:336:THR:OG1	2.25	0.49
1:B:455:TYR:HA	1:B:471:TRP:HZ3	1.77	0.49
1:C:549:LEU:N	1:C:549:LEU:HD12	2.27	0.49
1:C:540:ARG:CZ	1:C:627:TYR:CE1	2.96	0.49
1:C:650:THR:C	1:C:652:ALA:N	2.66	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: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
2:D:92:PHE:CE2	2:D:108:VAL:HG11	2.48	0.48
2:E:20:ASP:C	2:E:22:ASP:H	2.16	0.48
1:C:505:LYS:HD3	2:F:112:LEU:O	2.13	0.48
2:F:95:ASP:OD2	2:F:97:ASN:HB3	2.13	0.48
1:A:307:LEU:HD12	1:A:307:LEU:H	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:730:ASN:CG	1:B:730:ASN:O	2.51	0.48
2:F:103:ALA:O	2:F:106:ARG:HB3	2.13	0.48
2:F:37:ARG:HA	2:F:41:GLN:O	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: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
1:B:318:ILE:HG21	1:B:556:MET:CE	2.43	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:C:437:SER:C	1:C:439:ASN:H	2.18	0.48
1:C:661:ALA:O	1:C:663:PHE:N	2.38	0.48
1:A:513:TRP:HH2	2:D:114:GLU:N	2.12	0.48
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: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:C:755:ARG:O	1:C:756:ILE:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:GLN:NE2	1:B:797:ILE:HD13	2.29	0.47
1:C:661:ALA:C	1:C:663:PHE:H	2.16	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:438:ASN:ND2	1:C:438:ASN:C	2.65	0.47
1:C:502:THR:O	1:C:505:LYS:HB3	2.14	0.47
1:C:670:ILE:HD11	1:C:744:GLU:C	2.35	0.47
2:E:5:THR:O	2:E:8:GLN:HB2	2.15	0.47
1:C:540:ARG:NH2	2:F:87:GLU:OE1	2.48	0.47
1:A:349:ASN:H	1:A:349:ASN:ND2	2.12	0.47
1:A:577:HIS:O	1:A:578:GLY:C	2.51	0.47
1:C:530:THR:O	1:C:534:ILE:HG13	2.14	0.47
1:C:761:GLN:NE2	1:C:761:GLN:HA	2.30	0.47
2:F:20:ASP:C	2:F:22:ASP:H	2.16	0.47
1:A:353:LYS:N	1:A:368:GLN:HE22	2.12	0.47
1:A:515:LYS:O	1:A:515:LYS:HG2	2.14	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:A:759:GLN:HE21	1:A:759:GLN:CA	2.27	0.47
1:B:360:VAL:HG21	1:B:365:PRO:HB3	1.95	0.47
1:B:438:ASN:ND2	1:B:438:ASN:C	2.67	0.47
2:E:8:GLN:NE2	2:E:8:GLN:HA	2.30	0.47
1:B:660:SER:N	1:B:662:GLU:H	2.11	0.47
1:B:655:ASN:HA	1:B:759:GLN:NE2	2.30	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
2:E:144:MET:SD	2:E:145:MET:HE2	2.55	0.47
2:F:81:SER:O	2:F:82:GLU:C	2.54	0.47
1:A:670:ILE:HG23	1:A:670:ILE:O	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
2:D:107:HIS:O	2:D:108:VAL:C	2.53	0.47
1:A:364:ILE:HB	1:A:477:MET:HB2	1.98	0.46
1:B:437:SER:C	1:B:439:ASN:H	2.17	0.46
1:B:587:PRO:HD2	1:B:639:ASN:HD21	1.79	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
1:C:695:LYS:NZ	2:F:18:LEU:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:65:PHE:CD1	2:F:65:PHE:N	2.83	0.46
1:C:323:ASN:HD22	1:C:598:PRO:CB	2.28	0.46
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:C:661:ALA:C	1:C:663:PHE:N	2.69	0.46
1:A:463:THR:HG22	1:A:464:VAL:N	2.30	0.46
1:B:561:ASN:O	1:B:562:GLU:C	2.54	0.46
1:C:459:GLU:C	1:C:461:LYS:H	2.18	0.46
1:C:514:ASP:C	1:C:516:VAL:N	2.68	0.46
1:B:663:PHE:CB	2:E:14:GLU:HG3	2.45	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:B:733:GLU:C	1:B:735:VAL:N	2.69	0.46
2:E:81:SER:O	2:E:82:GLU:C	2.53	0.46
2:F:65:PHE:HB2	2:F:66:PRO:CD	2.42	0.46
1:A:459:GLU:C	1:A:461:LYS:H	2.19	0.46
1:B:720:ILE:HB	1:B:724:ARG:HE	1.81	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:120:GLU:O	2:F:123:GLU:HB2	2.16	0.46
2:F:8:GLN:HA	2:F:8:GLN:NE2	2.31	0.46
1:A:338:LEU:O	1:A:343:VAL:HG23	2.16	0.46
1:A:700:TYR:O	1:A:703:ASP:HB2	2.16	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:A:723:PHE:HB2	1:A:793:PHE:CE2	2.50	0.46
1:A:755:ARG:O	1:A:756:ILE:C	2.53	0.46
1:B:629:ASN:ND2	1:B:631:SER:CB	2.75	0.46
1:B:658:PRO:C	1:B:659:THR:O	2.53	0.46
1:C:657:ILE:HG12	1:C:756:ILE:HD13	1.96	0.46
1:A:526:GLN:OE1	2:D:124:MET:HB3	2.15	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
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:CA	1:C:759:GLN:HE21	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:THR:C	2:D:63:ILE:HD12	2.37	0.46
2:D:65:PHE:N	2:D:65:PHE:CD1	2.84	0.46
1:B:734:ASN:C	1:B:736:LEU:H	2.18	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:B:346:LYS:HZ1	4:B:2999:EMA:PG	2.39	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
2:F:62:THR:C	2:F:63:ILE:HD12	2.36	0.45
1:A:718:ARG:HD2	1:A:767:GLN:OE1	2.15	0.45
1:B:323:ASN:CG	1:B:500:SER:HB3	2.36	0.45
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.29	0.45
1:A:586:PHE:HA	1:A:639:ASN:ND2	2.30	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
1:B:521:ASN:C	1:B:521:ASN:HD22	2.19	0.45
1:C:462:ILE:HG12	1:C:466:GLY:HA2	1.97	0.45
2:D:120:GLU:O	2:D:123:GLU:HB2	2.16	0.45
2:D:95:ASP:OD1	2:D:104:GLU:OE2	2.35	0.45
1:A:307:LEU:N	1:A:307:LEU:HD12	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:86:ARG:HA	2:D:138:TYR:CE1	2.51	0.45
2:D:79:THR:O	2:D:81:SER:N	2.49	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:A:785:ASN:ND2	1:A:785:ASN:H	2.10	0.45
1:B:384:ASN:O	1:B:385:LEU:C	2.55	0.45
1:B:459:GLU:C	1:B:461:LYS:H	2.19	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
1:A:549:LEU:HD12	1:A:549:LEU:N	2.30	0.45
1:A:633:ASN:H	1:A:633:ASN:HD22	1.64	0.45
1:A:657:ILE:HB	1:A:756:ILE:HD13	1.98	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:ASN:HD22	1:C:782:PHE:N	2.05	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:A:789:ASN:ND2	1:A:789:ASN:N	2.63	0.45
1:B:538:ILE:CD1	1:B:538:ILE:N	2.80	0.45
1:B:316:LYS:HD3	1:B:600:GLY:O	2.17	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
1:C:730:ASN:C	1:C:732:ILE:H	2.20	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: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:51:MET:C	2:E:53:ASN:H	2.20	0.45
1:A:295:VAL:HG22	1:A:603:ILE:HG22	1.91	0.44
1:B:525:LYS:C	1:B:528:GLY:H	2.20	0.44
2:D:51:MET:C	2:D:53:ASN:H	2.21	0.44
2:D:81:SER:O	2:D:82:GLU:C	2.55	0.44
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.52	0.44
1:A:525:LYS:C	1:A:527:LYS:N	2.71	0.44
1:A:540:ARG:HD2	1:A:582:ASP:OD1	2.17	0.44
1:A:730:ASN:C	1:A:732:ILE:H	2.20	0.44
1:B:580:GLU:CD	1:B:583:ASN:HD22	2.20	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
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:B:395:GLU:C	1:B:397:GLU:H	2.21	0.44
1:B:415:GLU:C	1:B:417:GLY:H	2.21	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:437:SER:C	1:A:439:ASN:H	2.20	0.44
1:B:298:GLY:O	1:B:299:GLU:C	2.56	0.44
1:C:307:LEU:N	1:C:307:LEU:HD12	2.32	0.44
1:B:526:GLN:HG3	2:E:124:MET:CE	2.47	0.44
2:E:79:THR:O	2:E:81:SER:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASN:O	1:C:451:ASN:HB2	2.18	0.44
1:A:317:LYS:HB2	1:A:317:LYS:HE2	1.88	0.44
1:A:432:TYR:CE1	1:A:471:TRP:HZ3	2.35	0.44
1:B:717:LYS:O	1:B:720:ILE:HG12	2.18	0.44
1:C:628:PHE:O	1:C:628:PHE:CD1	2.71	0.44
2:F:107:HIS:O	2:F:108:VAL:C	2.56	0.44
2:F:51:MET:C	2:F:53:ASN:H	2.21	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:537:GLY:C	1:B:538:ILE:HD12	2.38	0.44
1:B:607:ASN:O	1:B:610:MET:N	2.51	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:C:789:ASN:ND2	1:C:789:ASN:N	2.63	0.44
2:F:86:ARG:HA	2:F:138:TYR:CE1	2.53	0.44
1:A:395:GLU:C	1:A:397:GLU:H	2.21	0.43
1:A:447:SER:O	1:A:451:ASN:HA	2.18	0.43
1:A:305:SER:HB3	1:A:594:PHE:CD1	2.53	0.43
1:C:395:GLU:C	1:C:397:GLU:H	2.21	0.43
1:C:415:GLU:C	1:C:417:GLY:H	2.21	0.43
1:C:424:LYS:HG3	1:C:425:GLU:N	2.32	0.43
1:C:628:PHE:CD1	1:C:628:PHE:C	2.91	0.43
1:C:672:ARG:NE	1:C:672:ARG:HA	2.33	0.43
1:C:786:GLU:OE1	1:C:786:GLU:HA	2.18	0.43
1:A:415:GLU:C	1:A:417:GLY:H	2.21	0.43
1:B:717:LYS:HA	1:B:720:ILE:CG1	2.45	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:320:ARG:HA	1:C:598:PRO:O	2.17	0.43
2:E:107:HIS:O	2:E:108:VAL:C	2.56	0.43
2:E:95:ASP:OD1	2:E:104:GLU:OE2	2.36	0.43
1:C:695:LYS:HG3	2:F:18:LEU:HD22	2.00	0.43
1:B:296:LEU:HD21	1:B:606:LYS:CE	2.49	0.43
1:C:324:THR:OG1	1:C:499:PRO:CA	2.66	0.43
1:C:530:THR:HG21	2:F:145:MET:SD	2.58	0.43
1:B:415:GLU:C	1:B:417:GLY:N	2.72	0.43
1:B:657:ILE:HG13	1:B:658:PRO:N	2.33	0.43
1:B:744:GLU:CD	1:C:397:GLU:HG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLU:O	1:C:417:GLY:N	2.51	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:660:SER:O	1:C:663:PHE:HB3	2.18	0.43
2:E:62:THR:C	2:E:63:ILE:HD12	2.38	0.43
1:A:415:GLU:C	1:A:417:GLY:N	2.72	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:C:652:ALA:C	1:C:654:ILE:H	2.22	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:A:628:PHE:CD1	1:A:628:PHE:C	2.92	0.43
1:A:639:ASN:ND2	1:A:639:ASN:N	2.60	0.43
1:A:783:THR:C	1:A:784:GLU:OE1	2.57	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
1:C:294:ASP:O	1:C:610:MET:HE1	2.18	0.43
2:E:86:ARG:HA	2:E:138:TYR:HE1	1.84	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:HB2	1:B:317:LYS:HE2	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:415:GLU:C	1:C:417:GLY:N	2.70	0.43
1:A:294:ASP:O	1:A:610:MET:CE	2.66	0.43
1:B:654:ILE:HG13	1:B:654:ILE:O	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:C:695:LYS:HZ2	2:F:18:LEU:HB3	1.83	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:714:GLN:HA	1:B:717:LYS:CE	2.49	0.42
1:A:514:ASP:C	1:A:516:VAL:H	2.21	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:THR:O	1:A:651:LYS:C	2.57	0.42
1:C:505:LYS:HE3	1:C:513:TRP:CE2	2.54	0.42
2:F:137:ASN:OD1	2:F:137:ASN:C	2.58	0.42
1:A:360:VAL:CG2	1:A:360:VAL:O	2.65	0.42
1:A:516:VAL:O	1:A:517:VAL:C	2.58	0.42
1:A:628:PHE:O	1:A:628:PHE:CD1	2.72	0.42
1:A:776:LEU:HD12	1:A:776:LEU:N	2.35	0.42
1:A:644:GLU:OE2	1:B:400:LYS:NZ	2.53	0.42
1:B:450:ASN:O	1:B:451:ASN:HB2	2.18	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:HD12	1:C:776:LEU:N	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
1:A:346:LYS:HE3	4:A:1999:EMA:O2G	2.18	0.42
1:A:295:VAL:HG23	1:A:604:LEU:O	2.20	0.42
1:A:355:SER:HB2	1:A:371:SER:HA	2.01	0.42
1:A:394:HIS:O	1:A:395:GLU:C	2.57	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: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: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: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
1:B:312:ALA:O	1:B:315:PHE:HB2	2.19	0.42
1:B:370:LEU:HA	1:B:370:LEU:HD23	1.87	0.42
1:B:731:GLU:HG2	1:B:733:GLU:HB2	2.02	0.42
1:C:340:LYS:C	1:C:342:GLY:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:298:GLY:O	1:A:299:GLU:C	2.58	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: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:647:ASP:O	1:B:648:PRO:C	2.58	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:108:VAL:O	2:E:112:LEU:HG	2.20	0.41
2:E:7:GLU:O	2:E:11:GLU:HG3	2.20	0.41
2:F:108:VAL:O	2:F:112:LEU:HG	2.19	0.41
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.78	0.41
1:A:636:ALA:O	1:A:640:LYS:HA	2.20	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: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
1:C:740:GLN:CD	1:C:740:GLN:H	2.23	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:540:ARG:NH1	1:A:627:TYR:CE1	2.88	0.41
1:B:385:LEU:O	1:B:385:LEU:HD13	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:470:ASN:CG	1:C:471:TRP:H	2.24	0.41
1:C:581:GLN:O	1:C:629:ASN:HA	2.20	0.41
1:C:740:GLN:N	1:C:740:GLN:CD	2.74	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:C:322:LEU:O	1:C:323:ASN:C	2.59	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:730:ASN:C	1:C:732:ILE:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:PRO:HB3	1:C:755:ARG:NH2	2.34	0.41
1:C:759:GLN:CA	1:C:759:GLN:NE2	2.83	0.41
2:D:105:LEU:HD12	2:D:125:ILE:HD13	2.02	0.41
1:C:665:LYS:HG2	2:F:11:GLU:CD	2.41	0.41
1:A:340:LYS:C	1:A:342:GLY:H	2.23	0.41
1:A:664:ILE:O	1:A:667:LEU:N	2.43	0.41
1:A:730:ASN:C	1:A:732:ILE:N	2.74	0.41
1:B:394:HIS:O	1:B:397:GLU:CB	2.69	0.41
1:B:628:PHE:C	1:B:628:PHE:CD1	2.93	0.41
1:C:308:VAL:O	1:C:311:HIS:HB2	2.21	0.41
1:C:752:LEU:O	1:C:753:LYS:C	2.58	0.41
1:A:699:GLY:O	1:A:702:SER:N	2.52	0.41
1:B:654:ILE:C	1:B:655:ASN:ND2	2.74	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:HG3	1:C:510:GLN:O	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: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: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:658:PRO:HB3	1:A:755:ARG:NH2	2.35	0.41
1:A:775:LEU:HD12	1:A:776:LEU:CD1	2.50	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
1:C:526:GLN:HB2	2:F:124:MET:CE	2.51	0.41
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:F:83:GLU:O	2:F:87:GLU:HG3	2.21	0.41
1:A:322:LEU:O	1:A:323:ASN:C	2.58	0.41
1:A:349:ASN:H	1:A:349:ASN:HD22	1.69	0.41
1:A:713:SER:O	1:A:714:GLN:C	2.58	0.41
1:B:639:ASN:OD1	1:B:641:ALA:HB2	2.21	0.41
1:A:581:GLN:O	1:A:629:ASN:HA	2.21	0.41
1:C:456:LYS:HD3	1:C:471:TRP:CE2	2.56	0.41
1:C:364:ILE:HB	1:C:477:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:SER:O	1:C:632:TYR:C	2.59	0.41
1:C:587:PRO:HD2	1:C:639:ASN:HD21	1.86	0.41
1:A:391:ILE:HD13	1:A:399:GLY:HA2	2.03	0.41
1:B:322:LEU:O	1:B:323:ASN:C	2.60	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: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: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
1:B:391:ILE:HD13	1:B:399:GLY:HA2	2.03	0.40
1:B:556:MET:HE2	1:B:560:LEU:CG	2.52	0.40
1:B:537:GLY:C	1:B:625:LEU:HD21	2.40	0.40
1:B:792:VAL:O	1:B:796:ILE:HG12	2.20	0.40
1:C:450:ASN:CG	1:C:452:GLU:HG3	2.42	0.40
2:F:29:THR:HG22	2:F:29:THR:O	2.21	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
2:D:14:GLU:OE1	2:D:14:GLU:HA	2.21	0.40
1:A:346:LYS:NZ	1:A:352:GLY:O	2.49	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:B:791:GLU:HG3	1:B:792:VAL:N	2.36	0.40
1:A:400:LYS:NZ	1:C:644:GLU:OE2	2.53	0.40
2:E:137:ASN:C	2:E:137:ASN:OD1	2.59	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:695:LYS:N	2:D:18:LEU:HD21	2.36	0.40
1:B:526:GLN:HA	2:E:124:MET:HE2	2.04	0.40
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.56	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:E:79:THR:C	2:E:81:SER:N	2.75	0.40
2:F:105:LEU:O	2:F:109:MET:HG2	2.21	0.40
1:A:752:LEU:O	1:A:753:LYS:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ILE:HA	1:B:755:ARG:CD	2.48	0.40
1:B:761:GLN:O	1:B:764:LEU:HB2	2.22	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:137:ASN:C	2:D:137:ASN:OD1	2.60	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 [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	478/507 (94%)	399 (84%)	69 (14%)	10 (2%)	7	31
1	B	462/507 (91%)	372 (80%)	69 (15%)	21 (4%)	2	15
1	C	499/507 (98%)	416 (83%)	68 (14%)	15 (3%)	4	24
2	D	141/147 (96%)	112 (79%)	26 (18%)	3 (2%)	7	31
2	E	141/147 (96%)	113 (80%)	25 (18%)	3 (2%)	7	31
2	F	141/147 (96%)	112 (79%)	26 (18%)	3 (2%)	7	31
All	All	1862/1962 (95%)	1524 (82%)	283 (15%)	55 (3%)	4	24

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	392 (91%)	40 (9%)	9	30
1	B	414/452 (92%)	369 (89%)	45 (11%)	6	24
1	C	448/452 (99%)	411 (92%)	37 (8%)	11	36
2	D	121/125 (97%)	118 (98%)	3 (2%)	47	72
2	E	121/125 (97%)	117 (97%)	4 (3%)	38	66
2	F	121/125 (97%)	117 (97%)	4 (3%)	38	66
All	All	1657/1731 (96%)	1524 (92%)	133 (8%)	12	37

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	VAL
1	A	303	LYS
1	A	309	PRO
1	A	346	LYS
1	A	373	LYS
1	A	385	LEU
1	A	400	LYS
1	A	406	ASP
1	A	419	ILE
1	A	438	ASN
1	A	445	ARG

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Mol	Chain	Res	Type
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	521	ASN
1	A	524	GLU
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	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	646	THR
1	A	659	THR
1	A	670	ILE
1	A	693	SER
1	A	694	VAL
1	A	707	SER
1	A	759	GLN
1	A	775	LEU
1	A	781	ASN
1	A	784	GLU
1	B	295	VAL
1	B	299	GLU
1	B	303	LYS
1	B	320	ARG
1	B	373	LYS
1	B	385	LEU
1	B	400	LYS
1	B	406	ASP
1	B	434	LEU
1	B	438	ASN
1	B	447	SER
1	B	455	TYR
1	B	458	LYS

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Mol	Chain	Res	Type
1	B	459	GLU
1	B	462	ILE
1	B	476	VAL
1	B	485	LEU
1	B	501	LEU
1	B	521	ASN
1	B	536	TYR
1	B	540	ARG
1	B	545	THR
1	B	546	LYS
1	B	552	TRP
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	629	ASN
1	B	633	ASN
1	B	639	ASN
1	B	646	THR
1	B	714	GLN
1	B	729	TYR
1	B	739	LYS
1	B	744	GLU
1	B	747	ASN
1	B	761	GLN
1	B	784	GLU
1	B	789	ASN
1	B	790	PHE
1	C	295	VAL
1	C	303	LYS
1	C	320	ARG
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	434	LEU

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Mol	Chain	Res	Type
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	531	ASN
1	C	535	LYS
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	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	646	THR
1	C	707	SER
1	C	759	GLN
1	C	775	LEU
1	C	781	ASN
1	C	784	GLU
2	D	76	MET
2	D	110	THR
2	D	135	GLN
2	E	58	ASP
2	E	76	MET
2	E	110	THR
2	E	135	GLN
2	F	58	ASP
2	F	76	MET
2	F	110	THR
2	F	135	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) 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	507	GLN
1	A	518	ASN
1	A	521	ASN
1	A	553	GLN
1	A	581	GLN
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	758	ASN
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	438	ASN
1	B	507	GLN
1	B	521	ASN
1	B	551	ASN
1	B	553	GLN
1	B	581	GLN
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

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Mol	Chain	Res	Type
1	B	789	ASN
1	B	794	GLN
1	C	323	ASN
1	C	351	HIS
1	C	368	GLN
1	C	438	ASN
1	C	507	GLN
1	C	518	ASN
1	C	553	GLN
1	C	581	GLN
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	758	ASN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	C	3999	3	22,27,27	2.81	10 (45%)	22,41,41	2.31	5 (22%)
4	EMA	B	2999	3	22,27,27	2.38	5 (22%)	22,41,41	2.10	4 (18%)
4	EMA	A	1999	3	22,27,27	2.23	6 (27%)	22,41,41	2.20	7 (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	C	3999	3	-	4/17/20/20	0/2/2/2
4	EMA	B	2999	3	-	3/17/20/20	0/2/2/2
4	EMA	A	1999	3	-	2/17/20/20	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3999	EMA	PA-C5'	-7.72	1.60	1.80
4	A	1999	EMA	PA-C5'	-7.69	1.61	1.80
4	B	2999	EMA	PA-C5'	-7.05	1.62	1.80
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	C4-N3	4.69	1.42	1.35
4	B	2999	EMA	C2-N3	3.18	1.37	1.32
4	C	3999	EMA	C1'-N9	3.12	1.57	1.49
4	C	3999	EMA	PA-O2A	-3.12	1.49	1.56
4	A	1999	EMA	PA-O2A	-2.99	1.49	1.56
4	B	2999	EMA	C4-N3	2.98	1.39	1.35
4	A	1999	EMA	C2-N3	2.89	1.36	1.32
4	C	3999	EMA	C1'-C4'	2.86	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3999	EMA	O5'-C4'	2.67	1.53	1.42
4	B	2999	EMA	PA-O2A	-2.37	1.50	1.56
4	C	3999	EMA	C2-N3	2.33	1.35	1.32
4	A	1999	EMA	C8-N7	-2.12	1.30	1.34
4	A	1999	EMA	O5'-C5'	2.11	1.45	1.42
4	C	3999	EMA	PG-O1G	-2.10	1.46	1.54
4	A	1999	EMA	PG-O1G	-2.05	1.47	1.54
4	C	3999	EMA	C5-C4	-2.02	1.35	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3999	EMA	C4'-C1'-N9	8.83	128.28	111.19
4	B	2999	EMA	C4'-C1'-N9	7.49	125.69	111.19
4	A	1999	EMA	C4'-C1'-N9	6.37	123.52	111.19
4	A	1999	EMA	C4-C5-N7	3.54	113.09	109.40
4	A	1999	EMA	C5'-O5'-C4'	-3.31	104.82	112.90
4	C	3999	EMA	O2A-PA-O1A	2.68	119.01	110.07
4	B	2999	EMA	O5'-C4'-C1'	2.59	119.78	109.92
4	A	1999	EMA	O5'-C4'-C1'	2.56	119.65	109.92
4	C	3999	EMA	C1'-N9-C8	2.53	138.69	126.15
4	A	1999	EMA	O2A-PA-O1A	2.33	117.86	110.07
4	C	3999	EMA	O1A-PA-C5'	-2.33	104.66	112.92
4	A	1999	EMA	N6-C6-N1	2.26	123.25	118.57
4	C	3999	EMA	O3B-PG-O2G	-2.17	99.16	111.19
4	A	1999	EMA	O3B-PG-O2G	-2.13	99.36	111.19
4	B	2999	EMA	O2A-PA-O1A	2.08	117.01	110.07
4	B	2999	EMA	O3B-PG-O2G	-2.06	99.75	111.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

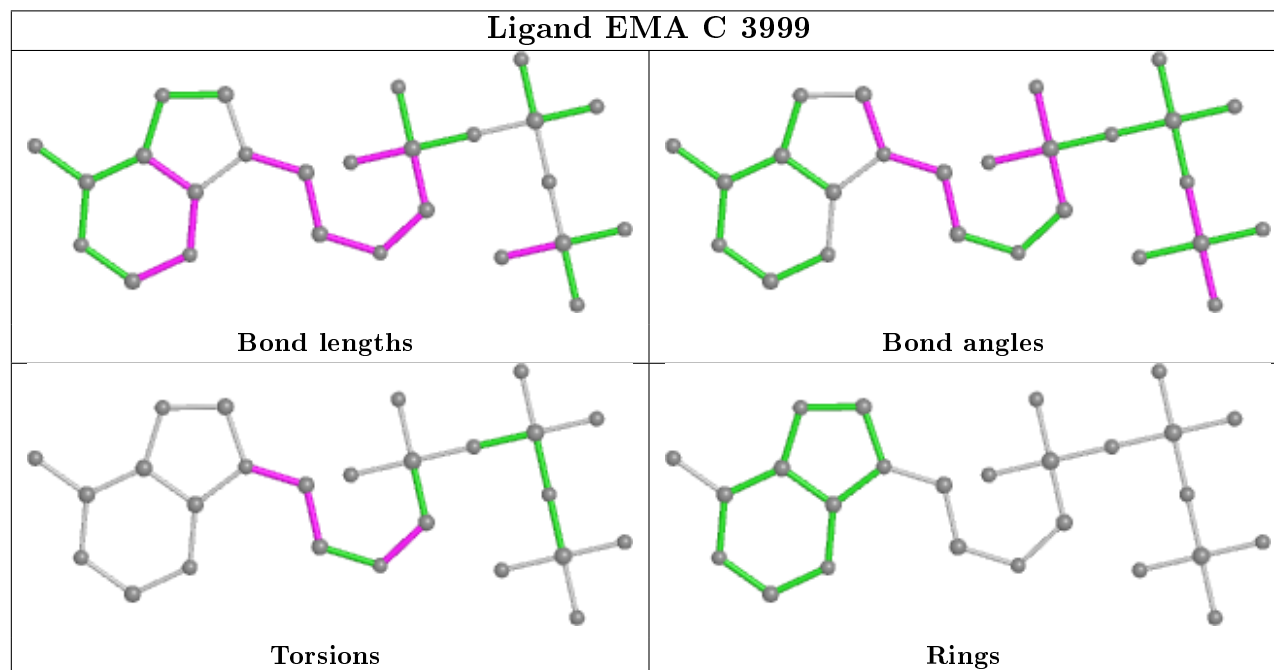
Mol	Chain	Res	Type	Atoms
4	A	1999	EMA	PA-C5'-O5'-C4'
4	A	1999	EMA	N9-C1'-C4'-O5'
4	C	3999	EMA	PA-C5'-O5'-C4'
4	C	3999	EMA	N9-C1'-C4'-O5'
4	C	3999	EMA	C4'-C1'-N9-C8
4	C	3999	EMA	C4'-C1'-N9-C4
4	B	2999	EMA	PA-C5'-O5'-C4'
4	B	2999	EMA	N9-C1'-C4'-O5'
4	B	2999	EMA	C4'-C1'-N9-C8

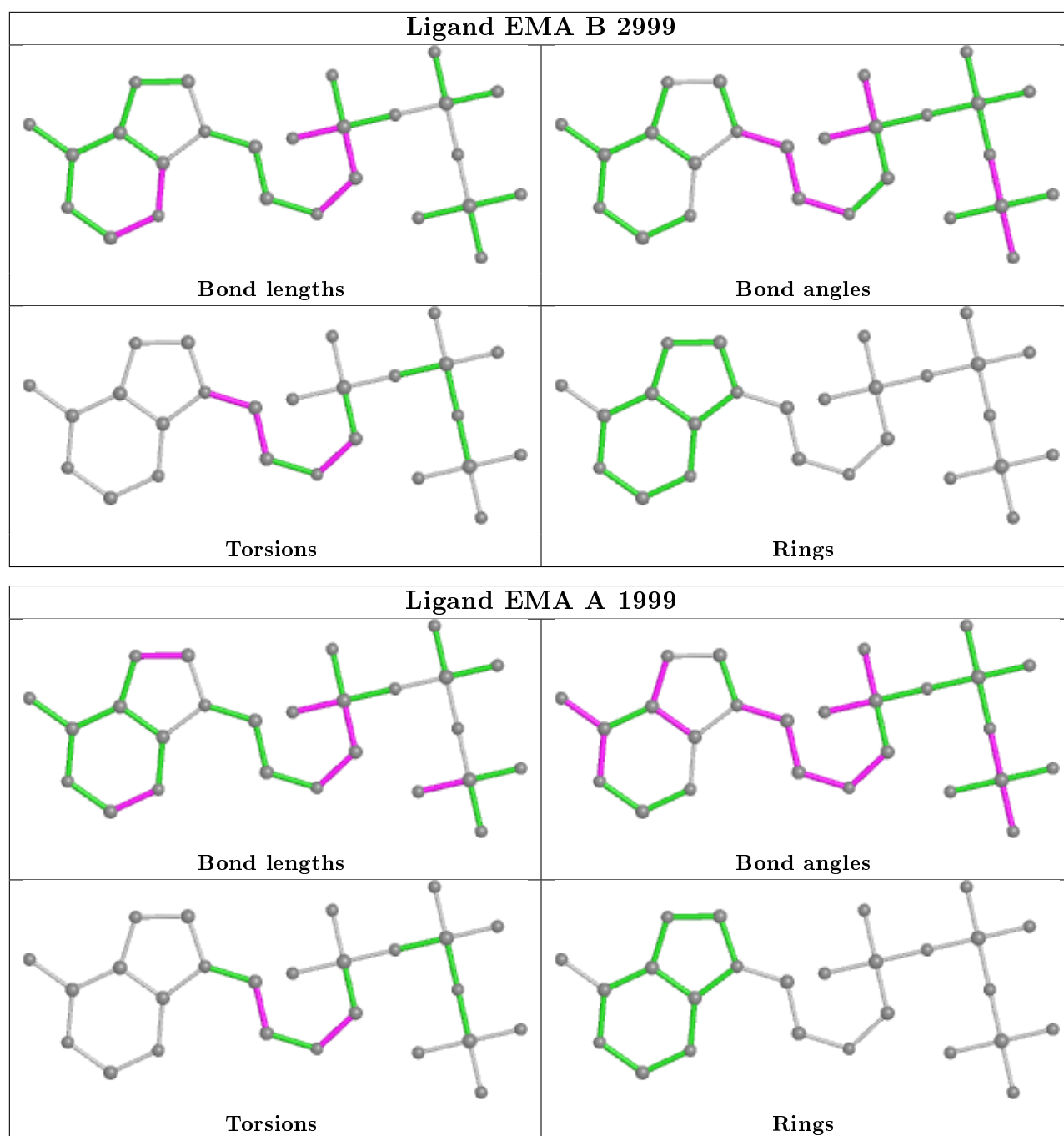
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3999	EMA	7	0
4	B	2999	EMA	5	0
4	A	1999	EMA	1	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	484/507 (95%)	-0.17	12 (2%)	57	54	11, 51, 126, 154	16 (3%)
1	B	462/507 (91%)	0.02	17 (3%)	41	38	13, 54, 141, 149	12 (2%)
1	C	491/507 (96%)	-0.11	15 (3%)	49	48	12, 53, 129, 152	19 (3%)
2	D	143/147 (97%)	0.70	23 (16%)	1	2	34, 123, 158, 160	0
2	E	143/147 (97%)	0.68	22 (15%)	2	2	36, 130, 158, 160	0
2	F	143/147 (97%)	0.64	22 (15%)	2	2	37, 128, 157, 159	0
All	All	1866/1962 (95%)	0.09	111 (5%)	22	22	11, 58, 150, 160	47 (2%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	693	SER	13.4
1	B	697	ILE	8.1
1	B	773	PHE	6.4
2	D	24	ASP	5.6
2	F	62	THR	5.4
2	D	79	THR	5.4
1	C	783	THR	5.1
2	F	73	ALA	5.1
2	D	57	ALA	5.0
2	D	78	ASP	4.8
2	D	77	LYS	4.8
2	F	24	ASP	4.7
2	E	21	LYS	4.6
2	F	29	THR	4.6
1	A	694	VAL	4.4
1	B	785	ASN	4.3
2	D	43	PRO	4.2
1	A	784	GLU	4.2
2	E	19	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	48	LEU	4.1
1	A	783	THR	4.1
2	D	53	ASN	4.1
2	D	56	ASP	4.0
1	B	786	GLU	3.9
1	C	675	ASN	3.9
1	C	785	ASN	3.9
2	F	46	ALA	3.9
1	C	689	ALA	3.8
1	C	786	GLU	3.8
1	B	711	ILE	3.7
1	B	747	ASN	3.6
2	E	51	MET	3.6
1	B	765	THR	3.6
1	A	737	LYS	3.5
2	F	61	GLY	3.5
1	C	741	ILE	3.5
2	E	77	LYS	3.5
2	E	24	ASP	3.4
2	E	55	VAL	3.3
1	B	740	GLN	3.3
2	D	73	ALA	3.3
2	E	59	GLY	3.3
2	E	58	ASP	3.2
2	E	73	ALA	3.2
2	E	76	MET	3.2
2	E	42	ASN	3.2
1	C	518	ASN	3.1
2	F	77	LYS	3.1
2	D	52	ILE	3.1
1	B	783	THR	3.1
2	D	76	MET	3.1
1	C	784	GLU	3.0
2	F	80	ASP	3.0
2	F	21	LYS	3.0
2	E	48	LEU	3.0
1	A	787	THR	2.9
1	C	692	GLU	2.9
2	D	51	MET	2.8
2	F	51	MET	2.8
1	B	751	TYR	2.8
1	C	779	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	30	LYS	2.8
2	F	44	THR	2.7
2	E	57	ALA	2.7
2	D	66	PRO	2.7
2	F	53	ASN	2.7
1	A	798	ASP	2.7
2	D	49	GLN	2.7
1	B	787	THR	2.7
2	F	57	ALA	2.7
2	F	74	ARG	2.6
1	C	707	SER	2.6
1	A	779	GLN	2.6
1	C	787	THR	2.6
1	B	705	TYR	2.6
2	F	59	GLY	2.5
2	E	69	LEU	2.5
2	D	50	ASP	2.5
2	F	78	ASP	2.5
1	A	429	GLY	2.5
1	B	782	PHE	2.5
1	C	688	PHE	2.4
2	E	147	ALA	2.4
2	E	53	ASN	2.4
2	F	43	PRO	2.4
2	E	116	LEU	2.4
2	D	58	ASP	2.3
2	E	80	ASP	2.3
2	F	20	ASP	2.3
2	F	147	ALA	2.3
1	B	766	HIS	2.3
2	D	45	GLU	2.2
2	D	60	ASN	2.2
1	B	702	SER	2.2
2	D	30	LYS	2.2
2	F	70	THR	2.2
2	E	72	MET	2.1
2	D	28	THR	2.1
2	E	29	THR	2.1
2	F	19	PHE	2.1
2	D	55	VAL	2.1
2	E	54	GLU	2.1
1	B	779	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	520	PRO	2.1
1	B	518	ASN	2.1
1	A	292	ARG	2.0
1	C	740	GLN	2.0
1	A	741	ILE	2.0
2	E	78	ASP	2.0
1	A	695	LYS	2.0
2	D	42	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

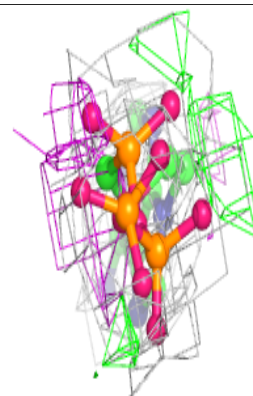
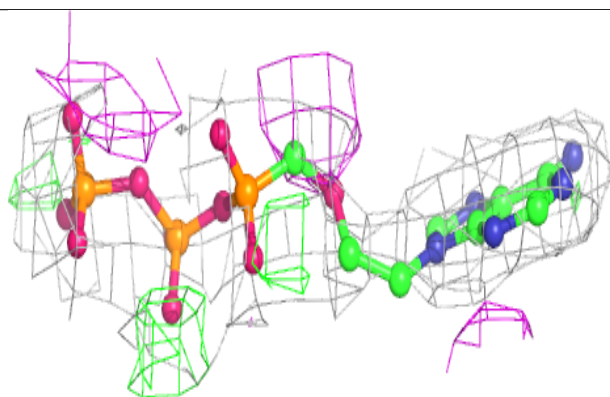
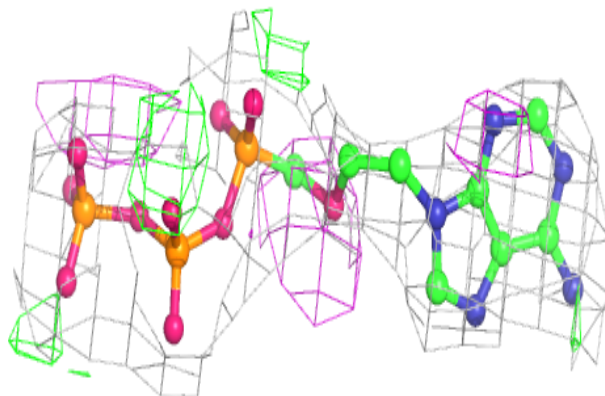
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EMA	B	2999	26/26	0.88	0.25	43,55,60,63	0
4	EMA	C	3999	26/26	0.89	0.25	46,63,71,72	0
4	EMA	A	1999	26/26	0.94	0.19	29,37,41,41	0
5	CA	F	804	1/1	0.95	0.08	44,44,44,44	0
5	CA	E	802	1/1	0.97	0.08	83,83,83,83	0
5	CA	F	805	1/1	0.97	0.04	48,48,48,48	0
3	YB	B	902	1/1	0.98	0.06	82,82,82,82	0
5	CA	D	800	1/1	0.98	0.09	30,30,30,30	0
3	YB	A	901	1/1	0.99	0.06	77,77,77,77	0
5	CA	E	803	1/1	0.99	0.05	47,47,47,47	0
5	CA	D	801	1/1	0.99	0.04	37,37,37,37	0
3	YB	C	903	1/1	0.99	0.06	86,86,86,86	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.

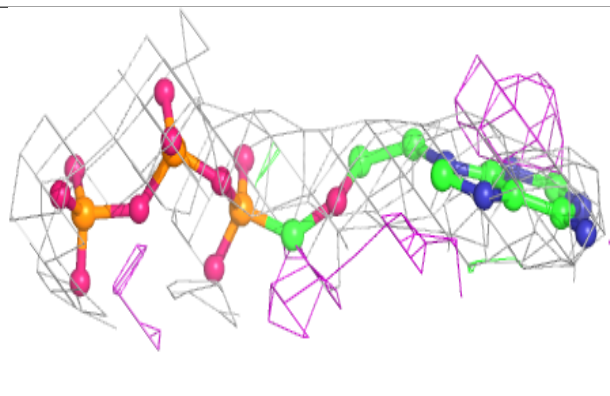
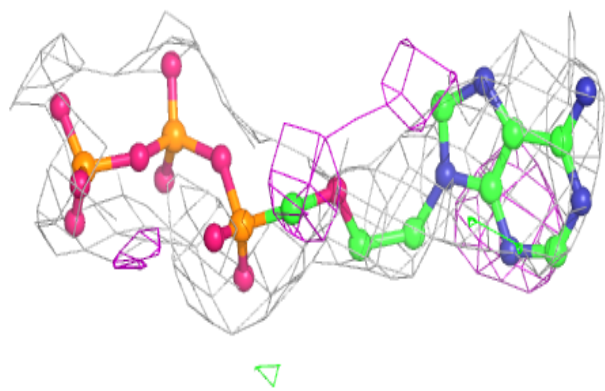
Electron density around EMA B 2999:

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



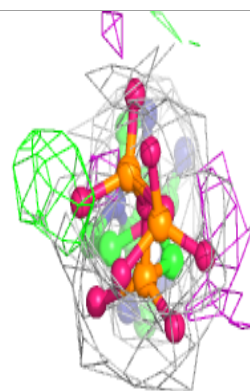
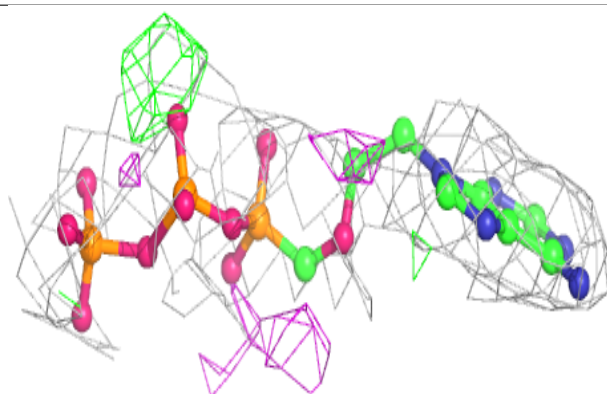
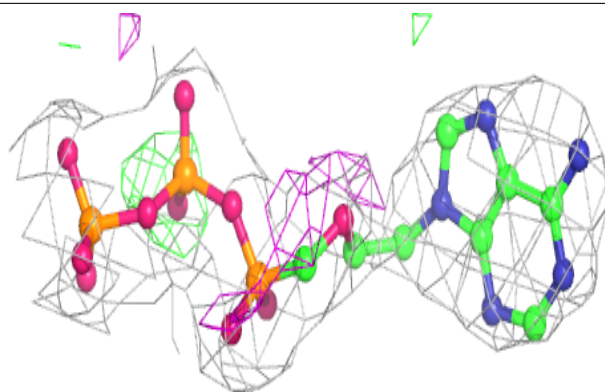
Electron density around EMA C 3999:

$2mF_o-DF_c$ (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.