



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 PM UTC

PDB ID : 1GKI / pdb_00001gki
Title : Plasmid coupling protein TrwB in complex with ADP and Mg2+.
Authors : Gomis-Ruth, F.X.; Moncalian, G.; De La cruz, F.; Coll, M.
Deposited on : 2001-08-14
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

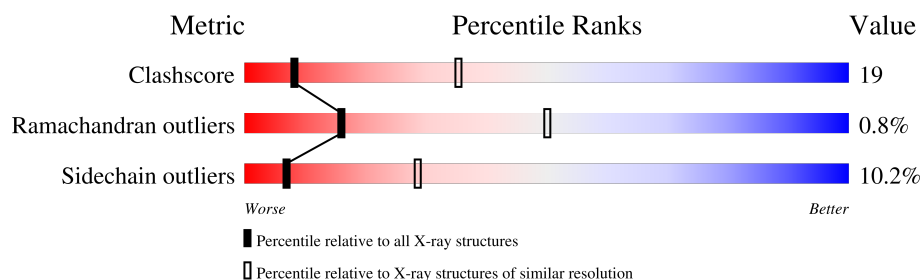
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	60% 29% 5% 5%
1	B	437	59% 30% 5% • 5%
1	D	437	59% 31% 5% 5%
1	E	437	60% 27% 7% 5%
1	F	437	59% 29% 6% 6%
1	G	437	56% 31% 6% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPE	E	1505	-	-	X	-
4	EPE	E	1506	-	X	-	-

2 Entry composition (i)

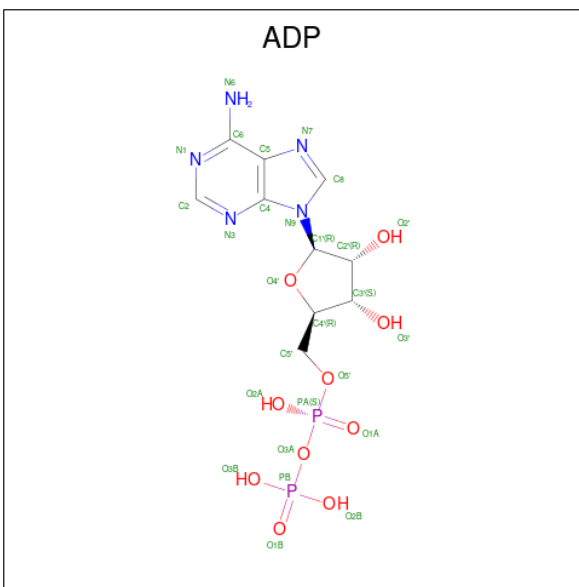
There are 5 unique types of molecules in this entry. The entry contains 20150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CONJUGAL TRANSFER PROTEIN TRWB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total 3261	C 2063	N 582	O 606	S 10	0	0	0
1	B	417	Total 3274	C 2069	N 587	O 608	S 10	0	0	0
1	D	416	Total 3269	C 2067	N 586	O 606	S 10	0	0	0
1	E	414	Total 3254	C 2059	N 581	O 604	S 10	0	0	0
1	F	412	Total 3237	C 2048	N 578	O 601	S 10	0	0	0
1	G	413	Total 3241	C 2050	N 579	O 602	S 10	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

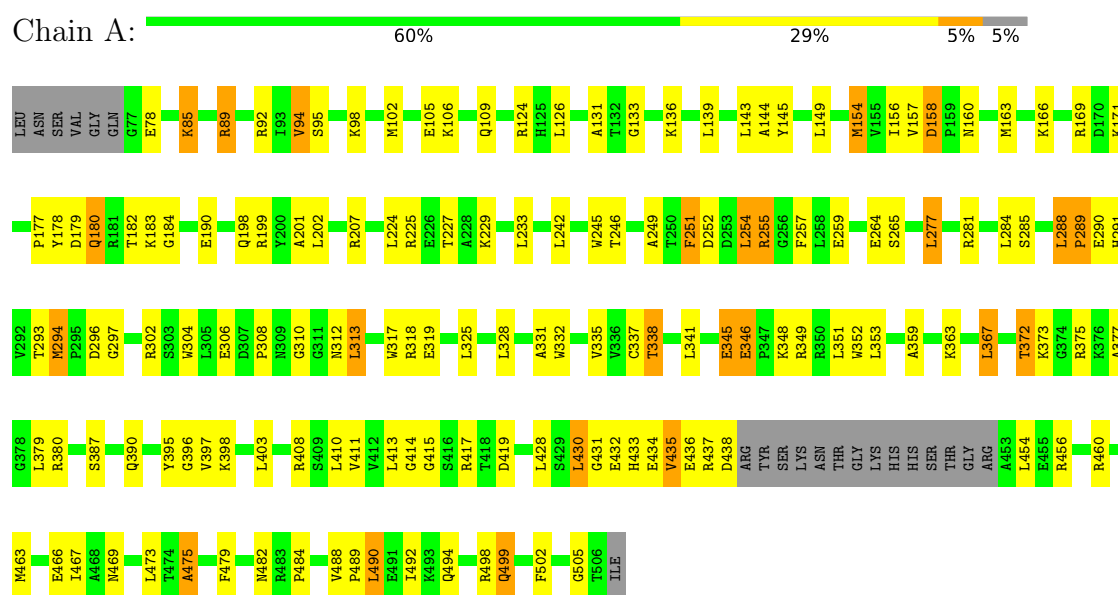
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	86	Total	O	0	0
			86	86		
5	D	85	Total	O	0	0
			85	85		
5	E	75	Total	O	0	0
			75	75		
5	F	51	Total	O	0	0
			51	51		
5	G	48	Total	O	0	0
			48	48		

3 Residue-property plots [i](#)

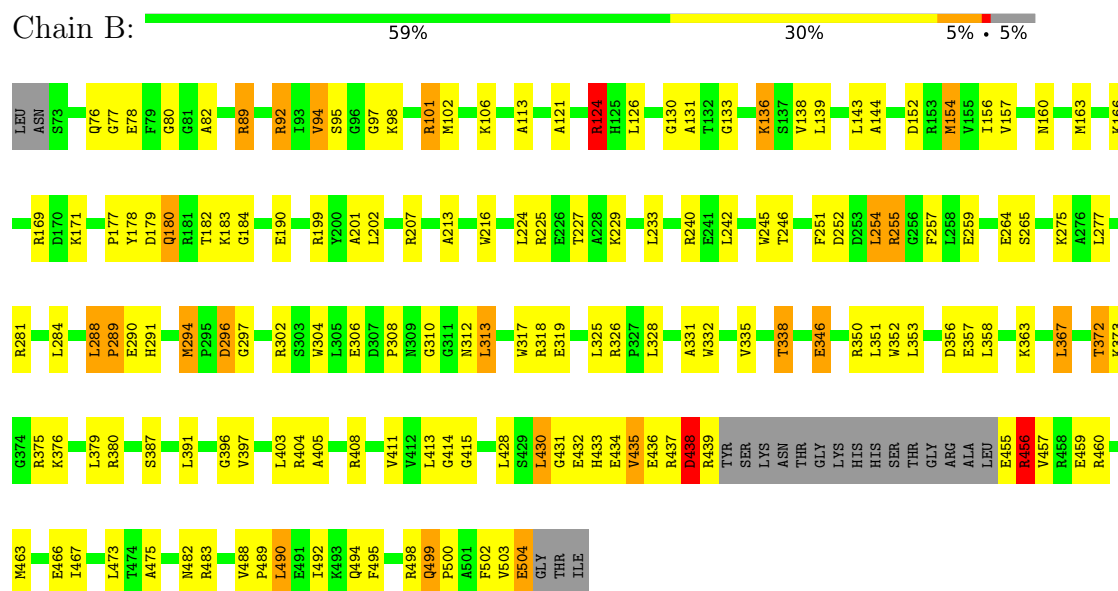
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

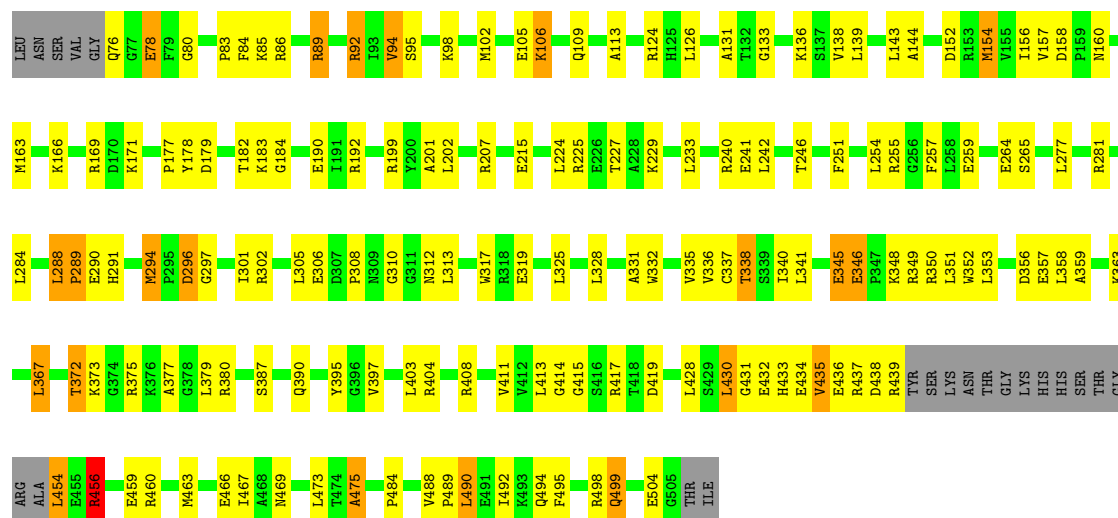


• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

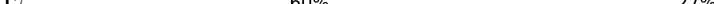


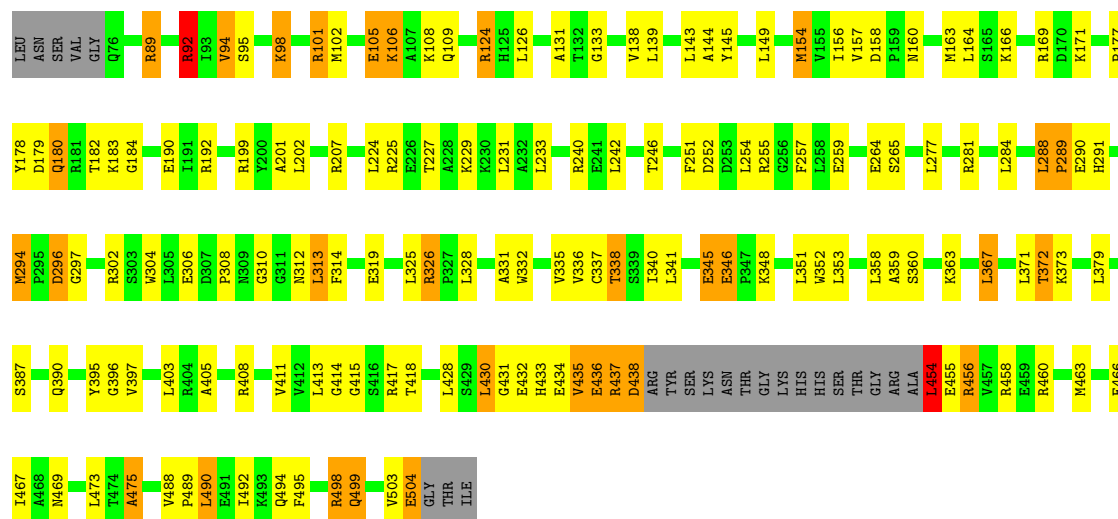
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain D:  59% 31% 5% 5%



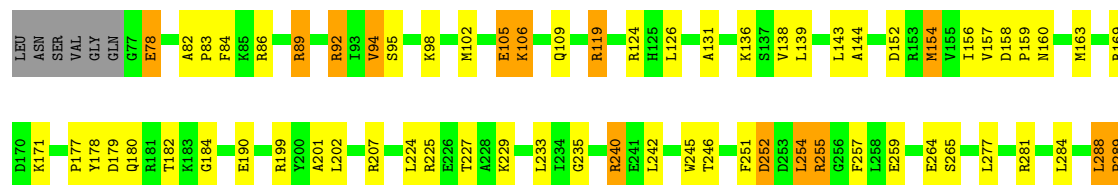
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

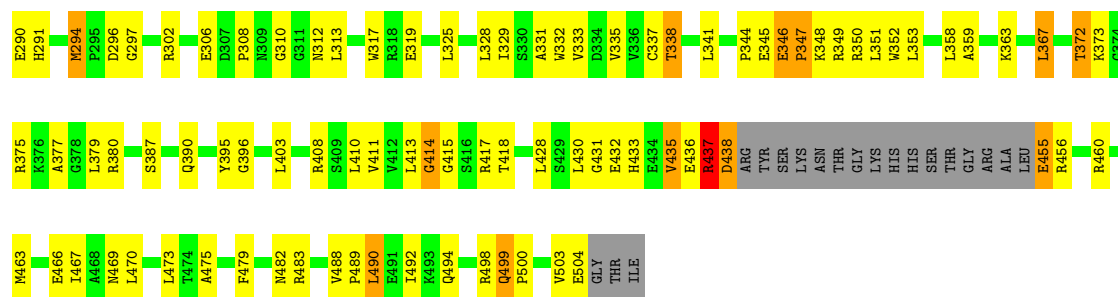
Chain E:  60% 27% 7% 5%



- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

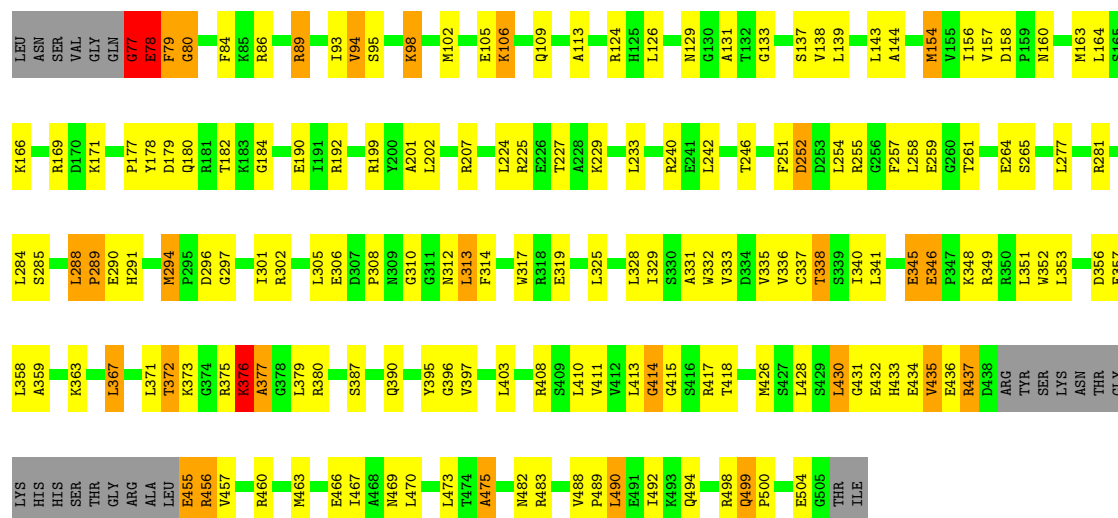
Chain F: 59% 29% 6% 6%





• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain G: 56% 31% 6% • 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.10Å 151.10Å 251.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (50.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20150	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, EPE, MG

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	0.49	0/3325	0.94	13/4495 (0.3%)
1	B	0.58	1/3338 (0.0%)	1.05	19/4511 (0.4%)
1	D	0.54	1/3333 (0.0%)	0.96	15/4504 (0.3%)
1	E	0.78	13/3318 (0.4%)	1.15	33/4485 (0.7%)
1	F	0.70	7/3301 (0.2%)	1.11	26/4462 (0.6%)
1	G	0.82	11/3305 (0.3%)	1.23	33/4467 (0.7%)
All	All	0.66	33/19920 (0.2%)	1.08	139/26924 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	1	3
All	All	1	4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	77	GLY	N-CA	22.80	1.82	1.45
1	G	79	PHE	C-O	-12.61	1.08	1.23
1	G	78	GLU	CA-C	-11.90	1.36	1.52
1	E	456	ARG	CZ-NH1	-10.32	1.18	1.32
1	E	92	ARG	CD-NE	-9.99	1.32	1.46
1	F	437	ARG	CA-C	-9.24	1.41	1.52
1	G	79	PHE	CA-CB	8.74	1.67	1.53
1	E	106	LYS	C-N	8.41	1.45	1.33
1	F	105	GLU	CA-C	-8.32	1.42	1.52
1	E	456	ARG	NE-CZ	7.94	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	79	PHE	CD2-CE2	7.87	1.62	1.38
1	E	436	GLU	CA-C	-7.81	1.43	1.52
1	G	456	ARG	CG-CD	-7.75	1.29	1.52
1	F	438	ASP	C-O	7.63	1.38	1.23
1	F	346	GLU	N-CA	-7.58	1.39	1.46
1	G	78	GLU	N-CA	-7.55	1.36	1.46
1	E	437	ARG	C-O	-7.17	1.15	1.24
1	E	437	ARG	CA-CB	-6.70	1.42	1.53
1	E	438	ASP	CA-CB	6.70	1.66	1.53
1	E	456	ARG	CD-NE	-6.51	1.37	1.46
1	G	375	ARG	CA-C	-6.37	1.45	1.52
1	E	326	ARG	CZ-NH2	6.35	1.41	1.33
1	G	78	GLU	C-N	5.90	1.41	1.33
1	G	456	ARG	CA-C	-5.84	1.45	1.52
1	E	180	GLN	CD-NE2	-5.61	1.21	1.33
1	F	345	GLU	N-CA	-5.61	1.38	1.46
1	F	437	ARG	N-CA	-5.49	1.38	1.45
1	G	456	ARG	NE-CZ	-5.45	1.27	1.33
1	E	438	ASP	CG-OD2	5.33	1.35	1.25
1	D	456	ARG	CG-CD	-5.32	1.36	1.52
1	E	438	ASP	CB-CG	5.20	1.65	1.52
1	B	92	ARG	CA-C	-5.06	1.46	1.52
1	F	119	ARG	CD-NE	-5.05	1.39	1.46

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	78	GLU	N-CA-C	24.89	163.82	110.80
1	G	79	PHE	N-CA-C	21.74	142.57	109.96
1	E	438	ASP	CA-C-O	17.68	150.86	120.80
1	E	456	ARG	CG-CD-NE	-14.17	80.83	112.00
1	G	78	GLU	N-CA-CB	-12.70	89.03	110.49
1	G	79	PHE	N-CA-CB	-11.54	92.65	109.85
1	G	437	ARG	NE-CZ-NH1	-11.40	110.09	121.50
1	B	92	ARG	NH1-CZ-NH2	10.15	132.49	119.30
1	G	377	ALA	N-CA-C	-9.99	101.09	113.38
1	G	77	GLY	O-C-N	9.72	138.55	123.00
1	F	310	GLY	N-CA-C	-9.56	100.31	112.54
1	E	456	ARG	NE-CZ-NH2	9.50	127.75	119.20
1	E	326	ARG	NE-CZ-NH2	9.48	127.73	119.20
1	G	78	GLU	CA-C-N	9.37	134.07	120.95
1	G	78	GLU	C-N-CA	9.37	134.07	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	78	GLU	CA-CB-CG	9.32	132.75	114.10
1	B	92	ARG	CG-CD-NE	-9.12	91.93	112.00
1	F	344	PRO	CA-C-N	-8.98	109.53	122.19
1	F	344	PRO	C-N-CA	-8.98	109.53	122.19
1	B	92	ARG	NE-CZ-NH1	-8.91	112.59	121.50
1	G	201	ALA	N-CA-C	-8.90	101.49	111.82
1	F	346	GLU	CA-C-N	8.82	128.84	119.05
1	F	346	GLU	C-N-CA	8.82	128.84	119.05
1	E	201	ALA	N-CA-C	-8.64	101.79	111.82
1	F	105	GLU	CA-C-N	8.61	131.64	120.44
1	F	105	GLU	C-N-CA	8.61	131.64	120.44
1	D	201	ALA	N-CA-C	-8.59	101.85	111.82
1	B	201	ALA	N-CA-C	-8.54	101.91	111.82
1	F	201	ALA	N-CA-C	-8.50	101.96	111.82
1	A	201	ALA	N-CA-C	-8.38	101.67	112.23
1	G	437	ARG	NE-CZ-NH2	8.30	126.67	119.20
1	G	455	GLU	CA-C-N	-8.29	111.75	122.77
1	G	455	GLU	C-N-CA	-8.29	111.75	122.77
1	E	326	ARG	NE-CZ-NH1	-8.09	113.41	121.50
1	F	345	GLU	N-CA-C	7.97	122.70	109.46
1	G	456	ARG	CG-CD-NE	-7.88	94.66	112.00
1	F	456	ARG	N-CA-C	-7.55	96.92	109.07
1	E	105	GLU	CA-C-N	7.08	129.64	120.44
1	E	105	GLU	C-N-CA	7.08	129.64	120.44
1	F	431	GLY	N-CA-C	6.94	121.42	112.68
1	G	77	GLY	CA-C-O	-6.86	106.39	120.80
1	D	92	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	G	310	GLY	N-CA-C	-6.79	104.86	112.33
1	E	326	ARG	CB-CG-CD	6.78	126.89	111.30
1	E	296	ASP	N-CA-C	6.76	120.88	110.20
1	E	101	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	D	296	ASP	N-CA-C	6.63	119.84	110.50
1	F	455	GLU	CB-CG-CD	-6.54	101.49	112.60
1	A	288	LEU	N-CA-C	6.48	122.46	113.45
1	A	157	VAL	N-CA-C	-6.30	98.43	107.37
1	A	310	GLY	N-CA-C	-6.21	105.50	112.33
1	F	288	LEU	N-CA-C	6.18	121.28	113.25
1	E	310	GLY	N-CA-C	-6.15	105.57	112.33
1	G	80	GLY	N-CA-C	6.13	121.27	113.24
1	G	288	LEU	N-CA-C	6.12	121.20	113.25
1	G	346	GLU	CA-C-N	6.11	125.83	119.05
1	G	346	GLU	C-N-CA	6.11	125.83	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	ARG	CB-CG-CD	-6.09	97.29	111.30
1	E	288	LEU	N-CA-C	6.03	121.83	113.45
1	B	438	ASP	N-CA-C	6.02	119.46	109.46
1	B	346	GLU	CA-C-N	6.02	125.73	119.05
1	B	346	GLU	C-N-CA	6.02	125.73	119.05
1	B	288	LEU	N-CA-C	5.97	121.74	113.45
1	B	310	GLY	N-CA-C	-5.96	105.07	111.93
1	D	310	GLY	N-CA-C	-5.91	105.83	112.33
1	D	346	GLU	CA-C-N	5.89	125.59	119.05
1	D	346	GLU	C-N-CA	5.89	125.59	119.05
1	E	438	ASP	N-CA-CB	5.88	120.49	110.50
1	B	77	GLY	N-CA-C	-5.86	107.79	115.47
1	E	456	ARG	CD-NE-CZ	-5.86	116.20	124.40
1	E	106	LYS	CA-C-O	5.83	126.94	120.82
1	F	347	PRO	N-CA-C	-5.82	105.44	113.53
1	E	92	ARG	CB-CG-CD	-5.81	97.94	111.30
1	B	397	VAL	N-CA-C	5.80	116.26	110.23
1	G	397	VAL	N-CA-C	5.78	116.24	110.23
1	F	157	VAL	N-CA-C	-5.77	99.17	107.37
1	A	397	VAL	N-CA-C	5.76	116.22	110.23
1	D	288	LEU	N-CA-C	5.76	121.45	113.45
1	F	240	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	F	345	GLU	N-CA-CB	5.72	119.60	110.16
1	B	396	GLY	N-CA-C	-5.72	104.52	112.18
1	A	431	GLY	N-CA-C	5.70	121.24	112.81
1	D	431	GLY	N-CA-C	5.68	121.21	112.81
1	B	157	VAL	N-CA-C	-5.67	99.32	107.37
1	G	376	LYS	CG-CD-CE	-5.66	98.28	111.30
1	D	157	VAL	N-CA-C	-5.63	99.37	107.37
1	F	240	ARG	NE-CZ-NH2	5.63	124.26	119.20
1	F	345	GLU	CA-CB-CG	5.62	125.34	114.10
1	D	183	LYS	N-CA-C	-5.57	103.34	110.53
1	E	437	ARG	CA-C-O	5.51	128.39	120.51
1	G	157	VAL	N-CA-C	-5.50	99.55	107.37
1	E	106	LYS	N-CA-CB	-5.49	102.05	110.01
1	A	337	CYS	N-CA-C	5.47	116.92	111.07
1	B	183	LYS	N-CA-C	-5.46	103.48	110.53
1	E	157	VAL	N-CA-C	-5.43	99.66	107.37
1	E	397	VAL	N-CA-C	5.41	115.86	110.23
1	E	454	LEU	CA-C-N	-5.41	113.36	122.29
1	E	454	LEU	C-N-CA	-5.41	113.36	122.29
1	D	397	VAL	N-CA-C	5.41	115.86	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	ALA	N-CA-C	5.39	117.59	109.23
1	G	437	ARG	N-CA-C	5.39	117.61	109.41
1	B	92	ARG	CB-CA-C	-5.39	100.96	109.80
1	E	337	CYS	N-CA-C	5.38	117.15	111.28
1	E	431	GLY	N-CA-C	5.37	120.76	112.81
1	F	438	ASP	CB-CG-OD2	5.33	130.66	118.40
1	F	438	ASP	N-CA-CB	5.32	119.54	110.50
1	G	457	VAL	N-CA-C	5.32	116.32	108.45
1	F	337	CYS	N-CA-C	5.31	117.06	111.28
1	G	475	ALA	N-CA-C	5.31	117.46	109.23
1	G	78	GLU	CB-CA-C	-5.30	99.88	110.42
1	D	158	ASP	N-CA-C	5.29	119.97	109.01
1	B	124	ARG	N-CA-C	-5.28	106.88	113.38
1	E	92	ARG	CD-NE-CZ	-5.28	117.00	124.40
1	G	455	GLU	CA-CB-CG	5.27	124.65	114.10
1	B	456	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	346	GLU	CA-C-N	5.21	124.84	119.05
1	A	346	GLU	C-N-CA	5.21	124.84	119.05
1	G	396	GLY	N-CA-C	-5.21	105.20	112.18
1	A	475	ALA	N-CA-C	5.17	117.25	109.23
1	E	437	ARG	CB-CA-C	-5.17	100.14	110.42
1	A	158	ASP	N-CA-C	5.15	118.93	109.10
1	F	438	ASP	CA-CB-CG	-5.12	107.47	112.60
1	D	92	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	E	396	GLY	N-CA-C	-5.10	105.35	112.18
1	F	396	GLY	N-CA-C	-5.08	105.37	112.18
1	D	337	CYS	N-CA-C	5.07	116.81	111.28
1	B	431	GLY	N-CA-C	5.07	120.31	112.81
1	E	183	LYS	N-CA-C	-5.05	103.26	110.59
1	F	437	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	G	337	CYS	N-CA-C	5.05	116.47	111.07
1	G	455	GLU	N-CA-C	5.05	125.13	111.00
1	A	183	LYS	N-CA-C	-5.04	104.03	110.53
1	A	396	GLY	N-CA-C	-5.04	105.43	112.18
1	B	457	VAL	N-CA-C	5.04	115.91	108.45
1	G	431	GLY	N-CA-C	5.04	120.67	112.61
1	E	475	ALA	N-CA-C	5.03	117.03	109.23
1	E	437	ARG	N-CA-C	5.03	121.51	110.80
1	E	346	GLU	CA-C-N	5.00	124.60	119.05
1	E	346	GLU	C-N-CA	5.00	124.60	119.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	78	GLU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	437	ARG	Sidechain
1	G	77	GLY	Peptide,Mainchain
1	G	78	GLU	Mainchain

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	3261	0	3290	122	0
1	B	3274	0	3302	131	1
1	D	3269	0	3299	135	1
1	E	3254	0	3283	142	1
1	F	3237	0	3264	129	1
1	G	3241	0	3266	141	0
2	A	27	0	12	3	0
2	B	27	0	12	4	0
2	D	27	0	12	3	0
2	E	27	0	12	3	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	E	30	0	33	13	0
5	A	72	0	0	2	0
5	B	86	0	0	3	0
5	D	85	0	0	5	0
5	E	75	0	0	2	0
5	F	51	0	0	1	0
5	G	48	0	0	1	0
All	All	20150	0	19809	762	2

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 19.

All (762) 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:G:77:GLY:N	1:G:77:GLY:CA	1.82	1.41
1:E:101:ARG:HH12	4:E:1505:EPE:H101	1.05	1.14
1:E:438:ASP:HB3	1:E:454:LEU:CD1	1.88	1.03
1:E:438:ASP:HB3	1:E:454:LEU:CG	1.90	1.01
1:B:98:LYS:O	1:B:102:MET:HG3	1.60	1.01
1:D:215:GLU:HG2	5:D:2044:HOH:O	1.62	0.99
1:G:169:ARG:HH11	1:G:171:LYS:HD3	1.25	0.99
1:E:169:ARG:HH11	1:E:171:LYS:HD3	1.28	0.98
1:G:437:ARG:O	1:G:455:GLU:HB3	1.65	0.96
1:D:192:ARG:HD3	5:D:2028:HOH:O	1.67	0.94
1:F:347:PRO:HA	5:F:2037:HOH:O	1.66	0.94
1:E:438:ASP:HB3	1:E:454:LEU:HG	1.47	0.93
1:E:101:ARG:NH1	4:E:1505:EPE:H101	1.83	0.93
1:A:169:ARG:HH11	1:A:171:LYS:HD3	1.32	0.93
1:B:92:ARG:HD2	5:B:2003:HOH:O	1.68	0.92
1:B:503:VAL:O	1:B:504:GLU:HB2	1.67	0.92
1:F:169:ARG:HH11	1:F:171:LYS:HD3	1.36	0.91
1:E:101:ARG:HH22	4:E:1505:EPE:C2	1.84	0.90
1:F:156:ILE:HD13	1:F:163:MET:HE3	1.53	0.90
1:B:180:GLN:HE21	1:B:504:GLU:HG2	1.37	0.89
1:E:192:ARG:HD3	5:E:2025:HOH:O	1.72	0.89
1:F:413:LEU:HD23	1:F:475:ALA:HB2	1.57	0.87
1:B:169:ARG:HH11	1:B:171:LYS:HD3	1.40	0.86
1:E:156:ILE:HD13	1:E:163:MET:HE3	1.56	0.85
1:E:367:LEU:HD13	1:E:403:LEU:HD11	1.58	0.85
1:E:437:ARG:O	1:E:455:GLU:HG2	1.76	0.84
1:B:144:ALA:HB1	1:B:154:MET:HE1	1.57	0.84
1:E:131:ALA:HB2	1:E:415:GLY:HA2	1.60	0.84
1:G:367:LEU:HD13	1:G:403:LEU:HD11	1.60	0.84
1:E:438:ASP:HB3	1:E:454:LEU:HD12	1.61	0.83
1:A:131:ALA:HB2	1:A:415:GLY:HA2	1.61	0.83
1:D:131:ALA:HB2	1:D:415:GLY:HA2	1.59	0.83
1:B:130:GLY:O	1:B:136:LYS:HE3	1.78	0.83
1:G:131:ALA:HB2	1:G:415:GLY:HA2	1.61	0.82
1:G:144:ALA:HB1	1:G:154:MET:HE1	1.62	0.82
1:B:180:GLN:NE2	1:B:504:GLU:HG2	1.95	0.81
1:D:144:ALA:HB1	1:D:154:MET:HE1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:413:LEU:HD23	1:G:475:ALA:HB2	1.61	0.81
1:B:131:ALA:HB2	1:B:415:GLY:HA2	1.63	0.81
1:D:169:ARG:HH21	1:D:312:ASN:ND2	1.79	0.81
1:E:105:GLU:HB2	1:E:109:GLN:NE2	1.96	0.81
1:F:131:ALA:HB2	1:F:415:GLY:HA2	1.61	0.80
1:D:456:ARG:HG3	1:D:456:ARG:HH11	1.46	0.80
1:A:198:GLN:HG2	5:A:2025:HOH:O	1.82	0.80
1:F:432:GLU:HG2	1:F:460:ARG:HD3	1.64	0.80
1:A:144:ALA:HB1	1:A:154:MET:HE1	1.64	0.80
1:B:437:ARG:HD2	1:D:456:ARG:HH12	1.47	0.79
1:A:437:ARG:HD2	1:B:456:ARG:NH2	1.98	0.79
1:A:413:LEU:HD23	1:A:475:ALA:HB2	1.64	0.79
1:F:144:ALA:HB1	1:F:154:MET:HE1	1.63	0.79
1:G:432:GLU:HG2	1:G:460:ARG:HD3	1.63	0.78
1:E:144:ALA:HB1	1:E:154:MET:HE1	1.65	0.78
1:A:94:VAL:HG13	1:A:98:LYS:HB3	1.66	0.78
1:D:156:ILE:HD13	1:D:163:MET:HE3	1.64	0.78
1:E:101:ARG:HH22	4:E:1505:EPE:C3	1.96	0.78
1:F:346:GLU:OE2	1:F:347:PRO:HD2	1.82	0.78
1:B:432:GLU:HG2	1:B:460:ARG:HD3	1.66	0.77
1:F:367:LEU:HD13	1:F:403:LEU:HD11	1.65	0.77
1:B:156:ILE:HD13	1:B:163:MET:HE3	1.66	0.77
1:G:77:GLY:N	1:G:78:GLU:HG3	2.00	0.76
1:A:432:GLU:HG2	1:A:460:ARG:HD3	1.67	0.76
1:A:133:GLY:C	2:A:701:ADP:H5'2	2.09	0.76
1:D:432:GLU:HG2	1:D:460:ARG:HD3	1.67	0.76
1:B:180:GLN:HE21	1:B:504:GLU:CG	1.98	0.76
1:D:94:VAL:HG13	1:D:98:LYS:HB3	1.67	0.75
1:D:413:LEU:HD23	1:D:475:ALA:HB2	1.68	0.75
1:B:94:VAL:HG13	1:B:98:LYS:HB3	1.67	0.75
1:G:156:ILE:HD13	1:G:163:MET:HE3	1.69	0.75
1:B:413:LEU:HD23	1:B:475:ALA:HB2	1.69	0.74
1:E:101:ARG:HH22	4:E:1505:EPE:H22	1.53	0.74
1:E:154:MET:CE	1:E:156:ILE:HD11	2.17	0.74
1:E:94:VAL:HG13	1:E:98:LYS:HB3	1.69	0.73
1:F:473:LEU:HD11	1:F:492:ILE:HD11	1.69	0.73
1:B:154:MET:HE2	1:B:156:ILE:HD11	1.69	0.73
1:F:437:ARG:O	1:F:455:GLU:CB	2.36	0.73
1:A:473:LEU:HD11	1:A:492:ILE:HD11	1.70	0.73
1:E:432:GLU:HG2	1:E:460:ARG:HD3	1.69	0.72
1:F:463:MET:SD	1:G:89:ARG:HD3	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:THR:O	1:D:281:ARG:HD2	1.87	0.72
1:F:413:LEU:CD2	1:F:475:ALA:HB2	2.19	0.72
1:B:246:THR:O	1:B:281:ARG:HD2	1.89	0.72
1:G:473:LEU:HD11	1:G:492:ILE:HD11	1.72	0.72
1:E:473:LEU:HD11	1:E:492:ILE:HD11	1.72	0.72
1:G:498:ARG:O	1:G:499:GLN:HB2	1.88	0.72
1:B:177:PRO:CA	1:B:294:MET:HE2	2.20	0.71
1:B:367:LEU:HD13	1:B:403:LEU:HD11	1.71	0.71
1:D:456:ARG:HH11	1:D:456:ARG:CG	2.02	0.71
1:F:94:VAL:HG13	1:F:98:LYS:HB3	1.72	0.71
1:G:177:PRO:HG2	1:G:178:TYR:CD1	2.25	0.71
1:G:246:THR:O	1:G:281:ARG:HD2	1.89	0.71
1:E:463:MET:SD	1:F:89:ARG:HD3	2.30	0.71
1:E:246:THR:O	1:E:281:ARG:HD2	1.90	0.71
1:D:215:GLU:HA	1:D:215:GLU:OE1	1.90	0.71
1:E:413:LEU:HD23	1:E:475:ALA:HB2	1.72	0.71
1:A:85:LYS:HD2	1:A:454:LEU:HD21	1.72	0.71
1:E:456:ARG:C	1:E:456:ARG:HD2	2.15	0.71
1:F:177:PRO:CA	1:F:294:MET:HE2	2.21	0.71
1:G:413:LEU:CD2	1:G:475:ALA:HB2	2.21	0.71
1:B:473:LEU:HD11	1:B:492:ILE:HD11	1.72	0.70
1:F:246:THR:O	1:F:281:ARG:HD2	1.89	0.70
1:F:437:ARG:O	1:F:455:GLU:HA	1.91	0.70
1:F:498:ARG:O	1:F:499:GLN:HB2	1.90	0.70
1:D:473:LEU:HD11	1:D:492:ILE:HD11	1.73	0.70
1:B:463:MET:HB2	1:B:466:GLU:HG3	1.72	0.70
1:F:438:ASP:HB2	1:F:455:GLU:HB3	1.73	0.69
1:G:463:MET:HB2	1:G:466:GLU:HG3	1.75	0.69
1:F:154:MET:CE	1:F:156:ILE:HD11	2.23	0.69
1:F:437:ARG:O	1:F:455:GLU:CA	2.41	0.69
1:G:77:GLY:N	1:G:77:GLY:C	2.51	0.69
1:G:177:PRO:CA	1:G:294:MET:HE2	2.23	0.69
1:D:463:MET:HB2	1:D:466:GLU:HG3	1.75	0.69
1:G:94:VAL:HG13	1:G:98:LYS:HB3	1.73	0.69
1:A:367:LEU:HD13	1:A:403:LEU:HD11	1.75	0.68
1:F:138:VAL:HG23	2:F:701:ADP:O2A	1.92	0.68
1:E:498:ARG:O	1:E:499:GLN:HB2	1.92	0.68
1:E:98:LYS:NZ	4:E:1505:EPE:O8	2.27	0.68
1:A:255:ARG:HH21	1:A:255:ARG:HG3	1.59	0.68
1:D:177:PRO:CA	1:D:294:MET:HE2	2.23	0.68
1:E:294:MET:HE3	1:E:332:TRP:CH2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:LEU:HB2	1:E:490:LEU:HD11	1.75	0.68
1:E:154:MET:HE2	1:E:156:ILE:HD11	1.73	0.68
1:F:463:MET:HB2	1:F:466:GLU:HG3	1.74	0.68
1:G:184:GLY:HA3	1:G:297:GLY:HA3	1.76	0.68
1:B:498:ARG:O	1:B:499:GLN:HB2	1.93	0.68
1:B:154:MET:CE	1:B:156:ILE:HD11	2.24	0.68
1:D:367:LEU:HD13	1:D:403:LEU:HD11	1.76	0.67
1:E:177:PRO:CA	1:E:294:MET:HE2	2.25	0.67
1:A:463:MET:HB2	1:A:466:GLU:HG3	1.77	0.67
1:B:437:ARG:HH22	1:B:459:GLU:CD	2.02	0.67
1:E:138:VAL:HG23	2:E:701:ADP:O2A	1.95	0.67
1:F:154:MET:HE2	1:F:156:ILE:HD11	1.74	0.67
1:F:177:PRO:HG2	1:F:178:TYR:CD1	2.30	0.67
1:A:498:ARG:O	1:A:499:GLN:HB2	1.92	0.67
1:B:294:MET:HE3	1:B:332:TRP:CH2	2.30	0.67
1:A:154:MET:HE2	1:A:156:ILE:HD11	1.77	0.66
1:A:177:PRO:HG2	1:A:178:TYR:CD1	2.30	0.66
1:A:89:ARG:HD3	1:G:463:MET:SD	2.35	0.66
1:F:346:GLU:OE2	1:F:347:PRO:CD	2.43	0.66
1:D:169:ARG:NH2	1:D:312:ASN:ND2	2.43	0.66
1:E:101:ARG:NH2	4:E:1505:EPE:C3	2.58	0.66
1:A:413:LEU:CD2	1:A:475:ALA:HB2	2.25	0.66
1:D:76:GLN:HE22	1:D:84:PHE:H	1.44	0.66
1:E:101:ARG:NH2	4:E:1505:EPE:H22	2.11	0.66
1:E:199:ARG:HE	1:E:338:THR:CG2	2.09	0.66
1:A:184:GLY:HA3	1:A:297:GLY:HA3	1.78	0.66
1:A:246:THR:O	1:A:281:ARG:HD2	1.96	0.65
1:A:294:MET:HE3	1:A:332:TRP:CH2	2.30	0.65
1:E:438:ASP:CB	1:E:454:LEU:HD12	2.26	0.65
1:D:413:LEU:CD2	1:D:475:ALA:HB2	2.27	0.65
1:G:154:MET:CE	1:G:156:ILE:HD11	2.26	0.65
1:A:177:PRO:CA	1:A:294:MET:HE2	2.27	0.65
1:B:413:LEU:CD2	1:B:475:ALA:HB2	2.27	0.65
1:F:184:GLY:HA3	1:F:297:GLY:HA3	1.78	0.64
1:A:488:VAL:HG13	1:A:489:PRO:HD2	1.77	0.64
1:D:498:ARG:O	1:D:499:GLN:HB2	1.96	0.64
1:E:177:PRO:HG2	1:E:178:TYR:CD1	2.32	0.64
1:B:294:MET:HE3	1:B:332:TRP:HH2	1.63	0.64
1:A:154:MET:CE	1:A:156:ILE:HD11	2.28	0.63
1:B:255:ARG:HH21	1:B:255:ARG:HG3	1.64	0.63
1:E:413:LEU:CD2	1:E:475:ALA:HB2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:VAL:HG23	2:G:701:ADP:O2A	1.98	0.63
1:F:294:MET:HE3	1:F:332:TRP:HH2	1.64	0.63
1:B:180:GLN:HB2	1:B:504:GLU:HG3	1.81	0.63
1:E:294:MET:HE3	1:E:332:TRP:HH2	1.64	0.62
1:F:83:PRO:O	1:F:437:ARG:HD3	1.99	0.62
1:F:294:MET:HE3	1:F:332:TRP:CH2	2.33	0.62
1:B:437:ARG:HD2	1:D:456:ARG:NH1	2.13	0.62
1:D:89:ARG:HD2	1:D:434:GLU:OE1	1.98	0.62
1:A:199:ARG:HE	1:A:338:THR:CG2	2.12	0.62
1:G:294:MET:HE3	1:G:332:TRP:CH2	2.33	0.62
1:E:133:GLY:HA2	1:F:375:ARG:HH12	1.64	0.62
1:D:372:THR:HG22	1:D:373:LYS:HG3	1.82	0.62
1:G:139:LEU:HB2	1:G:490:LEU:HD11	1.80	0.62
1:G:190:GLU:OE1	1:G:302:ARG:HG3	2.00	0.62
1:E:456:ARG:C	1:E:456:ARG:CD	2.73	0.62
1:E:456:ARG:CZ	1:E:456:ARG:HB3	2.28	0.61
1:F:488:VAL:HG13	1:F:489:PRO:HD2	1.82	0.61
1:G:154:MET:HE2	1:G:156:ILE:HD11	1.81	0.61
1:B:372:THR:HG22	1:B:373:LYS:HG3	1.81	0.61
1:A:346:GLU:OE2	1:A:346:GLU:HA	1.99	0.61
1:D:436:GLU:HG2	1:D:454:LEU:HD23	1.83	0.61
1:E:101:ARG:HH12	4:E:1505:EPE:C10	1.97	0.61
1:E:438:ASP:CB	1:E:454:LEU:CD1	2.73	0.61
1:E:463:MET:HB2	1:E:466:GLU:HG3	1.82	0.61
1:F:199:ARG:HE	1:F:338:THR:CG2	2.13	0.61
1:D:437:ARG:NH2	1:E:456:ARG:HH21	2.00	0.60
1:G:199:ARG:HE	1:G:338:THR:CG2	2.14	0.60
1:A:156:ILE:HD13	1:A:163:MET:HE3	1.82	0.60
1:B:177:PRO:HG2	1:B:178:TYR:CD1	2.35	0.60
1:B:199:ARG:HE	1:B:338:THR:CG2	2.15	0.60
1:F:78:GLU:OE1	1:F:95:SER:HB3	2.01	0.60
1:G:84:PHE:HA	1:G:437:ARG:HG3	1.83	0.60
1:E:101:ARG:HH22	4:E:1505:EPE:H32	1.64	0.60
1:E:101:ARG:NH2	4:E:1505:EPE:H32	2.16	0.60
1:E:488:VAL:HG13	1:E:489:PRO:HD2	1.84	0.60
1:D:294:MET:HE3	1:D:332:TRP:CH2	2.36	0.60
1:G:98:LYS:O	1:G:102:MET:HG3	2.01	0.60
1:G:77:GLY:N	1:G:78:GLU:CG	2.65	0.60
1:D:85:LYS:HD3	1:D:454:LEU:HD21	1.83	0.60
1:A:89:ARG:HD2	1:A:434:GLU:OE1	2.02	0.59
1:F:255:ARG:HH21	1:F:255:ARG:HG3	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:MET:HE3	1:G:332:TRP:HH2	1.68	0.59
1:D:84:PHE:HA	1:D:437:ARG:HG2	1.85	0.59
1:D:152:ASP:OD1	1:D:350:ARG:NH2	2.34	0.59
1:G:137:SER:HB2	2:G:701:ADP:PA	2.43	0.59
1:A:98:LYS:O	1:A:102:MET:HG3	2.03	0.59
1:G:331:ALA:O	1:G:335:VAL:HG23	2.03	0.59
1:D:139:LEU:HB2	1:D:490:LEU:HD11	1.85	0.59
1:E:180:GLN:HG2	1:E:504:GLU:CB	2.33	0.59
1:A:294:MET:HE3	1:A:332:TRP:HH2	1.68	0.59
1:G:169:ARG:HH11	1:G:171:LYS:CD	2.08	0.59
1:D:85:LYS:CD	1:D:454:LEU:HD21	2.33	0.58
1:D:177:PRO:HG2	1:D:178:TYR:CD1	2.38	0.58
1:A:259:GLU:HA	1:A:264:GLU:HG3	1.84	0.58
1:F:414:GLY:HA2	1:F:467:ILE:HG23	1.86	0.58
1:B:82:ALA:O	1:B:437:ARG:NH1	2.36	0.58
1:B:259:GLU:HA	1:B:264:GLU:HG3	1.85	0.58
1:E:190:GLU:OE1	1:E:302:ARG:HG3	2.02	0.58
1:G:144:ALA:HB2	1:G:163:MET:HE1	1.84	0.58
1:G:372:THR:HG22	1:G:373:LYS:HG3	1.85	0.58
1:D:169:ARG:NH1	1:D:171:LYS:HD3	2.19	0.58
1:F:98:LYS:O	1:F:102:MET:HG3	2.03	0.58
1:F:190:GLU:OE1	1:F:302:ARG:HG3	2.04	0.58
1:B:503:VAL:O	1:B:504:GLU:CB	2.49	0.58
1:F:144:ALA:HB2	1:F:163:MET:HE1	1.86	0.58
1:B:152:ASP:OD1	1:B:350:ARG:NH2	2.37	0.58
1:F:106:LYS:HD3	1:F:106:LYS:H	1.69	0.58
1:G:494:GLN:HA	1:G:494:GLN:HE21	1.69	0.58
1:D:154:MET:CE	1:D:156:ILE:HD11	2.34	0.58
1:F:177:PRO:N	1:F:294:MET:HE2	2.19	0.58
1:F:259:GLU:HA	1:F:264:GLU:HG3	1.87	0.57
1:A:494:GLN:HE21	1:A:494:GLN:HA	1.70	0.57
1:E:259:GLU:HA	1:E:264:GLU:HG3	1.86	0.57
1:B:331:ALA:O	1:B:335:VAL:HG23	2.04	0.57
1:D:199:ARG:HE	1:D:338:THR:CG2	2.17	0.57
1:D:255:ARG:HH21	1:D:255:ARG:HG3	1.70	0.57
1:D:346:GLU:OE2	1:D:346:GLU:HA	2.03	0.57
1:E:101:ARG:NH2	4:E:1505:EPE:C2	2.61	0.57
1:E:255:ARG:HH21	1:E:255:ARG:HG3	1.69	0.57
1:G:488:VAL:HG13	1:G:489:PRO:HD2	1.87	0.57
1:B:139:LEU:HB2	1:B:490:LEU:HD11	1.86	0.57
1:B:391:LEU:HD23	1:B:404:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:GLY:HA3	1:D:297:GLY:HA3	1.85	0.57
1:A:190:GLU:OE1	1:A:302:ARG:HG3	2.04	0.56
1:E:372:THR:HG22	1:E:373:LYS:HG3	1.86	0.56
1:A:177:PRO:N	1:A:294:MET:HE2	2.20	0.56
1:A:227:THR:HG23	1:A:257:PHE:HE2	1.70	0.56
1:B:144:ALA:HB1	1:B:154:MET:CE	2.33	0.56
1:B:177:PRO:N	1:B:294:MET:HE2	2.21	0.56
1:D:190:GLU:OE1	1:D:302:ARG:HG3	2.05	0.56
1:F:160:ASN:HD21	1:F:319:GLU:CD	2.13	0.56
1:D:488:VAL:HG13	1:D:489:PRO:HD2	1.87	0.56
1:A:319:GLU:OE2	1:B:376:LYS:NZ	2.38	0.56
1:F:152:ASP:OD1	1:F:350:ARG:NH2	2.37	0.56
1:B:133:GLY:HA2	2:B:701:ADP:H5'2	1.88	0.56
1:E:154:MET:HE3	1:E:156:ILE:HD11	1.88	0.56
1:D:294:MET:HE3	1:D:332:TRP:HH2	1.70	0.56
1:F:346:GLU:OE2	1:F:346:GLU:HA	2.06	0.56
1:A:139:LEU:HB2	1:A:490:LEU:HD11	1.86	0.56
1:D:160:ASN:HD21	1:D:319:GLU:CD	2.14	0.56
1:B:438:ASP:O	1:B:439:ARG:HB2	2.06	0.55
1:G:94:VAL:CG1	1:G:98:LYS:HB3	2.36	0.55
1:G:177:PRO:HA	1:G:294:MET:HE2	1.88	0.55
1:E:437:ARG:HG2	1:E:438:ASP:N	2.21	0.55
1:G:436:GLU:HA	1:G:455:GLU:O	2.05	0.55
1:A:372:THR:HG22	1:A:373:LYS:HG3	1.87	0.55
1:F:139:LEU:HB2	1:F:490:LEU:HD11	1.89	0.55
1:F:177:PRO:HB3	1:F:294:MET:HG2	1.88	0.55
1:B:89:ARG:HD2	1:B:434:GLU:OE1	2.05	0.55
1:D:438:ASP:OD2	1:D:454:LEU:HD11	2.06	0.55
1:F:177:PRO:HA	1:F:294:MET:HE2	1.88	0.55
1:G:160:ASN:HD21	1:G:319:GLU:CD	2.15	0.55
1:A:255:ARG:HG3	1:A:255:ARG:NH2	2.19	0.55
1:E:326:ARG:HD2	1:E:360:SER:O	2.06	0.55
1:F:331:ALA:O	1:F:335:VAL:HG23	2.07	0.55
1:G:346:GLU:HA	1:G:346:GLU:OE2	2.05	0.55
1:E:89:ARG:HD2	1:E:434:GLU:OE1	2.07	0.55
1:E:331:ALA:O	1:E:335:VAL:HG23	2.07	0.55
1:B:180:GLN:HB2	1:B:504:GLU:CG	2.35	0.55
1:E:346:GLU:HA	1:E:346:GLU:OE2	2.06	0.55
1:F:136:LYS:HB2	2:F:701:ADP:O3B	2.07	0.55
1:F:144:ALA:CB	1:F:163:MET:HE1	2.37	0.55
1:G:433:HIS:HD2	1:G:433:HIS:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:LYS:HE3	1:D:395:TYR:HA	1.88	0.55
1:E:494:GLN:NE2	1:E:494:GLN:HA	2.22	0.55
1:E:94:VAL:CG1	1:E:98:LYS:HB3	2.35	0.54
1:F:494:GLN:HE21	1:F:494:GLN:HA	1.73	0.54
1:A:160:ASN:HD21	1:A:319:GLU:CD	2.14	0.54
1:B:177:PRO:HA	1:B:294:MET:HE2	1.89	0.54
1:D:331:ALA:O	1:D:335:VAL:HG23	2.07	0.54
1:F:346:GLU:OE2	1:F:347:PRO:N	2.41	0.54
1:A:169:ARG:NH2	1:A:312:ASN:ND2	2.56	0.54
1:E:290:GLU:HG3	1:E:325:LEU:HD23	1.89	0.54
1:G:144:ALA:HB1	1:G:154:MET:CE	2.35	0.54
1:A:144:ALA:HB2	1:A:163:MET:HE1	1.90	0.54
1:B:169:ARG:NH2	1:B:312:ASN:ND2	2.54	0.54
1:D:437:ARG:HH12	1:D:459:GLU:CD	2.16	0.54
1:F:144:ALA:HB1	1:F:154:MET:CE	2.37	0.54
1:G:494:GLN:HA	1:G:494:GLN:NE2	2.22	0.54
1:A:463:MET:SD	1:B:89:ARG:HD3	2.47	0.54
1:B:80:GLY:O	1:D:89:ARG:HG2	2.08	0.54
1:D:169:ARG:HG2	1:D:498:ARG:NH2	2.22	0.54
1:D:177:PRO:N	1:D:294:MET:HE2	2.23	0.54
1:G:94:VAL:HG22	1:G:98:LYS:HE3	1.90	0.54
1:A:494:GLN:HA	1:A:494:GLN:NE2	2.23	0.54
1:D:133:GLY:C	2:D:701:ADP:H5'2	2.32	0.54
1:G:144:ALA:CB	1:G:154:MET:HE1	2.36	0.54
1:D:144:ALA:HB1	1:D:154:MET:CE	2.35	0.53
1:D:154:MET:HE2	1:D:156:ILE:HD11	1.90	0.53
1:E:494:GLN:HA	1:E:494:GLN:HE21	1.72	0.53
1:F:169:ARG:NH2	1:F:312:ASN:ND2	2.56	0.53
1:G:177:PRO:N	1:G:294:MET:HE2	2.24	0.53
1:E:454:LEU:N	1:E:454:LEU:HD23	2.23	0.53
1:G:139:LEU:C	1:G:139:LEU:HD23	2.33	0.53
1:B:255:ARG:HG3	1:B:255:ARG:NH2	2.23	0.53
1:D:404:ARG:NH1	5:D:2069:HOH:O	2.41	0.53
1:A:306:GLU:O	1:A:308:PRO:HD3	2.08	0.53
1:G:89:ARG:HD2	1:G:434:GLU:OE1	2.07	0.53
1:D:139:LEU:C	1:D:139:LEU:HD23	2.34	0.53
1:D:177:PRO:HA	1:D:294:MET:HE2	1.90	0.53
1:A:417:ARG:NH2	1:A:469:ASN:OD1	2.42	0.53
1:F:139:LEU:C	1:F:139:LEU:HD23	2.34	0.53
1:G:414:GLY:HA2	1:G:467:ILE:HG23	1.90	0.53
1:F:105:GLU:HB2	1:F:109:GLN:CD	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:GLU:OE2	1:F:346:GLU:CA	2.56	0.53
1:A:338:THR:O	1:A:341:LEU:HB2	2.09	0.53
1:B:190:GLU:OE1	1:B:302:ARG:HG3	2.09	0.53
1:F:494:GLN:HA	1:F:494:GLN:NE2	2.24	0.53
1:A:144:ALA:HB1	1:A:154:MET:CE	2.38	0.53
1:D:169:ARG:HH21	1:D:312:ASN:HD21	1.56	0.53
1:E:438:ASP:CB	1:E:454:LEU:HG	2.28	0.53
1:F:199:ARG:HE	1:F:338:THR:HG22	1.74	0.53
1:A:293:THR:HG21	5:A:2047:HOH:O	2.08	0.52
1:A:414:GLY:HA2	1:A:467:ILE:HG23	1.91	0.52
1:B:224:LEU:CD1	1:B:242:LEU:HD21	2.39	0.52
1:D:494:GLN:HA	1:D:494:GLN:NE2	2.23	0.52
1:D:494:GLN:HA	1:D:494:GLN:HE21	1.73	0.52
1:E:177:PRO:N	1:E:294:MET:HE2	2.24	0.52
1:D:414:GLY:HA2	1:D:467:ILE:HG23	1.91	0.52
1:A:136:LYS:HB2	2:A:701:ADP:O3B	2.09	0.52
1:B:488:VAL:HG13	1:B:489:PRO:HD2	1.91	0.52
1:D:417:ARG:NH2	1:D:469:ASN:OD1	2.43	0.52
1:F:306:GLU:O	1:F:308:PRO:HD3	2.08	0.52
1:F:433:HIS:HD2	1:F:433:HIS:O	1.93	0.52
1:B:433:HIS:HD2	1:B:433:HIS:O	1.91	0.52
1:E:492:ILE:HD13	2:E:701:ADP:C4	2.44	0.52
1:A:199:ARG:HE	1:A:338:THR:HG22	1.75	0.52
1:F:105:GLU:HB2	1:F:109:GLN:NE2	2.24	0.52
1:G:288:LEU:O	1:G:291:HIS:HB2	2.10	0.52
1:G:290:GLU:HG3	1:G:325:LEU:HD23	1.91	0.52
1:A:290:GLU:HG3	1:A:325:LEU:HD23	1.91	0.52
1:F:437:ARG:O	1:F:455:GLU:HB2	2.08	0.52
1:B:160:ASN:HD21	1:B:319:GLU:CD	2.17	0.52
1:G:169:ARG:NH1	1:G:171:LYS:HD3	2.10	0.52
1:G:227:THR:HG23	1:G:257:PHE:HE2	1.75	0.52
1:G:255:ARG:HH21	1:G:255:ARG:HG3	1.75	0.52
1:A:433:HIS:HD2	1:A:433:HIS:O	1.93	0.52
1:D:136:LYS:HB2	2:D:701:ADP:O3B	2.09	0.52
1:D:169:ARG:HH11	1:D:171:LYS:HD3	1.74	0.52
1:D:288:LEU:O	1:D:291:HIS:HB2	2.10	0.52
1:A:139:LEU:C	1:A:139:LEU:HD23	2.34	0.51
1:B:97:GLY:O	1:B:101:ARG:CD	2.58	0.51
1:B:414:GLY:HA2	1:B:467:ILE:HG23	1.92	0.51
1:B:492:ILE:HD13	2:B:701:ADP:N3	2.24	0.51
1:D:98:LYS:O	1:D:102:MET:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ARG:NH2	1:E:469:ASN:OD1	2.42	0.51
1:F:358:LEU:HD11	1:F:367:LEU:HD11	1.91	0.51
1:A:331:ALA:O	1:A:335:VAL:HG23	2.10	0.51
1:F:255:ARG:HG3	1:F:255:ARG:NH2	2.25	0.51
1:A:144:ALA:CB	1:A:154:MET:HE1	2.39	0.51
1:B:144:ALA:CB	1:B:154:MET:HE1	2.34	0.51
1:D:138:VAL:HG23	2:D:701:ADP:O2A	2.11	0.51
1:D:215:GLU:OE1	1:D:215:GLU:CA	2.55	0.51
1:G:456:ARG:HD3	5:G:2041:HOH:O	2.10	0.51
1:B:80:GLY:C	1:D:89:ARG:HG2	2.35	0.51
1:B:184:GLY:HA3	1:B:296:ASP:C	2.36	0.51
1:E:255:ARG:HG3	1:E:255:ARG:NH2	2.26	0.51
1:A:179:ASP:O	1:A:182:THR:HG22	2.10	0.51
1:A:281:ARG:NH2	1:B:265:SER:HB3	2.26	0.51
1:B:199:ARG:HE	1:B:338:THR:HG22	1.75	0.51
1:E:105:GLU:HB2	1:E:109:GLN:CD	2.35	0.51
1:E:179:ASP:O	1:E:182:THR:HG22	2.10	0.51
1:B:494:GLN:HE21	1:B:494:GLN:HA	1.75	0.51
1:E:414:GLY:HA2	1:E:467:ILE:HG23	1.93	0.51
1:G:417:ARG:NH2	1:G:469:ASN:OD1	2.44	0.51
1:E:126:LEU:HD11	1:E:411:VAL:HG23	1.92	0.51
1:E:144:ALA:HB2	1:E:163:MET:HE1	1.92	0.51
1:F:437:ARG:HG3	1:F:437:ARG:NH1	2.26	0.51
1:F:144:ALA:CB	1:F:154:MET:HE1	2.40	0.51
1:G:329:ILE:O	1:G:333:VAL:HG23	2.11	0.51
1:A:126:LEU:HD11	1:A:411:VAL:HG23	1.93	0.50
1:D:76:GLN:NE2	1:D:84:PHE:H	2.08	0.50
1:D:144:ALA:CB	1:D:154:MET:HE1	2.36	0.50
1:E:306:GLU:O	1:E:308:PRO:HD3	2.11	0.50
1:A:133:GLY:HA2	1:B:375:ARG:NH2	2.25	0.50
1:G:169:ARG:NH2	1:G:312:ASN:ND2	2.59	0.50
1:D:184:GLY:HA3	1:D:296:ASP:C	2.36	0.50
1:D:345:GLU:HA	1:D:345:GLU:OE1	2.12	0.50
1:E:139:LEU:HD23	1:E:139:LEU:C	2.36	0.50
1:B:180:GLN:NE2	1:B:504:GLU:CG	2.66	0.50
1:D:433:HIS:HD2	1:D:433:HIS:O	1.94	0.50
1:G:338:THR:O	1:G:341:LEU:HB2	2.12	0.50
1:B:133:GLY:HA2	1:D:375:ARG:NH1	2.26	0.50
1:B:288:LEU:O	1:B:291:HIS:HB2	2.11	0.50
1:D:338:THR:O	1:D:341:LEU:HB2	2.12	0.50
1:E:180:GLN:HG2	1:E:504:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:LEU:O	1:F:291:HIS:HB2	2.11	0.50
1:D:437:ARG:NH1	1:D:459:GLU:OE2	2.45	0.50
1:E:98:LYS:O	1:E:102:MET:HG3	2.12	0.50
1:E:199:ARG:HE	1:E:338:THR:HG22	1.76	0.50
1:F:372:THR:HG22	1:F:373:LYS:HG3	1.94	0.50
1:A:345:GLU:OE1	1:A:345:GLU:HA	2.11	0.49
1:D:259:GLU:HA	1:D:264:GLU:HG3	1.94	0.49
1:E:98:LYS:HG3	4:E:1505:EPE:H32	1.94	0.49
1:G:199:ARG:HE	1:G:338:THR:HG22	1.75	0.49
1:A:85:LYS:HD2	1:A:454:LEU:CD2	2.42	0.49
1:B:184:GLY:HA3	1:B:297:GLY:HA3	1.94	0.49
1:F:105:GLU:OE1	1:F:119:ARG:CG	2.60	0.49
1:B:76:GLN:C	1:B:78:GLU:H	2.21	0.49
1:B:97:GLY:O	1:B:101:ARG:HD2	2.12	0.49
1:B:224:LEU:HD11	1:B:242:LEU:HD21	1.93	0.49
1:G:345:GLU:HA	1:G:345:GLU:OE1	2.12	0.49
1:A:346:GLU:OE2	1:A:346:GLU:CA	2.57	0.49
1:B:494:GLN:HA	1:B:494:GLN:NE2	2.28	0.49
1:D:358:LEU:HD11	1:D:367:LEU:HD11	1.94	0.49
1:E:180:GLN:CG	1:E:504:GLU:HB2	2.43	0.49
1:E:180:GLN:HG3	1:E:503:VAL:HG12	1.94	0.49
1:F:227:THR:HG23	1:F:257:PHE:HE2	1.77	0.49
1:G:437:ARG:O	1:G:455:GLU:CB	2.50	0.49
1:B:306:GLU:O	1:B:308:PRO:HD3	2.13	0.49
1:E:503:VAL:O	1:E:504:GLU:HB3	2.12	0.49
1:F:417:ARG:NH2	1:F:469:ASN:OD1	2.45	0.49
1:G:192:ARG:HG3	1:G:302:ARG:NH1	2.27	0.49
1:G:494:GLN:HE21	1:G:494:GLN:CA	2.26	0.49
1:B:179:ASP:O	1:B:182:THR:HG22	2.12	0.49
1:B:275:LYS:HE2	5:B:2043:HOH:O	2.13	0.48
1:D:207:ARG:HB2	1:D:363:LYS:HB3	1.95	0.48
1:F:290:GLU:HG3	1:F:325:LEU:HD23	1.94	0.48
1:D:255:ARG:HG3	1:D:255:ARG:NH2	2.29	0.48
1:D:154:MET:HB3	1:D:352:TRP:HB2	1.95	0.48
1:E:227:THR:HG23	1:E:257:PHE:HE2	1.78	0.48
1:D:80:GLY:O	1:E:89:ARG:HG2	2.13	0.48
1:D:463:MET:SD	1:E:89:ARG:HD3	2.53	0.48
1:E:169:ARG:NH2	1:E:312:ASN:ND2	2.62	0.48
1:F:359:ALA:HB1	1:F:390:GLN:HB3	1.95	0.48
1:E:359:ALA:HB1	1:E:390:GLN:HB3	1.96	0.48
1:F:281:ARG:NH2	1:G:265:SER:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:PRO:HA	1:E:294:MET:HE2	1.96	0.48
1:F:126:LEU:HD11	1:F:411:VAL:HG23	1.96	0.48
1:G:259:GLU:HA	1:G:264:GLU:HG3	1.96	0.48
1:G:177:PRO:HG2	1:G:178:TYR:CE1	2.49	0.48
1:G:359:ALA:HB1	1:G:390:GLN:HB3	1.95	0.48
1:B:139:LEU:C	1:B:139:LEU:HD23	2.39	0.48
1:D:290:GLU:HG3	1:D:325:LEU:HD23	1.96	0.48
1:E:169:ARG:HH11	1:E:171:LYS:CD	2.14	0.48
1:E:469:ASN:O	1:F:482:ASN:HB2	2.14	0.48
1:G:126:LEU:HD11	1:G:411:VAL:HG23	1.96	0.48
1:A:177:PRO:HA	1:A:294:MET:HE2	1.96	0.48
1:B:290:GLU:HG3	1:B:325:LEU:HD23	1.94	0.48
1:D:346:GLU:OE2	1:D:346:GLU:CA	2.61	0.48
1:G:144:ALA:CB	1:G:163:MET:HE1	2.44	0.48
1:G:306:GLU:O	1:G:308:PRO:HD3	2.13	0.48
1:A:224:LEU:CD1	1:A:242:LEU:HD21	2.43	0.47
1:F:207:ARG:HB2	1:F:363:LYS:HB3	1.97	0.47
1:G:376:LYS:HD3	1:G:376:LYS:HA	1.16	0.47
1:D:306:GLU:O	1:D:308:PRO:HD3	2.14	0.47
1:E:458:ARG:NH1	5:E:2065:HOH:O	2.46	0.47
1:F:169:ARG:HH11	1:F:171:LYS:CD	2.17	0.47
1:G:124:ARG:HB3	1:G:408:ARG:CG	2.44	0.47
1:A:180:GLN:HE21	1:A:180:GLN:HB2	1.51	0.47
1:D:144:ALA:HB2	1:D:163:MET:HE1	1.96	0.47
1:E:199:ARG:HE	1:E:338:THR:HG21	1.79	0.47
1:F:84:PHE:HB3	1:F:437:ARG:HG3	1.96	0.47
1:G:154:MET:HE3	1:G:156:ILE:HD11	1.94	0.47
1:G:336:VAL:O	1:G:340:ILE:HG23	2.14	0.47
1:A:359:ALA:HB1	1:A:390:GLN:HB3	1.95	0.47
1:B:169:ARG:HH22	1:B:312:ASN:ND2	2.12	0.47
1:E:160:ASN:HD21	1:E:319:GLU:CD	2.23	0.47
1:E:345:GLU:OE1	1:E:345:GLU:HA	2.15	0.47
1:A:224:LEU:HD11	1:A:242:LEU:HD21	1.96	0.47
1:A:437:ARG:HG2	1:A:438:ASP:H	1.79	0.47
1:B:245:TRP:O	1:B:254:LEU:HG	2.14	0.47
1:B:352:TRP:CZ2	1:B:380:ARG:HD3	2.49	0.47
1:D:94:VAL:HG13	1:D:95:SER:N	2.29	0.47
1:D:179:ASP:O	1:D:182:THR:HG22	2.14	0.47
1:D:359:ALA:HB1	1:D:390:GLN:HB3	1.96	0.47
1:E:94:VAL:HG22	1:E:98:LYS:HD2	1.97	0.47
1:F:179:ASP:O	1:F:182:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:PHE:HB2	1:G:93:ILE:HG21	1.97	0.47
1:G:177:PRO:HB3	1:G:294:MET:HG2	1.97	0.47
1:A:435:VAL:HG13	1:A:436:GLU:N	2.29	0.47
1:B:433:HIS:C	1:B:433:HIS:CD2	2.93	0.47
1:G:154:MET:HB3	1:G:352:TRP:HB2	1.97	0.47
1:B:138:VAL:HG23	2:B:701:ADP:O2A	2.15	0.47
1:A:294:MET:HE3	1:A:332:TRP:CZ2	2.50	0.47
2:A:701:ADP:O3'	1:B:124:ARG:NH1	2.44	0.47
1:B:499:GLN:HG2	1:B:500:PRO:HD2	1.97	0.47
1:E:224:LEU:CD1	1:E:242:LEU:HD21	2.45	0.47
1:G:346:GLU:OE2	1:G:346:GLU:CA	2.63	0.46
1:F:414:GLY:CA	1:F:470:LEU:HD12	2.45	0.46
1:A:180:GLN:HB2	1:A:505:GLY:HA2	1.97	0.46
1:E:184:GLY:HA3	1:E:297:GLY:N	2.30	0.46
1:E:294:MET:HE3	1:E:332:TRP:CZ2	2.51	0.46
1:G:346:GLU:OE1	1:G:348:LYS:HB2	2.15	0.46
1:A:304:TRP:CZ2	1:A:313:LEU:HB2	2.51	0.46
1:F:154:MET:HE3	1:F:156:ILE:HD11	1.96	0.46
1:G:433:HIS:O	1:G:433:HIS:CD2	2.69	0.46
1:A:144:ALA:CB	1:A:163:MET:HE1	2.45	0.46
1:B:177:PRO:HB3	1:B:294:MET:HG2	1.98	0.46
1:E:338:THR:O	1:E:341:LEU:HB2	2.16	0.46
1:F:252:ASP:N	1:F:252:ASP:OD2	2.49	0.46
1:G:207:ARG:HB2	1:G:363:LYS:HB3	1.98	0.46
1:G:433:HIS:CD2	1:G:433:HIS:C	2.92	0.46
1:F:352:TRP:CE2	1:F:380:ARG:HD3	2.51	0.46
1:F:363:LYS:HE3	1:F:395:TYR:HA	1.97	0.46
1:F:494:GLN:HE21	1:F:494:GLN:CA	2.28	0.46
1:A:433:HIS:CD2	1:A:433:HIS:C	2.94	0.46
1:B:166:LYS:HD2	1:B:495:PHE:HB2	1.96	0.46
1:B:414:GLY:HA2	1:B:467:ILE:CG2	2.46	0.46
1:A:288:LEU:O	1:A:291:HIS:HB2	2.16	0.46
1:F:435:VAL:HG13	1:F:436:GLU:N	2.30	0.46
1:D:317:TRP:HB2	1:D:325:LEU:HD12	1.98	0.46
1:A:494:GLN:HE21	1:A:494:GLN:CA	2.27	0.45
1:B:435:VAL:HG13	1:B:436:GLU:N	2.31	0.45
1:E:346:GLU:OE2	1:E:346:GLU:CA	2.64	0.45
1:F:177:PRO:HG2	1:F:178:TYR:CE1	2.50	0.45
1:F:317:TRP:HB2	1:F:325:LEU:HD12	1.97	0.45
1:G:106:LYS:H	1:G:106:LYS:HG2	1.37	0.45
1:G:349:ARG:HD2	1:G:377:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.81	0.45
1:E:281:ARG:NH2	1:F:265:SER:HB3	2.31	0.45
1:F:338:THR:O	1:F:341:LEU:HB2	2.15	0.45
1:B:94:VAL:HG13	1:B:95:SER:N	2.31	0.45
1:E:94:VAL:HG13	1:E:95:SER:N	2.31	0.45
1:G:499:GLN:HG2	1:G:500:PRO:HD2	1.99	0.45
1:A:156:ILE:HG22	1:A:158:ASP:HB2	1.98	0.45
1:B:98:LYS:O	1:B:102:MET:CG	2.50	0.45
1:D:433:HIS:C	1:D:433:HIS:CD2	2.94	0.45
1:E:207:ARG:HB2	1:E:363:LYS:HB3	1.98	0.45
1:F:224:LEU:CD1	1:F:242:LEU:HD21	2.47	0.45
1:F:433:HIS:C	1:F:433:HIS:CD2	2.95	0.45
1:G:131:ALA:CB	1:G:415:GLY:HA2	2.41	0.45
1:A:207:ARG:HB2	1:A:363:LYS:HB3	1.99	0.45
1:D:225:ARG:O	1:D:229:LYS:HB2	2.17	0.45
1:E:154:MET:HB3	1:E:352:TRP:HB2	1.99	0.45
1:E:180:GLN:HG3	1:E:504:GLU:HB2	1.98	0.45
1:F:124:ARG:HB3	1:F:408:ARG:CG	2.47	0.45
1:D:113:ALA:O	1:D:488:VAL:HG11	2.17	0.45
1:D:352:TRP:CZ2	1:D:380:ARG:HD3	2.51	0.45
1:G:129:ASN:ND2	1:G:426:MET:SD	2.90	0.45
1:G:164:LEU:HA	1:G:314:PHE:CE2	2.52	0.45
1:D:177:PRO:HB3	1:D:294:MET:HG2	1.97	0.45
1:D:336:VAL:O	1:D:340:ILE:HG23	2.17	0.45
1:E:144:ALA:CB	1:E:163:MET:HE1	2.47	0.45
1:E:304:TRP:CH2	1:E:313:LEU:HB2	2.52	0.45
1:A:482:ASN:HB2	1:G:469:ASN:O	2.17	0.45
1:B:113:ALA:O	1:B:488:VAL:HG11	2.17	0.45
1:F:503:VAL:O	1:F:504:GLU:HB3	2.17	0.45
1:D:166:LYS:HD2	1:D:495:PHE:HB2	1.99	0.45
1:A:184:GLY:HA3	1:A:297:GLY:CA	2.46	0.44
1:A:304:TRP:CH2	1:A:313:LEU:HB2	2.53	0.44
1:D:144:ALA:CB	1:D:163:MET:HE1	2.47	0.44
1:E:145:TYR:CZ	1:E:149:LEU:HD11	2.52	0.44
1:F:352:TRP:CZ2	1:F:380:ARG:HD3	2.52	0.44
1:G:252:ASP:OD2	1:G:252:ASP:N	2.48	0.44
1:A:92:ARG:HG3	1:A:484:PRO:HB3	1.98	0.44
1:A:410:LEU:HB2	1:G:418:THR:HG22	2.00	0.44
1:B:94:VAL:CG1	1:B:98:LYS:HB3	2.41	0.44
1:D:105:GLU:HB2	1:D:109:GLN:NE2	2.32	0.44
1:E:346:GLU:OE1	1:E:348:LYS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ARG:HD2	1:F:377:ALA:O	2.18	0.44
1:G:105:GLU:HB2	1:G:109:GLN:NE2	2.32	0.44
1:A:363:LYS:HE3	1:A:395:TYR:HA	1.99	0.44
1:B:227:THR:HG23	1:B:257:PHE:HE2	1.81	0.44
1:D:199:ARG:HE	1:D:338:THR:HG22	1.82	0.44
1:E:336:VAL:O	1:E:340:ILE:HG23	2.17	0.44
1:E:430:LEU:HD12	1:E:430:LEU:HA	1.81	0.44
1:F:169:ARG:HH22	1:F:312:ASN:ND2	2.14	0.44
1:F:499:GLN:HG2	1:F:500:PRO:HD2	1.99	0.44
1:B:126:LEU:HD11	1:B:411:VAL:HG23	1.99	0.44
1:D:435:VAL:HG13	1:D:436:GLU:N	2.31	0.44
1:G:156:ILE:HG22	1:G:158:ASP:HB2	1.99	0.44
1:G:179:ASP:O	1:G:182:THR:HG22	2.17	0.44
1:A:154:MET:HB3	1:A:352:TRP:HB2	1.99	0.44
1:A:166:LYS:O	1:A:498:ARG:HD3	2.18	0.44
1:A:352:TRP:CZ2	1:A:380:ARG:HD3	2.52	0.44
1:D:456:ARG:HG3	1:D:456:ARG:NH1	2.16	0.44
1:D:494:GLN:HE21	1:D:494:GLN:CA	2.29	0.44
1:G:184:GLY:HA3	1:G:297:GLY:CA	2.45	0.44
1:G:255:ARG:HG3	1:G:255:ARG:NH2	2.32	0.44
1:G:301:ILE:O	1:G:305:LEU:HG	2.18	0.44
1:A:169:ARG:HH11	1:A:171:LYS:CD	2.17	0.44
5:D:2060:HOH:O	1:E:338:THR:HG23	2.17	0.44
1:E:177:PRO:HG2	1:E:178:TYR:CE1	2.52	0.44
1:E:288:LEU:O	1:E:291:HIS:HB2	2.16	0.44
1:F:154:MET:HB3	1:F:352:TRP:HB2	1.98	0.44
1:F:346:GLU:OE2	1:F:346:GLU:C	2.60	0.44
1:E:133:GLY:C	2:E:701:ADP:H5'2	2.43	0.44
1:E:438:ASP:CG	1:E:454:LEU:HD12	2.42	0.44
1:E:363:LYS:HE3	1:E:395:TYR:HA	1.99	0.44
1:G:376:LYS:N	1:G:376:LYS:CD	2.76	0.44
1:D:126:LEU:HD11	1:D:411:VAL:HG23	1.98	0.44
1:E:435:VAL:HG13	1:E:436:GLU:N	2.33	0.44
1:G:77:GLY:N	1:G:78:GLU:N	2.65	0.44
1:D:154:MET:HE3	1:D:156:ILE:HD11	2.00	0.43
1:E:358:LEU:HD11	1:E:367:LEU:HD11	2.00	0.43
1:E:433:HIS:HD2	1:E:433:HIS:O	2.01	0.43
1:F:94:VAL:HG13	1:F:95:SER:N	2.33	0.43
1:D:124:ARG:HB3	1:D:408:ARG:CG	2.47	0.43
1:E:304:TRP:CZ2	1:E:313:LEU:HB2	2.53	0.43
1:A:169:ARG:NH1	1:A:171:LYS:HD3	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:THR:HG23	1:D:257:PHE:HE2	1.83	0.43
1:E:124:ARG:HB3	1:E:408:ARG:CG	2.48	0.43
1:F:92:ARG:H	1:F:92:ARG:HG2	1.63	0.43
1:F:436:GLU:HA	1:F:455:GLU:O	2.17	0.43
1:A:177:PRO:HB3	1:A:294:MET:HG2	2.01	0.43
1:E:144:ALA:CB	1:E:154:MET:HE1	2.43	0.43
1:E:164:LEU:HA	1:E:314:PHE:CE2	2.53	0.43
1:B:225:ARG:O	1:B:229:LYS:HB2	2.19	0.43
1:F:245:TRP:O	1:F:254:LEU:HG	2.18	0.43
1:A:479:PHE:O	1:G:417:ARG:NH1	2.51	0.43
1:B:133:GLY:C	2:B:701:ADP:H5'2	2.43	0.43
1:F:418:THR:HG22	1:G:410:LEU:HB2	1.99	0.43
1:G:79:PHE:HB2	1:G:93:ILE:CG2	2.49	0.43
1:G:367:LEU:HD22	1:G:371:LEU:CD1	2.48	0.43
1:A:177:PRO:HG2	1:A:178:TYR:CE1	2.53	0.43
1:A:265:SER:HB3	1:G:281:ARG:NH2	2.34	0.43
1:G:224:LEU:CD1	1:G:242:LEU:HD21	2.49	0.43
1:G:435:VAL:HG13	1:G:436:GLU:N	2.33	0.43
1:A:94:VAL:CG1	1:A:98:LYS:HB3	2.42	0.43
1:A:352:TRP:CE2	1:A:380:ARG:HD3	2.54	0.43
1:D:94:VAL:CG1	1:D:98:LYS:HB3	2.43	0.43
1:E:225:ARG:O	1:E:229:LYS:HB2	2.19	0.43
1:F:105:GLU:OE1	1:F:119:ARG:HG3	2.19	0.43
1:B:433:HIS:O	1:B:433:HIS:CD2	2.71	0.43
1:F:158:ASP:HA	1:F:159:PRO:HD3	1.86	0.43
1:G:94:VAL:HG13	1:G:95:SER:N	2.34	0.43
1:A:89:ARG:HG2	1:G:80:GLY:C	2.43	0.42
1:D:76:GLN:HE21	1:D:83:PRO:HA	1.84	0.42
1:D:419:ASP:HB2	1:E:405:ALA:HB2	2.00	0.42
1:F:329:ILE:O	1:F:333:VAL:HG23	2.18	0.42
1:G:358:LEU:HD11	1:G:367:LEU:HD11	2.01	0.42
1:E:180:GLN:CG	1:E:504:GLU:CB	2.97	0.42
1:F:119:ARG:HA	1:F:119:ARG:HD3	1.90	0.42
1:A:414:GLY:HA2	1:A:467:ILE:CG2	2.49	0.42
1:D:166:LYS:O	1:D:498:ARG:HD3	2.20	0.42
1:D:281:ARG:NH2	1:E:265:SER:HB3	2.35	0.42
1:G:317:TRP:HB2	1:G:325:LEU:HD12	2.01	0.42
1:A:145:TYR:CZ	1:A:149:LEU:HD11	2.54	0.42
1:A:317:TRP:HB2	1:A:325:LEU:HD12	2.01	0.42
1:A:318:ARG:HD2	1:A:502:PHE:CE2	2.55	0.42
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:HB3	1:B:352:TRP:HB2	2.02	0.42
1:B:207:ARG:HB2	1:B:363:LYS:HB3	2.01	0.42
1:D:106:LYS:H	1:D:106:LYS:HG2	1.26	0.42
1:A:225:ARG:O	1:A:229:LYS:HB2	2.19	0.42
1:A:249:ALA:O	1:A:281:ARG:NH2	2.47	0.42
1:D:301:ILE:O	1:D:305:LEU:HG	2.20	0.42
1:F:225:ARG:O	1:F:229:LYS:HB2	2.20	0.42
1:G:184:GLY:CA	1:G:297:GLY:HA3	2.47	0.42
1:B:438:ASP:O	1:B:439:ARG:CB	2.68	0.42
1:E:156:ILE:HG22	1:E:158:ASP:HB2	2.02	0.42
1:G:138:VAL:HG12	1:G:490:LEU:HD22	2.02	0.42
1:G:169:ARG:HH22	1:G:312:ASN:ND2	2.18	0.42
1:G:224:LEU:HD11	1:G:242:LEU:HD21	2.02	0.42
1:A:94:VAL:HG13	1:A:95:SER:N	2.34	0.42
1:D:215:GLU:CG	5:D:2044:HOH:O	2.42	0.42
1:B:166:LYS:O	1:B:498:ARG:HD3	2.19	0.42
1:B:169:ARG:HG3	1:B:498:ARG:NH2	2.35	0.42
1:B:326:ARG:HH21	1:B:326:ARG:HD3	1.60	0.42
1:D:346:GLU:OE1	1:D:348:LYS:HB2	2.20	0.42
1:F:84:PHE:HA	1:F:437:ARG:HG2	2.00	0.42
1:F:414:GLY:HA2	1:F:467:ILE:CG2	2.49	0.42
1:G:225:ARG:O	1:G:229:LYS:HB2	2.19	0.42
1:B:177:PRO:HG2	1:B:178:TYR:CE1	2.55	0.42
1:F:184:GLY:HA3	1:F:297:GLY:CA	2.48	0.42
1:G:113:ALA:O	1:G:488:VAL:HG11	2.20	0.42
1:G:376:LYS:HD3	1:G:376:LYS:N	2.13	0.42
1:A:433:HIS:O	1:A:433:HIS:CD2	2.72	0.42
1:B:144:ALA:HB2	1:B:163:MET:HE1	2.00	0.42
1:B:213:ALA:HA	1:B:216:TRP:CE3	2.55	0.42
1:B:356:ASP:HB2	5:B:2010:HOH:O	2.19	0.42
1:B:463:MET:SD	1:D:89:ARG:HD3	2.60	0.42
1:F:224:LEU:HD11	1:F:242:LEU:HD21	2.01	0.42
1:G:414:GLY:CA	1:G:470:LEU:HD12	2.50	0.42
1:D:349:ARG:HD2	1:D:377:ALA:O	2.20	0.41
1:G:124:ARG:HB3	1:G:408:ARG:HB2	2.02	0.41
1:A:469:ASN:O	1:B:482:ASN:HB2	2.20	0.41
1:B:494:GLN:HE21	1:B:494:GLN:CA	2.30	0.41
1:F:435:VAL:CG1	1:F:436:GLU:N	2.83	0.41
1:B:352:TRP:CE2	1:B:380:ARG:HD3	2.55	0.41
1:B:437:ARG:O	1:B:455:GLU:HA	2.21	0.41
1:D:94:VAL:CG1	1:D:95:SER:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LYS:HD3	1:A:398:LYS:HA	1.85	0.41
1:B:304:TRP:CZ2	1:B:313:LEU:HB2	2.55	0.41
1:B:358:LEU:HD11	1:B:367:LEU:HD11	2.02	0.41
1:D:352:TRP:CE2	1:D:380:ARG:HD3	2.55	0.41
1:G:124:ARG:HB3	1:G:408:ARG:HG3	2.01	0.41
1:G:352:TRP:CE2	1:G:380:ARG:HD3	2.55	0.41
1:B:180:GLN:HE21	1:B:180:GLN:HB2	1.54	0.41
1:B:252:ASP:N	1:B:252:ASP:OD2	2.54	0.41
1:D:184:GLY:HA3	1:D:296:ASP:O	2.20	0.41
1:D:224:LEU:HD11	1:D:242:LEU:HD21	2.03	0.41
1:E:417:ARG:NH1	1:F:479:PHE:O	2.54	0.41
1:F:414:GLY:HA3	1:F:470:LEU:HD12	2.02	0.41
1:A:419:ASP:HB2	1:B:405:ALA:HB2	2.01	0.41
1:B:102:MET:HE2	1:B:102:MET:HB3	1.91	0.41
1:D:80:GLY:C	1:E:89:ARG:HG2	2.46	0.41
1:D:224:LEU:CD1	1:D:242:LEU:HD21	2.51	0.41
1:E:94:VAL:CG1	1:E:95:SER:N	2.84	0.41
1:E:433:HIS:CD2	1:E:433:HIS:C	2.99	0.41
1:E:456:ARG:HD2	1:E:456:ARG:O	2.21	0.41
1:F:463:MET:HG3	1:G:89:ARG:CZ	2.50	0.41
1:G:166:LYS:O	1:G:498:ARG:HD3	2.20	0.41
1:G:356:ASP:CG	1:G:357:GLU:N	2.78	0.41
1:A:124:ARG:HB3	1:A:408:ARG:CG	2.51	0.41
1:A:184:GLY:CA	1:A:297:GLY:HA3	2.49	0.41
1:A:251:PHE:CZ	1:A:277:LEU:HD13	2.56	0.41
1:A:375:ARG:NH1	1:G:133:GLY:HA2	2.36	0.41
1:A:438:ASP:OD2	1:A:454:LEU:HD23	2.21	0.41
1:G:363:LYS:HE3	1:G:395:TYR:HA	2.03	0.41
1:A:245:TRP:O	1:A:254:LEU:HG	2.20	0.41
1:D:177:PRO:HG2	1:D:178:TYR:CE1	2.56	0.41
1:A:252:ASP:OD2	1:A:252:ASP:N	2.54	0.41
1:A:436:GLU:HG2	1:A:454:LEU:HD13	2.03	0.41
1:B:124:ARG:HB3	1:B:408:ARG:CG	2.50	0.41
1:B:317:TRP:HB2	1:B:325:LEU:HD12	2.03	0.41
1:D:76:GLN:NE2	1:D:83:PRO:HA	2.36	0.41
1:E:231:LEU:HD23	1:E:231:LEU:HA	1.95	0.41
1:E:418:THR:HG22	1:F:410:LEU:HB2	2.03	0.41
1:F:169:ARG:HH22	1:F:312:ASN:HD21	1.69	0.41
1:F:492:ILE:HD11	2:F:701:ADP:HI'	2.03	0.41
1:A:105:GLU:HB2	1:A:109:GLN:NE2	2.35	0.41
1:B:318:ARG:HD2	1:B:502:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:LEU:O	1:G:261:THR:OG1	2.37	0.41
1:B:294:MET:HE3	1:B:332:TRP:CZ2	2.56	0.40
1:D:78:GLU:H	1:D:78:GLU:HG2	1.79	0.40
1:D:356:ASP:CG	1:D:357:GLU:N	2.80	0.40
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.78	0.40
1:E:166:LYS:HD2	1:E:495:PHE:HB2	2.03	0.40
1:E:252:ASP:OD2	1:E:252:ASP:N	2.54	0.40
1:B:94:VAL:CG1	1:B:95:SER:N	2.83	0.40
1:B:356:ASP:CG	1:B:357:GLU:N	2.79	0.40
1:F:433:HIS:O	1:F:433:HIS:CD2	2.73	0.40
1:G:105:GLU:HB2	1:G:109:GLN:CD	2.46	0.40
1:D:408:ARG:HH11	1:D:408:ARG:HG3	1.87	0.40
1:F:184:GLY:CA	1:F:297:GLY:HA3	2.50	0.40
1:G:138:VAL:CG1	1:G:490:LEU:HD22	2.51	0.40
1:G:313:LEU:HD23	1:G:314:PHE:N	2.36	0.40
1:A:346:GLU:OE1	1:A:348:LYS:HB2	2.20	0.40
1:A:349:ARG:HD2	1:A:377:ALA:O	2.22	0.40
1:B:121:ALA:HA	1:B:124:ARG:HG3	2.02	0.40
1:B:281:ARG:NH2	1:D:265:SER:HB3	2.36	0.40
1:E:367:LEU:HD22	1:E:371:LEU:HG	2.03	0.40
1:F:82:ALA:HA	1:F:83:PRO:HD3	1.97	0.40
1:F:469:ASN:O	1:G:482:ASN:HB2	2.22	0.40
1:G:352:TRP:CZ2	1:G:380:ARG:HD3	2.55	0.40
1:G:414:GLY:HA2	1:G:467:ILE:CG2	2.50	0.40
1:G:430:LEU:HD12	1:G:430:LEU:HA	1.84	0.40
1:D:92:ARG:HG3	1:D:484:PRO:HB3	2.03	0.40
1:D:433:HIS:O	1:D:433:HIS:CD2	2.73	0.40
1:G:294:MET:HE3	1:G:332:TRP:CZ2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:NZ	1:D:241:GLU:OE2[4_456]	2.13	0.07
1:E:92:ARG:NH1	1:F:235:GLY:O[5_565]	2.19	0.01

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	412/437 (94%)	388 (94%)	21 (5%)	3 (1%)	18	53
1	B	413/437 (94%)	394 (95%)	17 (4%)	2 (0%)	24	60
1	D	412/437 (94%)	390 (95%)	19 (5%)	3 (1%)	18	53
1	E	410/437 (94%)	387 (94%)	20 (5%)	3 (1%)	18	53
1	F	408/437 (93%)	389 (95%)	16 (4%)	3 (1%)	18	53
1	G	409/437 (94%)	385 (94%)	19 (5%)	5 (1%)	10	40
All	All	2464/2622 (94%)	2333 (95%)	112 (4%)	19 (1%)	16	50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	78	GLU
1	E	499	GLN
1	G	345	GLU
1	G	499	GLN
1	A	499	GLN
1	B	499	GLN
1	D	289	PRO
1	D	345	GLU
1	D	499	GLN
1	E	345	GLU
1	F	289	PRO
1	F	499	GLN
1	A	345	GLU
1	B	289	PRO
1	G	289	PRO
1	E	289	PRO
1	A	289	PRO
1	F	414	GLY
1	G	414	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/364 (95%)	313 (90%)	33 (10%)	8	31
1	B	348/364 (96%)	310 (89%)	38 (11%)	6	26
1	D	347/364 (95%)	314 (90%)	33 (10%)	8	31
1	E	346/364 (95%)	311 (90%)	35 (10%)	7	29
1	F	344/364 (94%)	307 (89%)	37 (11%)	6	26
1	G	344/364 (94%)	308 (90%)	36 (10%)	6	27
All	All	2075/2184 (95%)	1863 (90%)	212 (10%)	7	29

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	85	LYS
1	A	89	ARG
1	A	94	VAL
1	A	106	LYS
1	A	143	LEU
1	A	154	MET
1	A	180	GLN
1	A	202	LEU
1	A	233	LEU
1	A	251	PHE
1	A	254	LEU
1	A	255	ARG
1	A	277	LEU
1	A	284	LEU
1	A	285	SER
1	A	289	PRO
1	A	294	MET
1	A	296	ASP
1	A	313	LEU
1	A	328	LEU
1	A	338	THR

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Mol	Chain	Res	Type
1	A	351	LEU
1	A	353	LEU
1	A	367	LEU
1	A	372	THR
1	A	379	LEU
1	A	387	SER
1	A	428	LEU
1	A	430	LEU
1	A	435	VAL
1	A	456	ARG
1	A	490	LEU
1	B	89	ARG
1	B	94	VAL
1	B	101	ARG
1	B	106	LYS
1	B	124	ARG
1	B	136	LYS
1	B	143	LEU
1	B	154	MET
1	B	180	GLN
1	B	202	LEU
1	B	233	LEU
1	B	240	ARG
1	B	251	PHE
1	B	254	LEU
1	B	255	ARG
1	B	277	LEU
1	B	284	LEU
1	B	289	PRO
1	B	294	MET
1	B	296	ASP
1	B	313	LEU
1	B	328	LEU
1	B	338	THR
1	B	346	GLU
1	B	351	LEU
1	B	353	LEU
1	B	367	LEU
1	B	372	THR
1	B	379	LEU
1	B	387	SER
1	B	428	LEU

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Mol	Chain	Res	Type
1	B	430	LEU
1	B	435	VAL
1	B	438	ASP
1	B	456	ARG
1	B	483	ARG
1	B	490	LEU
1	B	504	GLU
1	D	78	GLU
1	D	86	ARG
1	D	89	ARG
1	D	94	VAL
1	D	106	LYS
1	D	143	LEU
1	D	154	MET
1	D	202	LEU
1	D	233	LEU
1	D	240	ARG
1	D	251	PHE
1	D	254	LEU
1	D	277	LEU
1	D	284	LEU
1	D	289	PRO
1	D	294	MET
1	D	313	LEU
1	D	328	LEU
1	D	338	THR
1	D	351	LEU
1	D	353	LEU
1	D	367	LEU
1	D	372	THR
1	D	379	LEU
1	D	387	SER
1	D	428	LEU
1	D	430	LEU
1	D	435	VAL
1	D	439	ARG
1	D	454	LEU
1	D	456	ARG
1	D	490	LEU
1	D	504	GLU
1	E	89	ARG
1	E	92	ARG

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Mol	Chain	Res	Type
1	E	94	VAL
1	E	98	LYS
1	E	106	LYS
1	E	108	LYS
1	E	124	ARG
1	E	143	LEU
1	E	154	MET
1	E	202	LEU
1	E	233	LEU
1	E	240	ARG
1	E	251	PHE
1	E	254	LEU
1	E	277	LEU
1	E	284	LEU
1	E	289	PRO
1	E	294	MET
1	E	296	ASP
1	E	313	LEU
1	E	328	LEU
1	E	338	THR
1	E	351	LEU
1	E	353	LEU
1	E	367	LEU
1	E	372	THR
1	E	379	LEU
1	E	387	SER
1	E	428	LEU
1	E	430	LEU
1	E	435	VAL
1	E	454	LEU
1	E	490	LEU
1	E	498	ARG
1	E	504	GLU
1	F	78	GLU
1	F	86	ARG
1	F	89	ARG
1	F	92	ARG
1	F	94	VAL
1	F	106	LYS
1	F	143	LEU
1	F	154	MET
1	F	180	GLN

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Mol	Chain	Res	Type
1	F	202	LEU
1	F	233	LEU
1	F	240	ARG
1	F	251	PHE
1	F	252	ASP
1	F	254	LEU
1	F	255	ARG
1	F	277	LEU
1	F	284	LEU
1	F	289	PRO
1	F	294	MET
1	F	296	ASP
1	F	313	LEU
1	F	328	LEU
1	F	338	THR
1	F	348	LYS
1	F	351	LEU
1	F	353	LEU
1	F	367	LEU
1	F	372	THR
1	F	379	LEU
1	F	387	SER
1	F	428	LEU
1	F	430	LEU
1	F	435	VAL
1	F	437	ARG
1	F	483	ARG
1	F	490	LEU
1	G	86	ARG
1	G	89	ARG
1	G	94	VAL
1	G	98	LYS
1	G	106	LYS
1	G	143	LEU
1	G	154	MET
1	G	180	GLN
1	G	202	LEU
1	G	233	LEU
1	G	240	ARG
1	G	251	PHE
1	G	252	ASP
1	G	254	LEU

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Mol	Chain	Res	Type
1	G	277	LEU
1	G	284	LEU
1	G	285	SER
1	G	289	PRO
1	G	294	MET
1	G	296	ASP
1	G	313	LEU
1	G	328	LEU
1	G	338	THR
1	G	351	LEU
1	G	353	LEU
1	G	367	LEU
1	G	372	THR
1	G	376	LYS
1	G	379	LEU
1	G	387	SER
1	G	428	LEU
1	G	430	LEU
1	G	435	VAL
1	G	483	ARG
1	G	490	LEU
1	G	504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	160	ASN
1	A	180	GLN
1	A	291	HIS
1	A	433	HIS
1	A	482	ASN
1	A	494	GLN
1	A	497	ASN
1	A	499	GLN
1	B	76	GLN
1	B	129	ASN
1	B	160	ASN
1	B	180	GLN
1	B	390	GLN
1	B	482	ASN
1	B	494	GLN

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Mol	Chain	Res	Type
1	B	497	ASN
1	B	499	GLN
1	D	76	GLN
1	D	129	ASN
1	D	160	ASN
1	D	291	HIS
1	D	312	ASN
1	D	482	ASN
1	D	494	GLN
1	D	497	ASN
1	D	499	GLN
1	E	76	GLN
1	E	129	ASN
1	E	160	ASN
1	E	180	GLN
1	E	291	HIS
1	E	386	GLN
1	E	482	ASN
1	E	494	GLN
1	E	497	ASN
1	E	499	GLN
1	F	160	ASN
1	F	180	GLN
1	F	312	ASN
1	F	386	GLN
1	F	482	ASN
1	F	494	GLN
1	F	497	ASN
1	F	499	GLN
1	G	129	ASN
1	G	160	ASN
1	G	180	GLN
1	G	433	HIS
1	G	482	ASN
1	G	494	GLN
1	G	497	ASN
1	G	499	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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$
2	ADP	E	701	3	28,29,29	1.58	2 (7%)	43,45,45	0.92	0
2	ADP	A	701	3	28,29,29	1.32	4 (14%)	43,45,45	0.89	1 (2%)
2	ADP	G	701	3	28,29,29	2.36	9 (32%)	43,45,45	1.63	8 (18%)
4	EPE	E	1505	-	15,15,15	1.77	4 (26%)	19,20,20	1.58	5 (26%)
2	ADP	B	701	3	28,29,29	1.50	5 (17%)	43,45,45	0.91	2 (4%)
4	EPE	E	1506	-	15,15,15	3.33	10 (66%)	19,20,20	2.99	10 (52%)
2	ADP	F	701	-	28,29,29	1.60	5 (17%)	43,45,45	0.90	0
2	ADP	D	701	3	28,29,29	1.43	2 (7%)	43,45,45	0.89	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	701	3	-	2/16/32/32	0/3/3/3
2	ADP	A	701	3	-	3/16/32/32	0/3/3/3
2	ADP	G	701	3	-	2/16/32/32	0/3/3/3
4	EPE	E	1505	-	-	3/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	701	3	-	3/16/32/32	0/3/3/3
4	EPE	E	1506	-	-	3/9/19/19	0/1/1/1
2	ADP	F	701	-	-	2/16/32/32	0/3/3/3
2	ADP	D	701	3	-	2/16/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1506	EPE	C6-N1	-6.47	1.29	1.46
2	G	701	ADP	C2-N3	6.12	1.44	1.33
4	E	1506	EPE	C3-N4	5.51	1.61	1.46
2	E	701	ADP	PA-O3A	4.65	1.64	1.59
2	F	701	ADP	PA-O3A	4.27	1.64	1.59
2	G	701	ADP	PA-O3A	4.14	1.64	1.59
4	E	1506	EPE	C7-N4	-4.12	1.38	1.47
4	E	1506	EPE	C6-C5	-4.06	1.36	1.51
4	E	1505	EPE	C7-N4	3.97	1.56	1.47
2	G	701	ADP	C1'-N9	3.93	1.57	1.46
2	D	701	ADP	PA-O3A	3.86	1.63	1.59
2	G	701	ADP	C5-C4	-3.60	1.32	1.39
2	G	701	ADP	C6-N1	3.58	1.45	1.35
4	E	1506	EPE	C2-N1	3.49	1.56	1.46
2	B	701	ADP	PA-O3A	3.47	1.63	1.59
2	G	701	ADP	C4-N9	3.45	1.44	1.37
4	E	1506	EPE	C7-C8	-3.35	1.38	1.51
2	F	701	ADP	C1'-N9	3.34	1.55	1.46
4	E	1506	EPE	C9-C10	3.33	1.61	1.52
2	G	701	ADP	O2'-C2'	3.31	1.51	1.43
2	E	701	ADP	C1'-N9	3.06	1.54	1.46
4	E	1506	EPE	C5-N4	-2.99	1.38	1.46
2	B	701	ADP	C1'-N9	2.95	1.54	1.46
2	A	701	ADP	C1'-N9	2.88	1.54	1.46
2	D	701	ADP	C1'-N9	2.75	1.53	1.46
4	E	1506	EPE	C10-S	2.72	1.81	1.77
2	G	701	ADP	C4-N3	2.63	1.39	1.34
4	E	1505	EPE	C9-N1	2.61	1.53	1.47
2	B	701	ADP	C5-C6	2.50	1.48	1.41
2	F	701	ADP	O4'-C4'	2.49	1.50	1.45
4	E	1506	EPE	C9-N1	2.40	1.52	1.47
4	E	1505	EPE	C7-C8	2.40	1.60	1.51
2	A	701	ADP	PA-O3A	2.39	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	ADP	C2'-C3'	2.32	1.59	1.53
2	A	701	ADP	C8-N9	-2.29	1.33	1.37
2	F	701	ADP	C5-C6	2.28	1.47	1.41
2	B	701	ADP	O2'-C2'	2.17	1.48	1.43
2	A	701	ADP	C5-C6	2.15	1.47	1.41
2	F	701	ADP	C8-N9	-2.15	1.33	1.37
2	B	701	ADP	C8-N9	-2.05	1.34	1.37
4	E	1505	EPE	C2-N1	2.00	1.52	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1506	EPE	C7-N4-C5	-5.85	95.64	111.24
4	E	1506	EPE	C5-N4-C3	-4.97	98.13	108.84
4	E	1506	EPE	C9-N1-C6	-4.95	98.05	111.24
4	E	1506	EPE	C9-N1-C2	4.34	122.81	111.24
4	E	1506	EPE	O8-C8-C7	-4.17	94.02	111.22
4	E	1506	EPE	C3-C2-N1	-4.09	102.41	110.65
2	G	701	ADP	O3'-C3'-C4'	-4.06	99.43	111.08
2	G	701	ADP	O5'-C5'-C4'	4.02	122.68	108.99
2	G	701	ADP	C5-C4-N3	3.47	131.49	126.72
4	E	1505	EPE	C7-N4-C3	3.22	119.82	111.24
4	E	1505	EPE	C9-N1-C6	-3.02	103.18	111.24
4	E	1506	EPE	O1S-S-C10	2.67	110.76	106.73
2	G	701	ADP	C2'-C1'-N9	2.59	119.74	113.30
2	G	701	ADP	N3-C2-N1	-2.55	124.73	128.58
4	E	1505	EPE	C6-N1-C2	-2.54	103.38	108.84
4	E	1506	EPE	C10-C9-N1	2.53	121.92	112.36
2	G	701	ADP	C4-C5-N7	2.42	113.35	110.58
4	E	1506	EPE	O2S-S-C10	-2.37	103.15	106.73
2	D	701	ADP	C4-N9-C8	2.28	108.13	105.74
4	E	1505	EPE	C3-C2-N1	-2.28	106.05	110.65
2	G	701	ADP	C5-C4-N9	-2.26	103.35	105.81
2	B	701	ADP	C4-N9-C8	2.25	108.10	105.74
4	E	1505	EPE	C7-N4-C5	-2.23	105.31	111.24
2	G	701	ADP	N6-C6-N1	2.22	123.32	118.38
2	A	701	ADP	C4-N9-C8	2.15	108.00	105.74
4	E	1506	EPE	C6-N1-C2	2.06	113.28	108.84
2	B	701	ADP	O5'-C5'-C4'	2.06	115.99	108.99

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	701	ADP	PA-O3A-PB-O2B
4	E	1505	EPE	C10-C9-N1-C2
4	E	1506	EPE	C10-C9-N1-C6
4	E	1505	EPE	N4-C7-C8-O8
4	E	1505	EPE	C10-C9-N1-C6
4	E	1506	EPE	N4-C7-C8-O8
2	A	701	ADP	PA-O3A-PB-O1B
2	B	701	ADP	PA-O3A-PB-O1B
2	A	701	ADP	PA-O3A-PB-O2B
2	B	701	ADP	C4'-C5'-O5'-PA
4	E	1506	EPE	C10-C9-N1-C2
2	F	701	ADP	C4'-C5'-O5'-PA
2	E	701	ADP	C4'-C5'-O5'-PA
2	B	701	ADP	PA-O3A-PB-O2B
2	D	701	ADP	PA-O3A-PB-O2B
2	D	701	ADP	PA-O3A-PB-O3B
2	F	701	ADP	PA-O3A-PB-O3B
2	G	701	ADP	PA-O3A-PB-O2B
2	G	701	ADP	PA-O3A-PB-O3B
2	A	701	ADP	C4'-C5'-O5'-PA

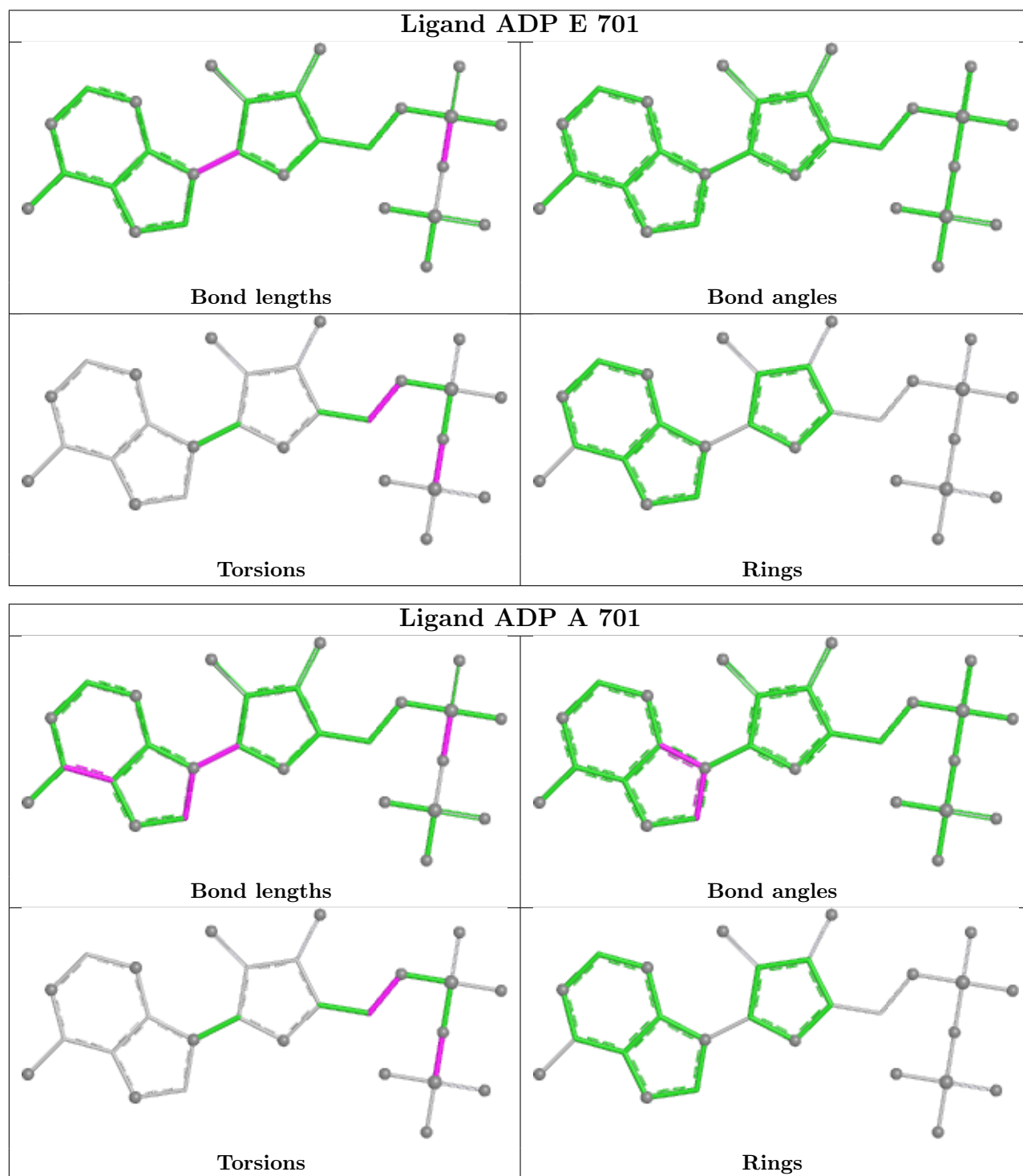
There are no ring outliers.

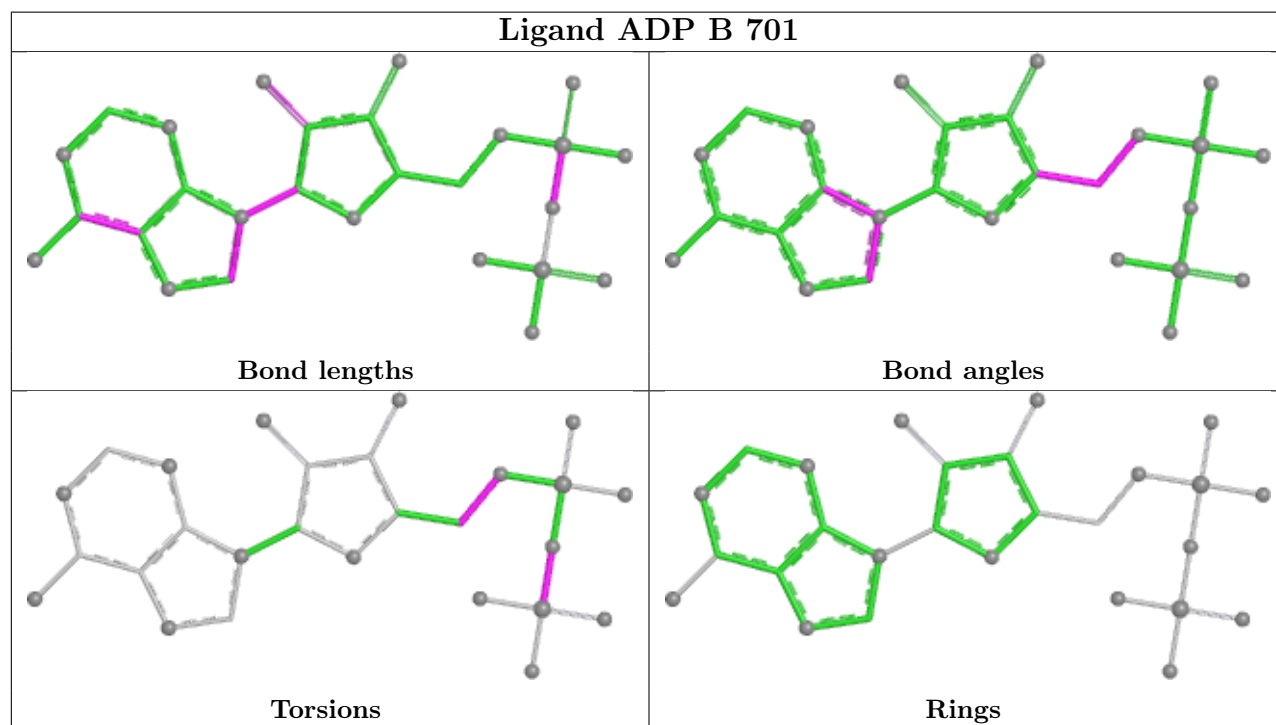
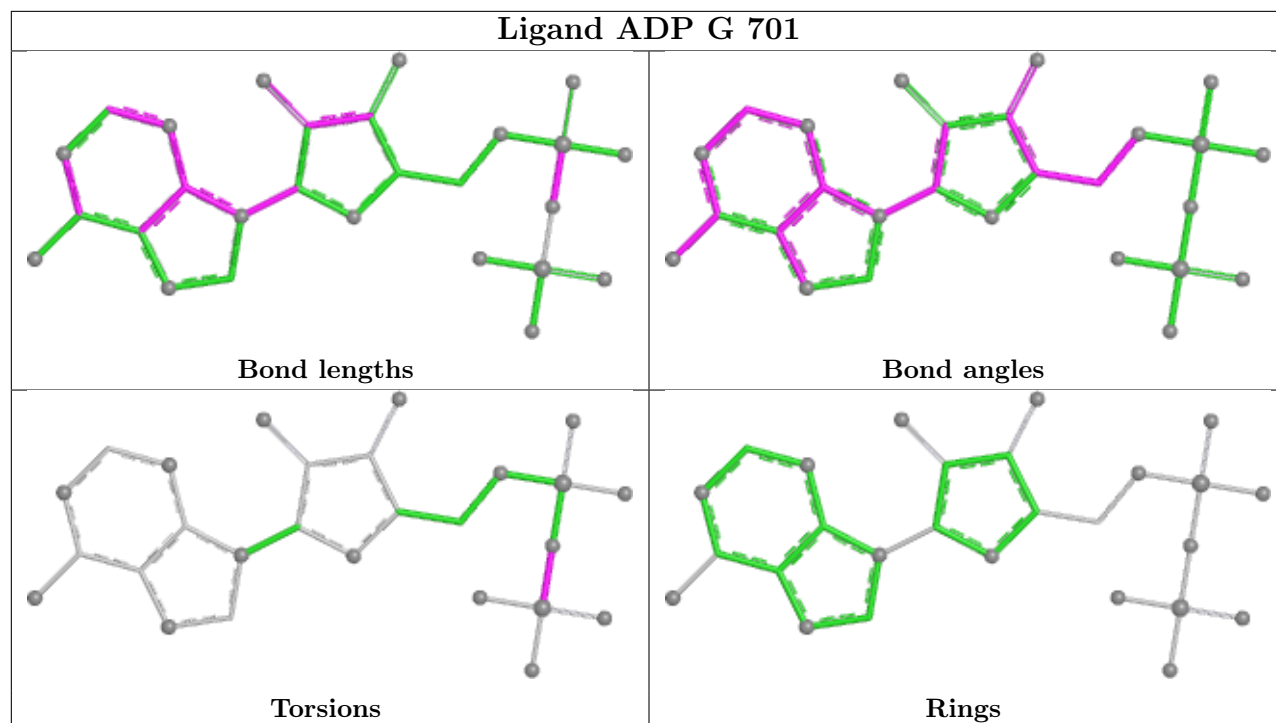
7 monomers are involved in 31 short contacts:

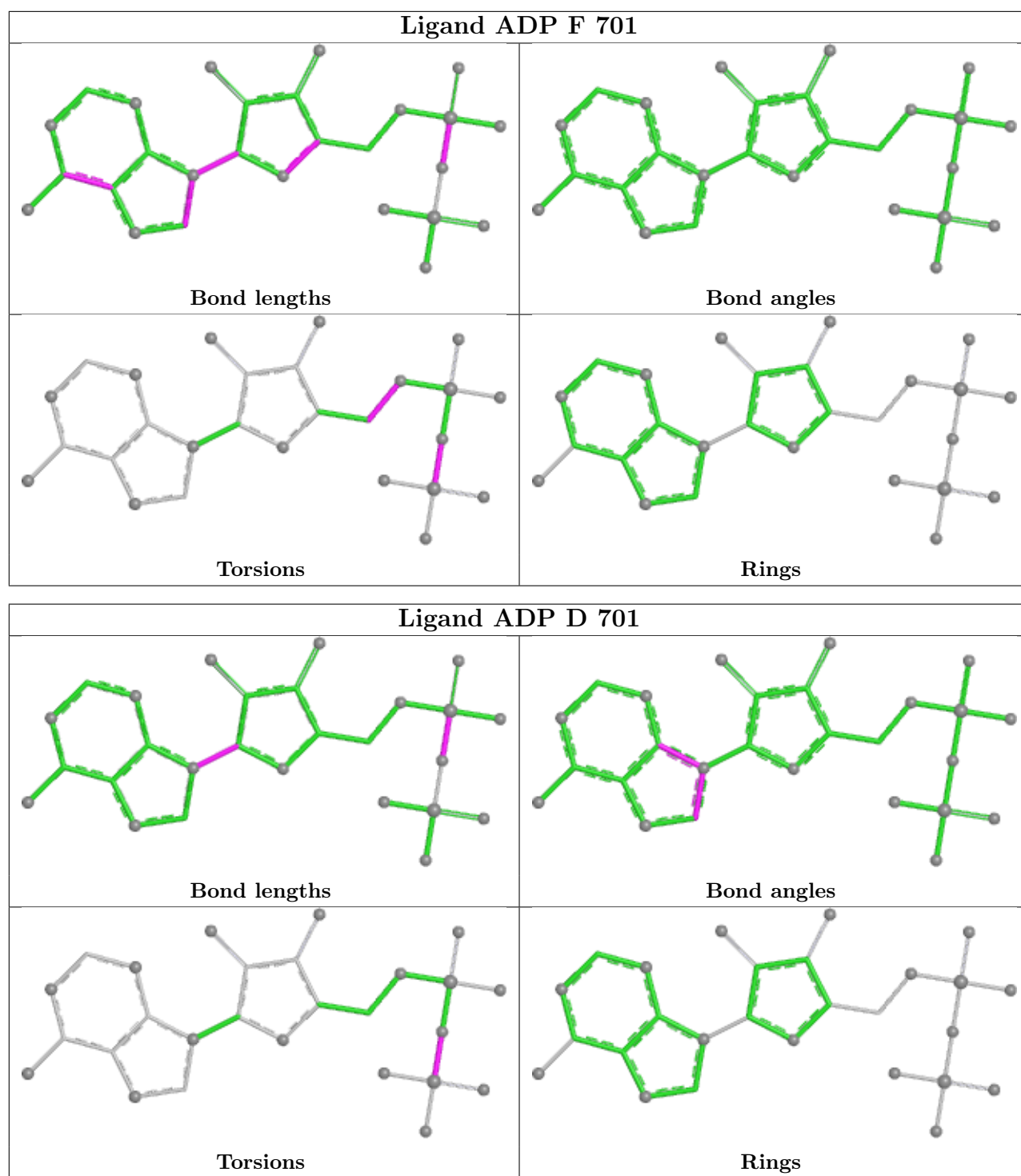
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	ADP	3	0
2	A	701	ADP	3	0
2	G	701	ADP	2	0
4	E	1505	EPE	13	0
2	B	701	ADP	4	0
2	F	701	ADP	3	0
2	D	701	ADP	3	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.