



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:34 PM UTC

PDB ID : 1ZM2 / pdb_00001zm2
Title : Structure of ADP-ribosylated eEF2 in complex with catalytic fragment of ETA
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.
Deposited on : 2005-05-10
Resolution : 3.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

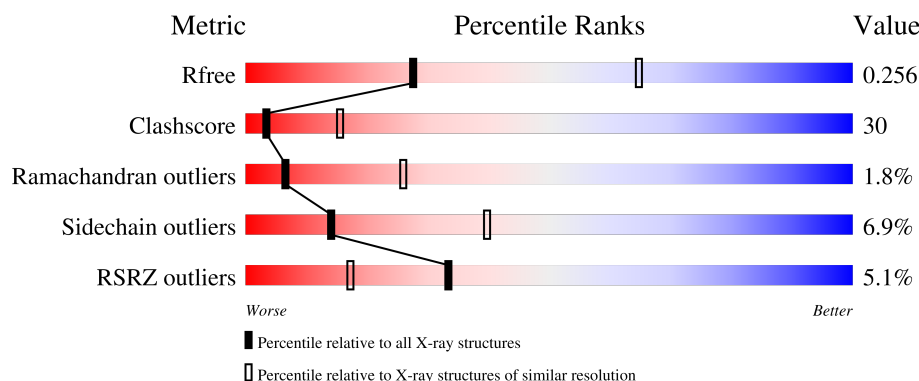
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	842	50% 43% • •
1	C	842	2% 44% 47% 7% •
1	E	842	16% 44% 49% 5% •
2	B	207	56% 37% 6% •
2	D	207	% 57% 35% 8%

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Mol	Chain	Length	Quality of chain
2	F	207	 A horizontal bar chart showing the quality of chain 2. The bar is divided into three segments: green (46%), yellow (43%), and orange (10%).

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	DDE	E	699	-	-	X	-
3	APR	E	843	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24024 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			

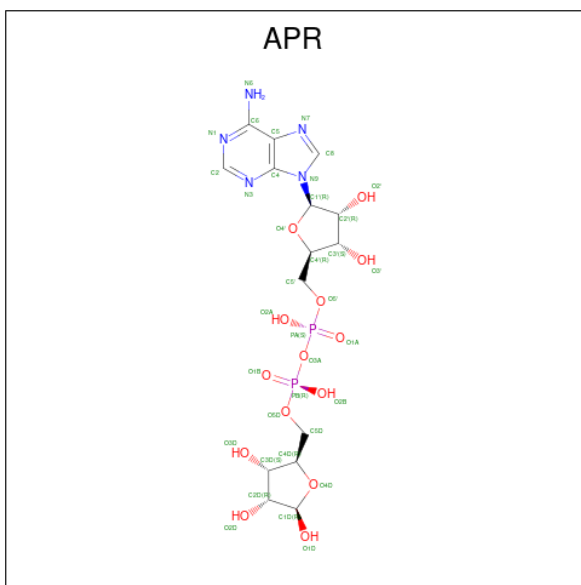
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	modified residue	UNP P32324
C	699	DDE	HIS	modified residue	UNP P32324
E	699	DDE	HIS	modified residue	UNP P32324

- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).

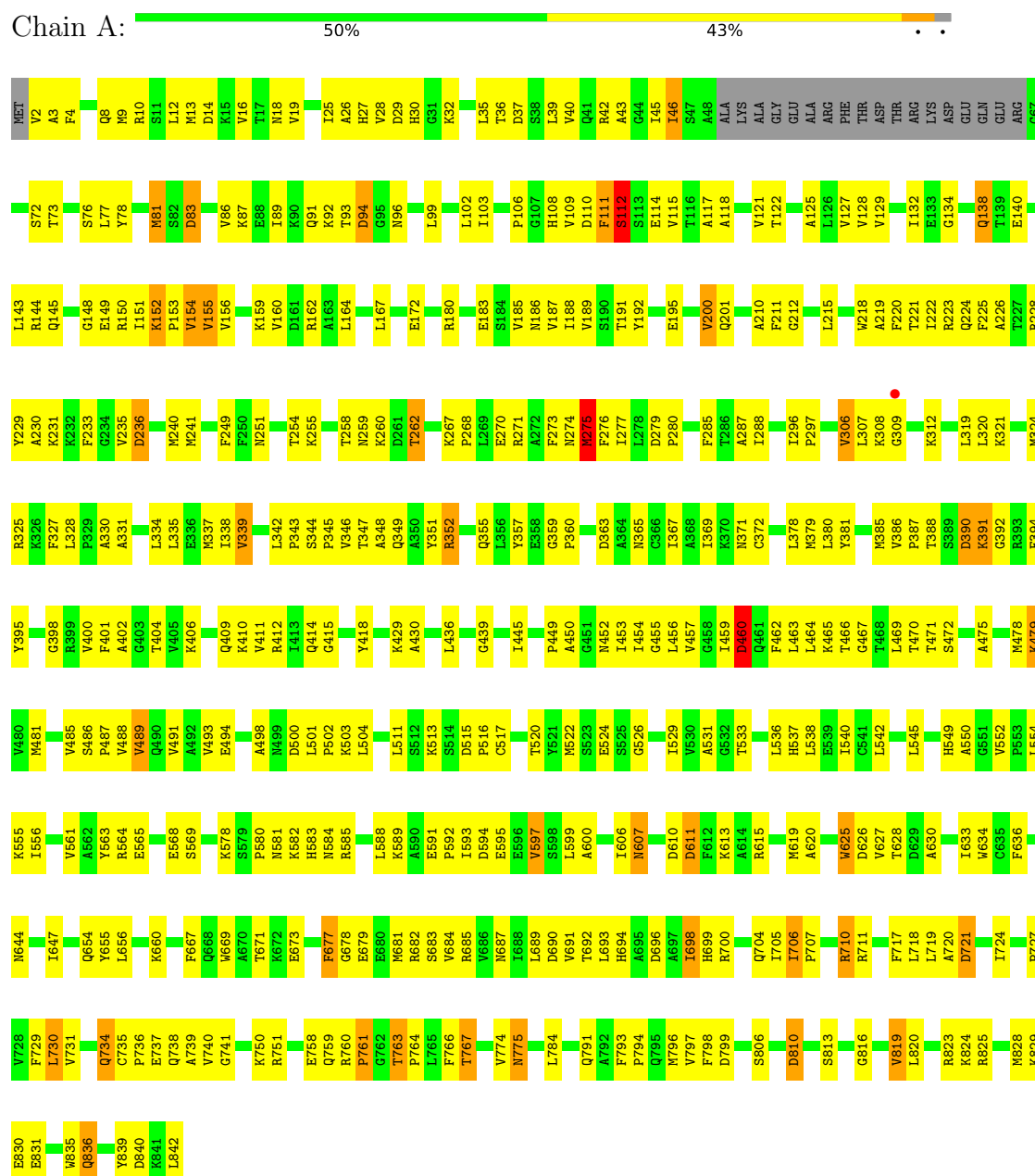


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

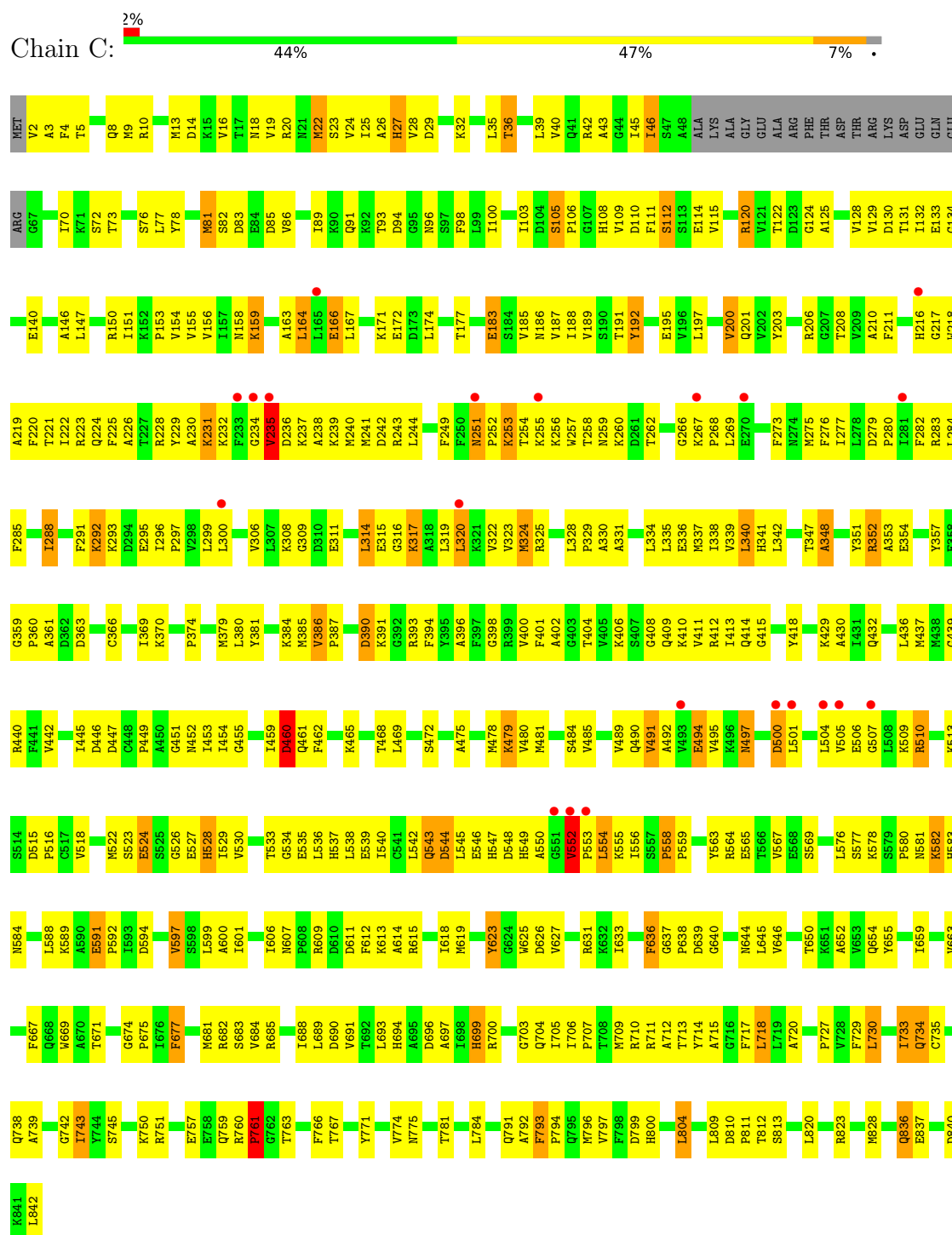
3 Residue-property plots

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

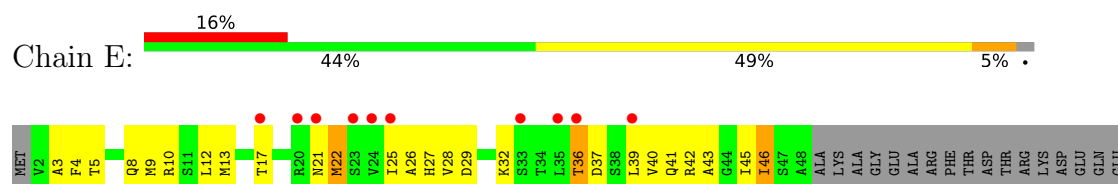
• Molecule 1: Elongation factor 2

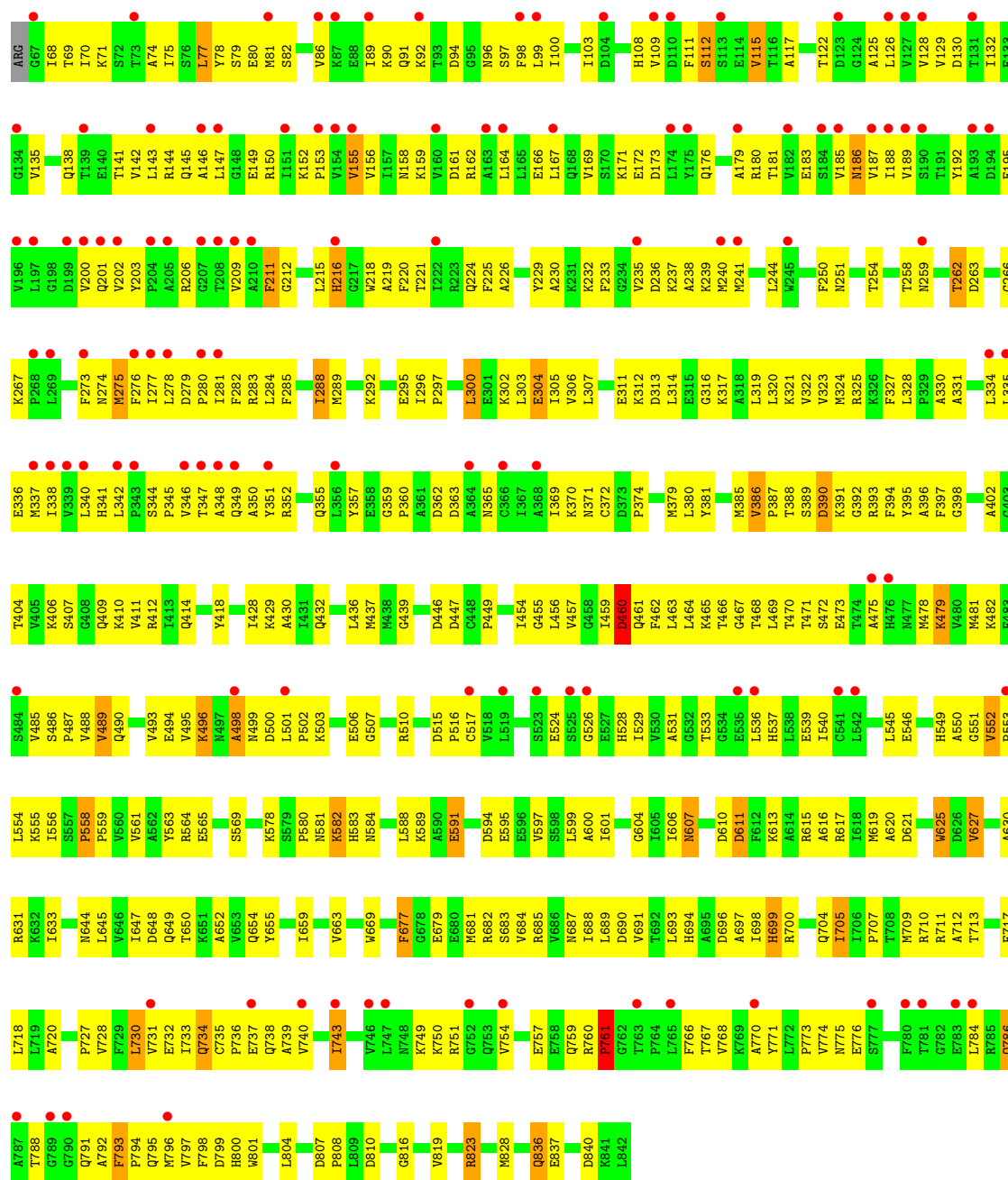


• Molecule 1: Elongation factor 2



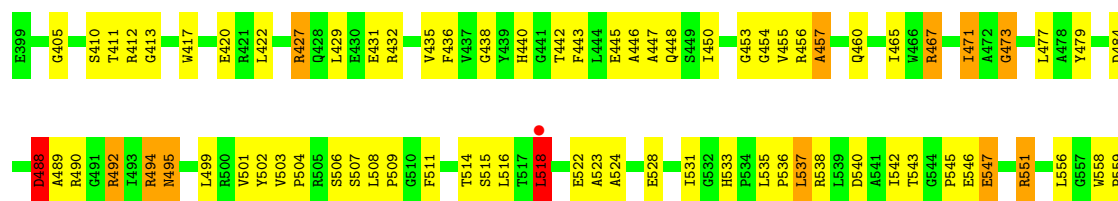
• Molecule 1: Elongation factor 2





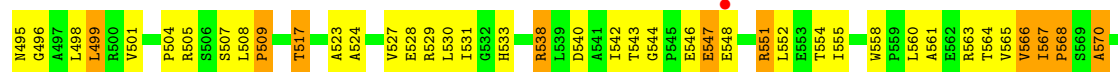
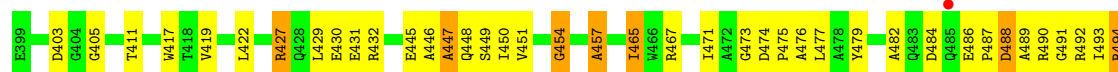
• Molecule 2: Exotoxin A

Chain B: 56% 37% 6%

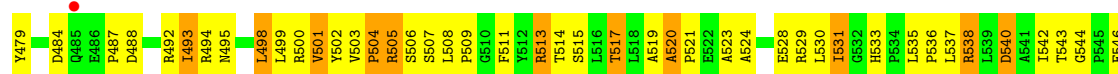
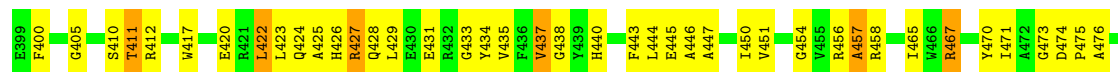




• Molecule 2: Exotoxin A



• Molecule 2: Exotoxin A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	330.63Å 67.84Å 191.50Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.07 30.00 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.07) 99.2 (30.00-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.06Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.265 0.229 , 0.256	Depositor DCC
R_{free} test set	1552 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24024	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0079e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: APR, DDE

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	0.58	1/6517 (0.0%)	1.04	28/8823 (0.3%)
1	C	0.54	0/6517	1.03	37/8823 (0.4%)
1	E	0.52	2/6517 (0.0%)	1.01	26/8823 (0.3%)
2	B	0.75	0/1627	1.21	15/2216 (0.7%)
2	D	0.73	0/1627	1.19	11/2216 (0.5%)
2	F	0.73	0/1627	1.24	15/2216 (0.7%)
All	All	0.59	3/24432 (0.0%)	1.07	132/33117 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	558	PRO	C-O	-8.47	1.17	1.24
1	A	706	ILE	CA-CB	-6.21	1.51	1.54
1	E	697	ALA	CA-CB	-5.00	1.45	1.53

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	VAL	N-CA-C	-9.08	101.89	110.42
2	F	520	ALA	CA-C-N	9.06	131.16	119.84
2	F	520	ALA	C-N-CA	9.06	131.16	119.84
1	E	558	PRO	CA-C-N	8.47	130.43	119.84
1	E	558	PRO	C-N-CA	8.47	130.43	119.84
2	F	517	THR	N-CA-C	-8.33	97.68	110.10
1	A	721	ASP	CA-C-N	8.32	128.08	119.76
1	A	721	ASP	C-N-CA	8.32	128.08	119.76
1	E	607	ASN	CA-C-N	7.87	128.29	119.32
1	E	607	ASN	C-N-CA	7.87	128.29	119.32
2	B	411	THR	N-CA-C	-7.79	102.78	111.82
1	A	115	VAL	N-CA-C	-7.76	103.29	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	554	LEU	N-CA-C	7.66	120.55	109.14
1	C	591	GLU	CA-C-N	7.63	127.56	119.85
1	C	591	GLU	C-N-CA	7.63	127.56	119.85
2	B	488	ASP	N-CA-C	-7.44	100.94	110.53
2	F	595	SER	N-CA-C	7.12	120.84	112.72
1	C	348	ALA	N-CA-C	7.09	119.08	111.36
1	E	471	THR	N-CA-C	-7.06	105.85	114.75
1	C	510	ARG	N-CA-C	-7.04	104.31	113.12
2	F	515	SER	N-CA-C	-6.93	104.86	113.38
2	F	411	THR	N-CA-C	-6.91	103.77	111.71
2	D	517	THR	N-CA-C	-6.88	100.79	110.50
1	E	652	ALA	N-CA-C	6.84	120.83	111.39
2	F	537	LEU	N-CA-C	-6.81	100.89	110.50
1	E	386	VAL	CA-C-N	6.79	126.75	119.76
1	E	386	VAL	C-N-CA	6.79	126.75	119.76
1	C	386	VAL	N-CA-C	6.75	115.25	107.89
1	E	498	ALA	N-CA-C	6.71	119.89	111.24
1	A	236	ASP	N-CA-C	-6.63	98.45	109.46
1	A	810	ASP	CA-C-N	6.61	127.13	119.47
1	A	810	ASP	C-N-CA	6.61	127.13	119.47
1	A	793	PHE	CA-C-N	6.59	126.50	119.85
1	A	793	PHE	C-N-CA	6.59	126.50	119.85
1	C	607	ASN	CA-C-N	6.58	127.11	119.47
1	C	607	ASN	C-N-CA	6.58	127.11	119.47
1	C	340	LEU	N-CA-C	6.49	120.46	112.54
2	F	587	ILE	N-CA-C	-6.47	101.22	107.76
2	F	457	ALA	N-CA-C	-6.38	101.93	110.55
1	C	552	VAL	CA-C-N	6.38	127.25	120.11
1	C	552	VAL	C-N-CA	6.38	127.25	120.11
2	F	501	VAL	N-CA-C	6.36	117.02	107.80
1	A	607	ASN	CA-C-N	6.34	125.96	119.56
1	A	607	ASN	C-N-CA	6.34	125.96	119.56
1	C	733	ILE	N-CA-C	6.29	116.92	108.11
1	C	359	GLY	CA-C-N	6.27	126.60	119.83
1	C	359	GLY	C-N-CA	6.27	126.60	119.83
2	B	457	ALA	N-CA-C	-6.24	102.29	110.53
2	F	438	GLY	N-CA-C	6.21	118.94	110.69
1	E	611	ASP	N-CA-C	-6.20	99.90	109.76
1	E	591	GLU	CA-C-N	6.19	126.70	120.14
1	E	591	GLU	C-N-CA	6.19	126.70	120.14
2	F	587	ILE	CB-CA-C	-6.15	104.13	110.71
2	B	573	THR	N-CA-C	-6.11	100.60	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	PRO	N-CA-C	-6.11	101.59	111.19
2	D	501	VAL	N-CA-C	6.09	117.07	108.36
2	F	544	GLY	CA-C-N	6.06	126.42	119.93
2	F	544	GLY	C-N-CA	6.06	126.42	119.93
1	E	496	LYS	N-CA-C	-6.06	105.70	114.12
1	C	22	MET	N-CA-C	6.03	117.36	108.86
2	F	504	PRO	N-CA-C	-6.01	101.72	110.80
1	E	705	ILE	N-CA-C	5.93	116.67	110.62
2	D	570	ALA	N-CA-C	-5.91	106.07	113.28
2	B	432	ARG	N-CA-C	-5.89	106.01	112.72
1	E	346	VAL	N-CA-C	-5.86	107.20	112.12
2	B	556	LEU	N-CA-C	-5.86	100.94	110.20
1	C	251	ASN	CA-C-N	5.83	125.37	119.19
1	C	251	ASN	C-N-CA	5.83	125.37	119.19
1	E	793	PHE	CA-C-N	5.83	125.74	119.85
1	E	793	PHE	C-N-CA	5.83	125.74	119.85
1	A	471	THR	N-CA-C	-5.82	107.98	114.62
1	A	706	ILE	CB-CA-C	-5.81	108.18	113.70
1	C	793	PHE	CA-C-N	5.79	125.75	119.78
1	C	793	PHE	C-N-CA	5.79	125.75	119.78
2	B	595	SER	N-CA-C	5.75	119.88	112.41
2	D	457	ALA	N-CA-C	-5.74	102.95	110.53
2	D	566	VAL	N-CA-C	5.71	116.80	108.53
1	E	267	LYS	CA-C-N	5.67	125.85	119.90
1	E	267	LYS	C-N-CA	5.67	125.85	119.90
1	E	288	ILE	N-CA-C	5.67	116.40	110.62
1	A	839	TYR	N-CA-C	-5.63	103.48	110.41
2	B	465	ILE	N-CA-C	5.61	119.89	112.76
1	A	339	VAL	N-CA-C	5.59	115.79	110.53
1	E	558	PRO	O-C-N	-5.59	118.52	121.15
1	A	611	ASP	N-CA-C	-5.56	100.22	109.46
1	A	155	VAL	N-CA-C	5.56	117.82	109.20
2	D	567	ILE	N-CA-C	5.56	115.29	109.01
2	D	544	GLY	CA-C-N	5.50	125.81	119.93
2	D	544	GLY	C-N-CA	5.50	125.81	119.93
1	C	652	ALA	N-CA-C	5.49	118.97	111.39
2	D	419	VAL	N-CA-C	-5.49	105.18	110.72
1	C	705	ILE	N-CA-C	5.48	115.68	110.53
1	A	415	GLY	CA-C-N	5.45	124.91	119.24
1	A	415	GLY	C-N-CA	5.45	124.91	119.24
1	C	369	ILE	CB-CA-C	-5.43	104.91	112.02
1	C	674	GLY	CA-C-N	5.40	126.45	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	674	GLY	C-N-CA	5.40	126.45	120.45
1	A	763	THR	N-CA-C	5.37	118.56	109.87
1	C	636	PHE	N-CA-C	-5.36	102.53	110.46
2	B	473	GLY	N-CA-C	-5.35	105.92	112.77
2	D	504	PRO	N-CA-C	-5.32	102.77	110.80
1	A	152	LYS	CA-C-N	-5.29	114.89	120.66
1	A	152	LYS	C-N-CA	-5.29	114.89	120.66
1	E	558	PRO	CB-CA-C	5.28	116.13	111.17
2	B	570	ALA	N-CA-C	-5.28	106.69	113.02
2	B	537	LEU	N-CA-C	-5.24	103.61	110.53
1	A	819	VAL	N-CA-C	5.24	115.68	110.23
1	A	275	MET	N-CA-C	5.23	117.79	111.40
1	E	155	VAL	N-CA-C	5.22	116.81	108.87
1	C	415	GLY	CA-C-N	5.19	124.99	119.28
1	C	415	GLY	C-N-CA	5.19	124.99	119.28
1	C	623	TYR	N-CA-C	5.19	120.26	112.94
1	C	317	LYS	N-CA-C	-5.19	106.90	113.18
2	B	427	ARG	N-CA-C	-5.17	104.90	111.11
1	C	288	ILE	N-CA-C	5.16	115.78	110.36
1	E	604	GLY	N-CA-C	5.14	122.38	115.59
1	A	154	VAL	N-CA-C	-5.13	101.24	108.27
1	A	636	PHE	N-CA-C	-5.13	102.56	109.95
1	C	192	TYR	N-CA-C	5.13	120.39	113.72
1	A	593	ILE	N-CA-C	-5.13	101.09	108.53
1	C	120	ARG	N-CA-C	5.12	119.00	112.34
2	B	518	LEU	N-CA-C	5.12	121.71	110.80
1	E	115	VAL	N-CA-C	-5.12	105.72	110.53
1	C	27	HIS	N-CA-C	-5.11	103.40	110.35
1	A	127	VAL	N-CA-C	5.10	115.69	107.98
1	E	22	MET	N-CA-C	5.09	115.26	108.38
1	C	267	LYS	N-CA-C	5.07	116.22	109.93
1	C	386	VAL	CA-C-N	5.05	124.96	119.76
1	C	386	VAL	C-N-CA	5.05	124.96	119.76
1	A	306	VAL	N-CA-C	5.03	115.58	107.73
2	B	571	ILE	CB-CA-C	-5.02	105.11	111.04
2	D	555	ILE	CB-CA-C	-5.02	105.76	111.59

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	6405	0	6472	372	0
1	C	6405	0	6472	406	0
1	E	6415	0	6487	448	0
2	B	1588	0	1539	72	0
2	D	1588	0	1539	77	0
2	F	1588	0	1539	91	0
3	E	35	0	19	6	0
All	All	24024	0	24067	1449	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 30.

All (1449) 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)
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.29	1.14
2:B:546:GLU:HG3	2:B:547:GLU:HG3	1.32	1.11
1:C:404:THR:HG22	1:C:449:PRO:HA	1.34	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.37	1.03
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.42	1.02
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.41	1.01
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.41	1.01
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.60	1.01
1:C:256:LYS:HD3	1:C:257:TRP:H	1.25	0.99
2:B:455:VAL:O	2:B:456:ARG:HD2	1.63	0.99
1:A:45:ILE:HD11	1:A:78:TYR:HB2	1.45	0.97
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.47	0.96
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.00	0.96
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.44	0.95
1:E:91:GLN:HE22	1:E:344:SER:H	1.13	0.94
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.48	0.94
1:A:694:HIS:HD2	1:A:696:ASP:H	1.15	0.94
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.50	0.93
1:C:552:VAL:HG22	1:C:553:PRO:HD2	1.49	0.93
2:F:513:ARG:HB2	2:F:513:ARG:HH11	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:HIS:HD2	1:E:696:ASP:H	1.11	0.90
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.35	0.90
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.53	0.90
1:A:409:GLN:HE21	1:A:411:VAL:HG22	1.37	0.89
1:A:731:VAL:HG12	1:A:796:MET:HB3	1.56	0.88
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.56	0.88
1:C:42:ARG:HG3	1:C:331:ALA:CB	2.04	0.87
1:A:258:THR:HG22	1:A:259:ASN:H	1.39	0.87
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.56	0.86
2:B:455:VAL:C	2:B:456:ARG:HD2	2.01	0.85
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.42	0.85
1:C:27:HIS:HD2	1:C:29:ASP:H	1.24	0.85
1:A:404:THR:HG22	1:A:449:PRO:HA	1.58	0.85
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.07	0.85
2:B:495:ASN:N	2:B:495:ASN:HD22	1.73	0.84
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.57	0.84
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.59	0.84
1:A:533:THR:H	1:A:537:HIS:CD2	1.95	0.83
1:A:533:THR:H	1:A:537:HIS:HD2	1.25	0.83
2:B:537:LEU:O	2:B:538:ARG:HD3	1.77	0.83
1:E:27:HIS:HD2	1:E:29:ASP:H	1.24	0.83
1:C:545:LEU:O	1:C:550:ALA:HB3	1.78	0.83
2:B:551:ARG:HG3	2:B:551:ARG:HH11	1.43	0.83
1:C:836:GLN:H	1:C:836:GLN:HE21	1.24	0.82
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.10	0.82
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.61	0.82
1:E:552:VAL:HG22	1:E:553:PRO:CD	2.10	0.82
2:B:477:LEU:HD22	2:B:551:ARG:HB2	1.61	0.81
1:E:289:MET:HE1	1:E:316:GLY:C	2.04	0.81
1:E:694:HIS:O	1:E:700:ARG:HD3	1.81	0.81
1:A:694:HIS:O	1:A:700:ARG:HD3	1.81	0.81
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.46	0.81
1:C:694:HIS:HD2	1:C:696:ASP:H	1.28	0.81
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.63	0.80
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.16	0.80
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.80
1:E:334:LEU:O	1:E:338:ILE:HG12	1.82	0.80
1:C:810:ASP:OD1	1:C:812:THR:HG22	1.81	0.80
1:C:225:PHE:HE2	1:C:277:ILE:HG23	1.45	0.80
2:D:477:LEU:HD13	2:D:551:ARG:NH1	1.96	0.80
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:LYS:HA	1:E:240:MET:HB3	1.63	0.80
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.63	0.79
1:C:644:ASN:ND2	1:C:684:VAL:H	1.78	0.79
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.64	0.79
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.63	0.79
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.18	0.79
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.63	0.79
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.82	0.79
1:C:256:LYS:HD3	1:C:257:TRP:N	1.97	0.78
1:C:615:ARG:HG2	1:C:619:MET:HE2	1.64	0.78
1:A:27:HIS:HD2	1:A:29:ASP:H	1.32	0.78
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.83	0.78
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.13	0.78
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.66	0.77
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.64	0.77
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.18	0.77
1:C:669:TRP:CD1	1:C:710:ARG:HE	2.03	0.77
1:E:404:THR:HG22	1:E:449:PRO:HA	1.66	0.77
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.66	0.77
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.84	0.77
1:E:694:HIS:CD2	1:E:696:ASP:H	1.99	0.77
1:C:311:GLU:HA	1:C:314:LEU:HD13	1.65	0.77
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.66	0.77
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.15	0.77
1:C:552:VAL:HG22	1:C:553:PRO:CD	2.14	0.76
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.67	0.76
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.67	0.76
1:C:644:ASN:HD22	1:C:684:VAL:H	1.30	0.76
1:C:225:PHE:CD2	1:C:277:ILE:HG12	2.20	0.76
1:C:578:LYS:HE3	1:C:840:ASP:OD1	1.85	0.76
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.19	0.76
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.68	0.76
1:A:819:VAL:O	1:A:823:ARG:HG3	1.85	0.76
1:C:836:GLN:H	1:C:836:GLN:NE2	1.84	0.76
1:A:45:ILE:HD11	1:A:78:TYR:CB	2.16	0.75
1:A:258:THR:HG22	1:A:259:ASN:N	2.00	0.75
1:A:734:GLN:HE21	1:A:734:GLN:N	1.84	0.75
1:C:543:GLN:HG2	1:C:544:ASP:N	2.01	0.75
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.69	0.75
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.50	0.75
1:C:2:VAL:HG22	1:C:3:ALA:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:THR:H	1:C:537:HIS:CD2	2.05	0.75
1:A:10:ARG:HD3	1:A:445:ILE:HD11	1.69	0.75
2:B:495:ASN:HD22	2:B:495:ASN:H	1.33	0.75
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.16	0.74
1:A:83:ASP:O	1:A:87:LYS:HD3	1.87	0.74
1:A:321:LYS:O	1:A:325:ARG:HG3	1.87	0.74
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.69	0.74
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.69	0.74
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.68	0.74
1:A:429:LYS:HG3	1:A:430:ALA:H	1.52	0.74
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.23	0.74
1:E:27:HIS:CD2	1:E:29:ASP:H	2.05	0.74
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.70	0.73
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.23	0.73
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.18	0.73
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.70	0.73
1:E:26:ALA:CB	1:E:128:VAL:HB	2.18	0.73
1:A:581:ASN:HB3	1:A:583:HIS:HD2	1.52	0.73
2:F:552:LEU:HD12	2:F:552:LEU:N	2.04	0.73
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.70	0.73
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.69	0.73
1:C:258:THR:HG22	1:C:260:LYS:H	1.51	0.73
2:F:487:PRO:HA	2:F:492:ARG:O	1.88	0.73
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.71	0.73
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.71	0.73
1:C:681:MET:HE2	1:C:717:PHE:CD1	2.24	0.73
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.71	0.73
1:C:536:LEU:HD12	1:C:537:HIS:N	2.04	0.72
1:C:584:ASN:ND2	1:C:694:HIS:H	1.87	0.72
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.24	0.72
1:C:492:ALA:HA	1:C:528:HIS:O	1.88	0.72
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.72	0.72
2:B:427:ARG:O	2:B:431:GLU:HG3	1.89	0.72
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.70	0.72
1:A:533:THR:N	1:A:537:HIS:HD2	1.88	0.71
1:A:149:GLU:HA	1:A:355:GLN:HE22	1.55	0.71
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.72	0.71
1:C:381:TYR:OH	1:C:481:MET:HE2	1.89	0.71
1:C:584:ASN:HD21	1:C:694:HIS:H	1.39	0.71
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.71	0.71
1:E:39:LEU:HD23	1:E:39:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:LYS:N	1:C:509:LYS:HD2	2.03	0.71
1:C:2:VAL:HG22	1:C:3:ALA:N	2.05	0.71
1:C:251:ASN:OD1	1:C:269:LEU:HD11	1.91	0.70
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.19	0.70
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.26	0.70
1:E:694:HIS:HD2	1:E:696:ASP:N	1.88	0.70
1:E:300:LEU:HG	1:E:305:ILE:HB	1.74	0.70
1:E:685:ARG:HE	1:E:687:ASN:HD21	1.39	0.70
1:C:523:SER:OG	1:C:527:GLU:HB2	1.91	0.70
1:C:535:GLU:O	1:C:539:GLU:HG3	1.92	0.70
2:D:531:ILE:HD11	2:D:533:HIS:O	1.91	0.70
2:D:465:ILE:HD13	2:D:465:ILE:H	1.57	0.70
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.25	0.70
1:E:185:VAL:O	1:E:189:VAL:HG23	1.91	0.70
1:E:578:LYS:HE3	1:E:840:ASP:OD1	1.91	0.70
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.55	0.70
1:C:494:GLU:O	1:C:555:LYS:HB3	1.91	0.70
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.56	0.70
2:B:551:ARG:HG3	2:B:551:ARG:NH1	2.01	0.69
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.54	0.69
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.75	0.69
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.74	0.69
1:C:545:LEU:O	1:C:550:ALA:CB	2.40	0.69
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.23	0.69
1:C:220:PHE:HA	1:C:224:GLN:OE1	1.91	0.69
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.73	0.69
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.91	0.69
1:E:524:GLU:HG3	1:E:669:TRP:CZ3	2.26	0.69
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.73	0.69
1:A:611:ASP:OD2	1:A:613:LYS:HB2	1.93	0.69
2:B:495:ASN:H	2:B:495:ASN:ND2	1.89	0.69
1:C:404:THR:HG22	1:C:449:PRO:CA	2.18	0.69
1:E:321:LYS:O	1:E:325:ARG:HG3	1.92	0.69
1:E:615:ARG:HG2	1:E:619:MET:HE2	1.75	0.69
1:E:700:ARG:O	1:E:705:ILE:HD13	1.93	0.69
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.74	0.69
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.92	0.69
1:E:699:DDE:HAA1	3:E:843:APR:H5'2	1.74	0.69
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.93	0.69
2:F:427:ARG:O	2:F:431:GLU:HG3	1.93	0.68
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.75	0.68
1:E:141:THR:HA	1:E:144:ARG:NH2	2.08	0.68
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.75	0.68
1:A:148:GLY:HA2	1:A:760:ARG:NH2	2.08	0.68
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.29	0.68
1:A:429:LYS:HE3	1:A:430:ALA:H	1.59	0.68
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.58	0.68
1:E:284:LEU:HD13	1:E:324:MET:HE1	1.73	0.68
1:A:828:MET:HE2	2:B:576:ARG:HE	1.59	0.68
1:E:338:ILE:O	1:E:342:LEU:HB2	1.94	0.68
1:E:581:ASN:O	1:E:582:LYS:HB2	1.94	0.68
1:E:647:ILE:HG13	1:E:685:ARG:NE	2.09	0.68
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.76	0.67
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.76	0.67
2:F:505:ARG:HG3	2:F:505:ARG:HH11	1.59	0.67
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.77	0.67
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.75	0.67
1:C:72:SER:HA	1:C:439:GLY:O	1.95	0.67
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.75	0.67
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.95	0.67
1:E:597:VAL:O	1:E:601:ILE:HG13	1.94	0.67
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.77	0.67
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.77	0.67
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.77	0.67
1:A:132:ILE:HD12	1:A:162:ARG:NE	2.09	0.67
1:C:348:ALA:O	1:C:352:ARG:HB2	1.95	0.67
1:C:591:GLU:O	1:C:685:ARG:HB3	1.95	0.67
2:B:524:ALA:O	2:B:528:GLU:HG3	1.95	0.66
1:E:699:DDE:HAA1	3:E:843:APR:C5'	2.26	0.66
1:A:27:HIS:CD2	1:A:29:ASP:H	2.14	0.66
1:C:284:LEU:O	1:C:288:ILE:HB	1.95	0.66
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.30	0.66
2:D:527:VAL:O	2:D:531:ILE:HG23	1.96	0.66
1:E:91:GLN:HE22	1:E:344:SER:N	1.91	0.66
1:E:707:PRO:O	1:E:711:ARG:HG3	1.95	0.66
1:C:277:ILE:O	1:C:280:PRO:HD2	1.96	0.66
1:C:546:GLU:HG3	1:C:547:HIS:CD2	2.31	0.66
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.30	0.66
1:C:659:ILE:O	1:C:663:VAL:HG23	1.95	0.66
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.31	0.65
1:A:391:LYS:HG3	1:A:392:GLY:H	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ILE:HG13	1:C:455:GLY:H	1.61	0.65
1:C:544:ASP:HB3	1:C:549:HIS:CD2	2.32	0.65
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.10	0.65
1:A:644:ASN:HD22	1:A:684:VAL:H	1.43	0.65
2:D:561:ALA:O	2:D:564:THR:HG23	1.96	0.65
1:E:709:MET:HE3	1:E:713:THR:OG1	1.96	0.65
1:E:734:GLN:N	1:E:734:GLN:HE21	1.94	0.65
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.79	0.65
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.25	0.65
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.77	0.65
2:B:546:GLU:HG3	2:B:547:GLU:CG	2.19	0.65
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.78	0.65
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.32	0.65
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.79	0.65
1:E:142:VAL:O	1:E:145:GLN:HB2	1.96	0.65
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.78	0.65
1:C:3:ALA:HA	1:C:46:ILE:O	1.97	0.65
1:E:563:TYR:O	1:E:564:ARG:HD2	1.96	0.65
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.27	0.65
1:C:533:THR:H	1:C:537:HIS:HD2	1.45	0.65
1:C:707:PRO:O	1:C:711:ARG:HG3	1.96	0.65
1:C:491:VAL:O	1:C:529:ILE:HA	1.97	0.65
1:A:454:ILE:HG13	1:A:455:GLY:H	1.62	0.64
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.37	0.64
1:A:156:VAL:HG22	1:A:210:ALA:HB3	1.79	0.64
1:C:530:VAL:HG13	1:C:530:VAL:O	1.97	0.64
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.79	0.64
1:E:739:ALA:HB2	1:E:791:GLN:OE1	1.97	0.64
1:A:581:ASN:HB3	1:A:583:HIS:CD2	2.31	0.64
1:E:584:ASN:HD21	1:E:694:HIS:H	1.45	0.64
1:E:186:ASN:CG	1:E:201:GLN:HE21	2.06	0.64
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.79	0.64
1:E:627:VAL:O	1:E:631:ARG:HG3	1.97	0.64
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.28	0.64
1:A:828:MET:HE2	2:B:576:ARG:NE	2.13	0.64
1:C:546:GLU:HB3	1:C:554:LEU:HD12	1.79	0.64
1:E:584:ASN:ND2	1:E:694:HIS:H	1.96	0.64
1:E:749:LYS:HG3	1:E:750:LYS:HD2	1.80	0.64
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.79	0.64
1:E:80:GLU:O	1:E:81:MET:HE2	1.98	0.64
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ALA:O	1:E:230:ALA:HB2	1.98	0.64
2:F:524:ALA:O	2:F:528:GLU:HG3	1.97	0.64
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.80	0.63
1:E:432:GLN:HB2	1:E:457:VAL:O	1.97	0.63
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.64	0.63
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.28	0.63
1:A:228:ARG:HH12	1:A:327:PHE:HE1	1.44	0.63
1:A:378:LEU:HD22	1:A:409:GLN:HE22	1.63	0.63
1:C:253:LYS:HE3	1:C:253:LYS:CA	2.24	0.63
1:E:275:MET:HE2	1:E:276:PHE:CE1	2.34	0.63
1:C:694:HIS:O	1:C:700:ARG:HD3	1.99	0.63
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.80	0.63
1:E:365:ASN:O	1:E:369:ILE:HG12	1.98	0.63
1:C:5:THR:OG1	1:C:8:GLN:HG3	1.99	0.63
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.28	0.63
2:D:432:ARG:CZ	2:D:432:ARG:HA	2.29	0.63
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.81	0.63
1:A:156:VAL:HG21	1:A:334:LEU:CD2	2.29	0.63
1:E:493:VAL:HA	1:E:556:ILE:CD1	2.29	0.63
1:A:155:VAL:O	1:A:337:MET:HE1	1.98	0.62
1:E:89:ILE:C	1:E:91:GLN:H	2.07	0.62
1:E:454:ILE:HG13	1:E:455:GLY:N	2.14	0.62
1:A:581:ASN:O	1:A:582:LYS:HB2	1.97	0.62
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.81	0.62
1:A:19:VAL:O	1:A:345:PRO:HD3	2.00	0.62
1:A:429:LYS:HG3	1:A:430:ALA:N	2.13	0.62
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.28	0.62
2:D:450:ILE:O	2:D:454:GLY:HA2	2.00	0.62
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.81	0.62
1:E:391:LYS:HG3	1:E:392:GLY:H	1.65	0.62
1:A:410:LYS:HA	1:A:430:ALA:HA	1.81	0.62
1:C:494:GLU:HG2	1:C:528:HIS:CE1	2.34	0.62
1:E:331:ALA:O	1:E:335:LEU:HG	1.99	0.62
1:A:710:ARG:HG3	1:A:710:ARG:NH1	2.09	0.62
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.15	0.62
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.64	0.62
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.80	0.62
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.30	0.62
2:F:517:THR:HG21	2:F:548:GLU:HA	1.81	0.62
1:A:466:THR:HG22	1:A:467:GLY:N	2.14	0.62
1:A:536:LEU:O	1:A:540:ILE:HG12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.15	0.62
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.35	0.62
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.64	0.62
1:E:74:ALA:O	1:E:439:GLY:HA2	2.00	0.61
1:A:501:LEU:C	1:A:501:LEU:HD23	2.25	0.61
1:C:385:MET:HE2	1:C:460:ASP:HA	1.82	0.61
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.83	0.61
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.36	0.61
1:C:703:GLY:HA2	2:D:493:ILE:CD1	2.30	0.61
1:E:552:VAL:HG22	1:E:553:PRO:HD3	1.81	0.61
1:E:836:GLN:H	1:E:836:GLN:HE21	1.49	0.61
1:A:19:VAL:HG22	1:A:99:LEU:HB3	1.81	0.61
1:C:522:MET:HA	1:C:527:GLU:O	1.99	0.61
1:E:39:LEU:HD21	1:E:77:LEU:CD2	2.31	0.61
1:C:239:LYS:O	1:C:243:ARG:HG3	2.01	0.61
1:C:591:GLU:HG2	1:C:685:ARG:HG2	1.81	0.61
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.36	0.61
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.82	0.61
1:A:731:VAL:HG12	1:A:796:MET:CB	2.30	0.61
1:C:275:MET:HE2	1:C:276:PHE:CE1	2.36	0.61
1:E:91:GLN:NE2	1:E:344:SER:H	1.91	0.61
1:E:381:TYR:O	1:E:398:GLY:HA3	1.99	0.61
1:A:681:MET:HE2	1:A:717:PHE:CD1	2.36	0.61
1:C:70:ILE:O	1:C:440:ARG:HG3	2.01	0.61
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.82	0.61
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.36	0.60
1:C:669:TRP:HD1	1:C:710:ARG:HE	1.44	0.60
1:E:39:LEU:CD2	1:E:77:LEU:HG	2.31	0.60
1:A:454:ILE:HG13	1:A:455:GLY:N	2.14	0.60
1:A:9:MET:O	1:A:13:MET:HG3	2.02	0.60
1:A:478:MET:O	1:A:479:LYS:C	2.44	0.60
1:C:76:SER:O	1:C:77:LEU:HD12	2.01	0.60
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.31	0.60
1:E:279:ASP:O	1:E:283:ARG:HG2	2.02	0.60
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.83	0.60
2:B:490:ARG:HH22	2:B:492:ARG:NE	1.99	0.60
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.36	0.60
1:E:240:MET:O	1:E:244:LEU:HG	2.00	0.60
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.36	0.60
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.84	0.60
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.82	0.60
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.83	0.60
1:A:823:ARG:NH1	1:A:829:LYS:O	2.35	0.60
2:B:488:ASP:OD2	2:B:492:ARG:HD2	2.01	0.60
1:E:132:ILE:HD12	1:E:132:ILE:N	2.17	0.60
1:A:2:VAL:HG22	1:A:3:ALA:N	2.16	0.60
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.66	0.60
1:C:386:VAL:HG11	1:C:437:MET:CE	2.32	0.60
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.31	0.60
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.67	0.60
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.82	0.60
2:F:484:ASP:OD2	2:F:494:ARG:HG2	2.02	0.60
1:E:43:ALA:HB1	1:E:78:TYR:O	2.02	0.60
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.84	0.59
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.02	0.59
1:C:529:ILE:N	1:C:529:ILE:HD12	2.17	0.59
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.17	0.59
2:B:551:ARG:HH11	2:B:551:ARG:CG	2.15	0.59
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.84	0.59
1:E:546:GLU:HB2	1:E:554:LEU:HD12	1.83	0.59
1:C:285:PHE:HE2	1:C:324:MET:SD	2.25	0.59
1:C:581:ASN:O	1:C:582:LYS:HB2	2.01	0.59
1:E:478:MET:O	1:E:479:LYS:C	2.46	0.59
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.37	0.59
1:E:284:LEU:CD1	1:E:324:MET:HE1	2.32	0.59
1:C:132:ILE:HG23	1:C:133:GLU:N	2.18	0.59
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.37	0.59
1:C:669:TRP:HE1	1:C:710:ARG:NH2	2.01	0.59
1:A:520:THR:HA	1:A:529:ILE:O	2.02	0.59
1:C:150:ARG:HD3	1:C:197:LEU:HD21	1.85	0.59
1:E:828:MET:HE2	2:F:576:ARG:HE	1.67	0.59
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.02	0.59
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.18	0.59
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.38	0.59
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.28	0.59
1:E:39:LEU:HG	1:E:335:LEU:HD21	1.84	0.59
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.38	0.59
1:A:30:HIS:HA	1:A:159:LYS:HE3	1.85	0.58
1:C:606:ILE:HD12	1:C:619:MET:HG2	1.84	0.58
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.38	0.58
2:F:493:ILE:O	2:F:493:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:GLU:HG3	1:A:767:THR:HG23	1.86	0.58
1:E:647:ILE:HB	1:E:687:ASN:HD22	1.67	0.58
1:E:685:ARG:NE	1:E:687:ASN:HD21	2.01	0.58
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.85	0.58
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.85	0.58
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.86	0.58
1:E:26:ALA:O	1:E:32:LYS:HD2	2.03	0.58
1:E:348:ALA:O	1:E:352:ARG:HB2	2.03	0.58
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.38	0.58
2:F:420:GLU:CD	2:F:420:GLU:H	2.12	0.58
1:A:690:ASP:OD1	1:A:691:VAL:N	2.35	0.58
1:A:698:ILE:HD13	1:A:698:ILE:N	2.18	0.58
1:C:225:PHE:HD2	1:C:277:ILE:HG12	1.67	0.58
1:C:256:LYS:HE2	1:C:256:LYS:HA	1.85	0.58
1:C:268:PRO:O	1:C:269:LEU:HD23	2.04	0.58
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.33	0.58
1:E:181:THR:O	1:E:185:VAL:HG23	2.04	0.58
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.38	0.58
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.32	0.58
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.17	0.58
1:A:584:ASN:ND2	1:A:694:HIS:H	2.01	0.58
1:A:584:ASN:HD21	1:A:694:HIS:H	1.51	0.58
1:A:3:ALA:HA	1:A:46:ILE:O	2.04	0.58
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.19	0.58
1:A:588:LEU:HD12	1:A:588:LEU:C	2.29	0.58
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.86	0.58
1:E:411:VAL:HG12	1:E:412:ARG:N	2.18	0.58
1:E:731:VAL:HG23	1:E:796:MET:HB3	1.84	0.58
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.34	0.58
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.86	0.58
1:C:501:LEU:C	1:C:501:LEU:HD23	2.29	0.58
1:E:581:ASN:HB3	1:E:583:HIS:HD2	1.69	0.58
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.86	0.57
2:F:508:LEU:N	2:F:509:PRO:CD	2.67	0.57
1:A:409:GLN:HE21	1:A:411:VAL:CG2	2.15	0.57
1:A:644:ASN:ND2	1:A:684:VAL:H	2.01	0.57
1:A:836:GLN:H	1:A:836:GLN:HE21	1.52	0.57
1:C:597:VAL:O	1:C:601:ILE:HG13	2.03	0.57
1:E:69:THR:OG1	1:E:389:SER:HB3	2.03	0.57
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.87	0.57
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HE3	1:A:840:ASP:OD1	2.05	0.57
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.05	0.57
1:C:211:PHE:O	1:C:219:ALA:HA	2.05	0.57
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.73	0.57
1:E:103:ILE:HD12	1:E:103:ILE:N	2.18	0.57
1:E:183:GLU:O	1:E:187:VAL:HG23	2.04	0.57
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.87	0.57
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.34	0.57
1:C:799:ASP:OD1	1:C:800:HIS:HD2	1.88	0.57
2:D:479:TYR:CD2	2:D:582:LEU:HB2	2.40	0.57
2:D:484:ASP:OD2	2:D:494:ARG:HG2	2.04	0.57
1:E:284:LEU:HD13	1:E:324:MET:CE	2.35	0.57
1:E:536:LEU:O	1:E:539:GLU:N	2.38	0.57
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.87	0.57
2:D:457:ALA:HB2	2:D:558:TRP:CE3	2.40	0.57
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.19	0.57
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.86	0.57
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.87	0.57
1:A:275:MET:HE2	1:A:276:PHE:CE1	2.39	0.57
1:A:836:GLN:H	1:A:836:GLN:NE2	2.02	0.57
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.85	0.57
1:E:229:TYR:CD1	1:E:232:LYS:HD2	2.40	0.57
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.05	0.57
1:C:569:SER:O	1:C:720:ALA:HB1	2.05	0.56
1:E:36:THR:O	1:E:40:VAL:HG23	2.06	0.56
1:C:273:PHE:CD1	1:C:277:ILE:HD12	2.40	0.56
1:C:311:GLU:HA	1:C:314:LEU:CD1	2.33	0.56
1:E:81:MET:O	1:E:96:ASN:HB3	2.05	0.56
1:A:155:VAL:HG12	1:A:156:VAL:N	2.19	0.56
1:A:226:ALA:CB	1:A:241:MET:HB3	2.34	0.56
1:C:200:VAL:CG1	1:C:200:VAL:O	2.53	0.56
1:C:226:ALA:CB	1:C:241:MET:HB3	2.35	0.56
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.19	0.56
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.35	0.56
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.87	0.56
1:A:251:ASN:HB3	1:A:254:THR:OG1	2.05	0.56
1:C:565:GLU:O	1:C:681:MET:HA	2.06	0.56
1:C:588:LEU:C	1:C:588:LEU:HD12	2.31	0.56
2:D:492:ARG:HH12	2:D:494:ARG:HD2	1.70	0.56
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.36	0.56
2:F:505:ARG:HG3	2:F:505:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASN:O	1:A:369:ILE:HG12	2.06	0.56
1:C:390:ASP:O	1:C:391:LYS:HB2	2.05	0.56
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.41	0.56
1:E:565:GLU:O	1:E:681:MET:HA	2.05	0.56
1:A:258:THR:CG2	1:A:259:ASN:H	2.16	0.56
2:B:488:ASP:OD1	2:B:489:ALA:N	2.39	0.56
1:E:555:LYS:O	1:E:556:ILE:HD13	2.05	0.56
1:A:381:TYR:O	1:A:398:GLY:HA3	2.05	0.56
2:B:563:ARG:HG3	2:B:563:ARG:HH11	1.71	0.56
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.36	0.56
1:E:258:THR:HG22	1:E:259:ASN:N	2.21	0.56
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.40	0.56
1:A:820:LEU:HD11	1:A:824:LYS:HE3	1.88	0.56
1:C:240:MET:O	1:C:244:LEU:HG	2.06	0.56
1:C:619:MET:HE1	1:C:633:ILE:HD11	1.88	0.56
1:A:153:PRO:HD2	1:A:200:VAL:HG13	1.87	0.56
1:A:411:VAL:HG12	1:A:412:ARG:N	2.19	0.56
1:C:669:TRP:HE1	1:C:710:ARG:HH21	1.52	0.56
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.88	0.56
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.87	0.56
1:C:694:HIS:CD2	1:C:696:ASP:H	2.17	0.55
1:E:810:ASP:O	1:E:816:GLY:HA3	2.07	0.55
1:A:698:ILE:HD13	1:A:698:ILE:H	1.71	0.55
1:C:9:MET:O	1:C:13:MET:HG3	2.05	0.55
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.89	0.55
1:C:490:GLN:O	1:C:491:VAL:HG13	2.06	0.55
1:C:192:TYR:HA	1:C:763:THR:CG2	2.36	0.55
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.36	0.55
1:C:231:LYS:HG2	1:C:232:LYS:N	2.20	0.55
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.36	0.55
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.47	0.55
1:E:278:LEU:O	1:E:282:PHE:HB2	2.06	0.55
1:E:681:MET:HE2	1:E:717:PHE:CD1	2.40	0.55
2:F:433:GLY:O	2:F:505:ARG:HB2	2.07	0.55
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.22	0.55
1:C:529:ILE:HG22	1:C:530:VAL:N	2.21	0.55
1:E:371:ASN:O	1:E:372:CYS:C	2.48	0.55
1:E:162:ARG:O	1:E:166:GLU:HB2	2.07	0.55
1:A:707:PRO:O	1:A:711:ARG:HG3	2.06	0.55
1:E:258:THR:HG22	1:E:259:ASN:H	1.71	0.55
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:THR:HB	1:A:764:PRO:HD2	1.87	0.55
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.07	0.55
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.89	0.55
1:E:186:ASN:OD1	1:E:186:ASN:C	2.50	0.55
1:E:581:ASN:O	1:E:582:LYS:CB	2.55	0.55
1:A:429:LYS:CG	1:A:430:ALA:H	2.19	0.55
1:C:538:LEU:O	1:C:542:LEU:HG	2.06	0.55
2:D:523:ALA:O	2:D:524:ALA:C	2.50	0.55
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.88	0.55
1:E:644:ASN:ND2	1:E:684:VAL:H	2.04	0.55
1:C:478:MET:O	1:C:479:LYS:C	2.49	0.55
1:E:9:MET:O	1:E:12:LEU:HB3	2.07	0.55
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.89	0.55
1:C:544:ASP:O	1:C:549:HIS:N	2.40	0.54
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.72	0.54
1:E:17:THR:HB	1:E:92:LYS:O	2.07	0.54
1:E:588:LEU:C	1:E:588:LEU:HD12	2.32	0.54
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.07	0.54
2:F:400:PHE:CD1	2:F:429:LEU:HD23	2.42	0.54
1:A:485:VAL:O	1:A:487:PRO:HD3	2.07	0.54
2:B:508:LEU:N	2:B:509:PRO:CD	2.69	0.54
1:C:251:ASN:H	1:C:251:ASN:HD22	1.54	0.54
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.42	0.54
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.22	0.54
2:F:529:ARG:NH1	2:F:604:PRO:HG2	2.22	0.54
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.43	0.54
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.90	0.54
1:C:576:LEU:HD12	1:C:577:SER:N	2.22	0.54
1:E:237:LYS:HA	1:E:240:MET:CB	2.35	0.54
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.90	0.54
2:F:429:LEU:O	2:F:434:TYR:HB2	2.07	0.54
1:A:81:MET:O	1:A:96:ASN:HB3	2.08	0.54
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.88	0.54
1:E:303:LEU:O	1:E:304:GLU:HB2	2.08	0.54
1:E:569:SER:O	1:E:720:ALA:HB1	2.07	0.54
1:A:784:LEU:CD2	1:A:794:PRO:HG3	2.37	0.54
1:C:581:ASN:ND2	1:C:699:DDE:O	2.40	0.54
1:C:627:VAL:O	1:C:631:ARG:HG3	2.08	0.54
1:C:650:THR:CG2	1:C:688:ILE:HG22	2.38	0.54
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.56	0.54
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:TRP:CZ2	2:B:490:ARG:NH1	2.76	0.54
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.43	0.54
1:E:495:VAL:HA	1:E:554:LEU:HA	1.90	0.54
2:B:410:SER:HB3	2:B:413:GLY:O	2.07	0.54
1:C:132:ILE:HG23	1:C:133:GLU:H	1.73	0.54
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.90	0.54
1:C:750:LYS:O	1:C:751:ARG:HB2	2.07	0.54
2:D:505:ARG:HG3	2:D:505:ARG:HH11	1.73	0.54
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.90	0.54
1:C:291:PHE:HE1	1:C:315:GLU:CB	2.20	0.54
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.89	0.54
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.90	0.53
1:A:727:PRO:HG2	1:A:774:VAL:HB	1.88	0.53
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.88	0.53
2:F:531:ILE:HG22	2:F:533:HIS:H	1.72	0.53
1:A:797:VAL:HG22	1:A:798:PHE:N	2.23	0.53
1:C:155:VAL:HG12	1:C:156:VAL:N	2.21	0.53
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.90	0.53
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.90	0.53
1:A:45:ILE:CD1	1:A:78:TYR:HB2	2.29	0.53
1:C:234:GLY:O	1:C:235:VAL:HG23	2.08	0.53
1:C:614:ALA:O	1:C:618:ILE:HG12	2.07	0.53
1:A:258:THR:HG22	1:A:260:LYS:H	1.73	0.53
1:A:694:HIS:CD2	1:A:696:ASP:H	2.07	0.53
1:C:36:THR:O	1:C:40:VAL:HG23	2.09	0.53
1:C:331:ALA:O	1:C:335:LEU:HG	2.09	0.53
2:D:427:ARG:O	2:D:431:GLU:HG3	2.09	0.53
1:E:108:HIS:O	1:E:111:PHE:HD2	1.90	0.53
1:A:155:VAL:CG1	1:A:156:VAL:N	2.72	0.53
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.44	0.53
1:C:606:ILE:HD12	1:C:619:MET:CG	2.39	0.53
1:C:669:TRP:NE1	1:C:710:ARG:HH21	2.05	0.53
1:E:235:VAL:HG11	1:E:239:LYS:HD3	1.91	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
2:F:456:ARG:HH21	2:F:458:ARG:HH21	1.57	0.53
1:C:591:GLU:HG2	1:C:685:ARG:CG	2.39	0.53
1:E:39:LEU:HD21	1:E:77:LEU:HG	1.90	0.53
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.38	0.53
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.22	0.53
1:C:619:MET:HE1	1:C:633:ILE:CD1	2.38	0.53
2:D:477:LEU:HD12	2:D:477:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LEU:HD12	1:E:167:LEU:H	1.73	0.53
2:F:427:ARG:HG2	2:F:428:GLN:N	2.24	0.53
1:C:576:LEU:HD12	1:C:577:SER:H	1.73	0.53
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.90	0.53
1:E:40:VAL:C	1:E:42:ARG:H	2.16	0.53
1:E:109:VAL:HG12	1:E:109:VAL:O	2.08	0.53
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.44	0.53
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.74	0.52
1:E:644:ASN:HD22	1:E:684:VAL:H	1.57	0.52
1:C:386:VAL:HG11	1:C:437:MET:HE1	1.90	0.52
2:D:486:GLU:HG3	2:D:487:PRO:HD2	1.91	0.52
2:D:446:ALA:O	2:D:447:ALA:C	2.53	0.52
1:E:337:MET:HA	1:E:341:HIS:CD2	2.45	0.52
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.49	0.52
1:A:550:ALA:O	1:A:552:VAL:HG23	2.09	0.52
2:D:542:ILE:HG12	2:D:543:THR:N	2.24	0.52
1:E:80:GLU:HA	1:E:96:ASN:O	2.09	0.52
1:C:291:PHE:O	1:C:293:LYS:N	2.43	0.52
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.73	0.52
2:F:548:GLU:HG2	2:F:548:GLU:O	2.10	0.52
2:F:552:LEU:HD12	2:F:552:LEU:H	1.72	0.52
1:C:314:LEU:HD21	1:C:322:VAL:HG21	1.91	0.52
2:D:508:LEU:N	2:D:509:PRO:CD	2.72	0.52
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.10	0.52
1:A:698:ILE:H	1:A:698:ILE:CD1	2.23	0.52
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.10	0.52
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.78	0.52
1:E:37:ASP:O	1:E:41:GLN:HG3	2.09	0.52
1:E:545:LEU:HD12	1:E:549:HIS:CB	2.35	0.52
1:A:277:ILE:O	1:A:280:PRO:HD2	2.09	0.52
1:A:486:SER:O	1:A:488:VAL:HG13	2.09	0.52
1:C:515:ASP:HB3	1:C:518:VAL:CG1	2.37	0.52
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.92	0.52
1:A:411:VAL:HG13	1:A:470:THR:O	2.10	0.52
1:E:337:MET:HA	1:E:341:HIS:HD2	1.75	0.52
1:E:750:LYS:O	1:E:751:ARG:HB2	2.10	0.52
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.45	0.52
1:E:4:PHE:HD1	1:E:8:GLN:CD	2.17	0.52
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.39	0.52
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.75	0.52
1:A:112:SER:CB	1:A:794:PRO:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.90	0.51
1:C:91:GLN:O	1:C:93:THR:HG23	2.11	0.51
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.45	0.51
1:C:226:ALA:O	1:C:230:ALA:HB2	2.10	0.51
2:D:488:ASP:CG	2:D:489:ALA:N	2.68	0.51
1:C:85:ASP:OD1	1:C:223:ARG:NH2	2.43	0.51
1:C:468:THR:C	1:C:469:LEU:HD12	2.34	0.51
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.92	0.51
1:A:685:ARG:HE	1:A:687:ASN:HD21	1.58	0.51
1:C:110:ASP:C	1:C:112:SER:H	2.19	0.51
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.25	0.51
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.75	0.51
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.36	0.51
1:A:615:ARG:HG2	1:A:619:MET:HE2	1.93	0.51
1:C:500:ASP:OD2	1:C:552:VAL:HG21	2.11	0.51
1:E:739:ALA:HB1	1:E:788:THR:HB	1.93	0.51
2:B:477:LEU:HD13	2:B:551:ARG:NH1	2.25	0.51
1:C:147:LEU:HD11	1:C:189:VAL:HA	1.92	0.51
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.93	0.51
1:E:176:GLN:O	1:E:180:ARG:HG3	2.10	0.51
1:E:773:PRO:HB2	1:E:776:GLU:HB2	1.91	0.51
2:B:471:ILE:HG21	2:B:501:VAL:HG21	1.91	0.51
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.91	0.51
1:C:581:ASN:O	1:C:582:LYS:CB	2.58	0.51
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.93	0.51
1:E:350:ALA:O	1:E:370:LYS:HG2	2.11	0.51
2:F:426:HIS:O	2:F:429:LEU:HB2	2.11	0.51
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.46	0.51
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.78	0.51
1:A:132:ILE:HD12	1:A:162:ARG:CZ	2.41	0.51
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.46	0.51
1:C:155:VAL:CG1	1:C:156:VAL:N	2.73	0.51
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.74	0.51
1:C:237:LYS:HA	1:C:240:MET:HB3	1.93	0.51
1:E:704:GLN:O	1:E:707:PRO:HD2	2.11	0.51
1:A:306:VAL:HG13	1:A:306:VAL:O	2.11	0.51
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.93	0.51
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.46	0.51
1:E:5:THR:OG1	1:E:8:GLN:HG3	2.11	0.51
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.93	0.51
2:F:504:PRO:HD3	2:F:563:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:542:ILE:HD12	2:F:543:THR:H	1.76	0.51
1:A:19:VAL:HA	1:A:99:LEU:O	2.11	0.50
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.40	0.50
1:C:258:THR:HG22	1:C:259:ASN:N	2.25	0.50
1:C:563:TYR:O	1:C:564:ARG:HD2	2.11	0.50
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.92	0.50
1:A:183:GLU:O	1:A:187:VAL:HG23	2.12	0.50
1:C:129:VAL:HG13	1:C:134:GLY:O	2.10	0.50
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.46	0.50
1:C:601:ILE:HG12	1:C:606:ILE:HB	1.92	0.50
2:D:531:ILE:CD1	2:D:533:HIS:CE1	2.90	0.50
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.93	0.50
1:E:454:ILE:HG13	1:E:455:GLY:H	1.75	0.50
1:E:607:ASN:HB3	1:E:610:ASP:OD2	2.10	0.50
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.93	0.50
1:C:306:VAL:HG23	1:C:306:VAL:O	2.11	0.50
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.44	0.50
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.46	0.50
1:E:786:GLN:N	1:E:786:GLN:OE1	2.45	0.50
1:A:371:ASN:O	1:A:372:CYS:C	2.54	0.50
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.92	0.50
1:C:27:HIS:CD2	1:C:29:ASP:H	2.15	0.50
1:C:410:LYS:HA	1:C:430:ALA:HA	1.93	0.50
1:C:644:ASN:HD22	1:C:684:VAL:N	2.03	0.50
1:E:150:ARG:NH1	1:E:351:TYR:O	2.44	0.50
1:E:186:ASN:HA	1:E:189:VAL:HB	1.93	0.50
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.75	0.50
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.93	0.50
1:C:192:TYR:HA	1:C:763:THR:HG22	1.94	0.50
1:C:494:GLU:HG2	1:C:528:HIS:HE1	1.74	0.50
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.38	0.50
1:E:129:VAL:HG12	1:E:130:ASP:N	2.27	0.50
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.46	0.50
2:B:542:ILE:HD12	2:B:543:THR:H	1.76	0.50
1:C:667:PHE:O	1:C:671:THR:HG23	2.12	0.50
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.94	0.50
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.92	0.50
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.94	0.50
1:C:697:ALA:HA	1:C:700:ARG:NE	2.26	0.50
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.46	0.50
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ARG:HH11	1:E:412:ARG:HG2	1.76	0.50
1:A:26:ALA:CB	1:A:128:VAL:HB	2.40	0.50
1:A:429:LYS:HE3	1:A:430:ALA:N	2.25	0.50
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.42	0.50
1:E:39:LEU:HD23	1:E:39:LEU:C	2.36	0.50
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.42	0.50
1:A:200:VAL:HG13	1:A:200:VAL:O	2.10	0.49
1:A:228:ARG:C	1:A:230:ALA:H	2.18	0.49
1:A:704:GLN:O	1:A:707:PRO:HD2	2.12	0.49
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.94	0.49
1:C:580:PRO:HD2	1:C:704:GLN:CD	2.37	0.49
1:A:43:ALA:HB1	1:A:78:TYR:O	2.12	0.49
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.47	0.49
1:A:429:LYS:CE	1:A:430:ALA:H	2.25	0.49
2:B:435:VAL:HG21	2:B:598:PRO:HG3	1.94	0.49
1:C:292:LYS:HD2	1:C:295:GLU:OE2	2.12	0.49
1:E:229:TYR:HD1	1:E:232:LYS:HD2	1.76	0.49
1:E:836:GLN:H	1:E:836:GLN:NE2	2.09	0.49
2:F:513:ARG:HB2	2:F:513:ARG:NH1	2.15	0.49
1:C:381:TYR:O	1:C:398:GLY:HA3	2.13	0.49
1:E:200:VAL:HG22	1:E:200:VAL:O	2.13	0.49
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.26	0.49
1:A:231:LYS:C	1:A:233:PHE:N	2.68	0.49
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.41	0.49
2:B:490:ARG:HH22	2:B:492:ARG:CZ	2.24	0.49
1:C:76:SER:C	1:C:77:LEU:HD12	2.37	0.49
1:C:191:THR:O	1:C:763:THR:HG22	2.12	0.49
1:C:401:PHE:CD2	1:C:478:MET:HE1	2.46	0.49
2:F:519:ALA:O	2:F:521:PRO:HD3	2.12	0.49
1:A:40:VAL:C	1:A:42:ARG:H	2.21	0.49
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.77	0.49
1:C:43:ALA:HB1	1:C:78:TYR:O	2.12	0.49
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.43	0.49
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.47	0.49
1:A:231:LYS:C	1:A:233:PHE:H	2.19	0.49
1:A:569:SER:O	1:A:720:ALA:HB1	2.13	0.49
1:A:591:GLU:O	1:A:685:ARG:HB3	2.12	0.49
1:C:231:LYS:CG	1:C:232:LYS:N	2.75	0.49
2:F:451:VAL:O	2:F:451:VAL:CG1	2.61	0.49
1:A:110:ASP:C	1:A:112:SER:H	2.20	0.49
1:A:191:THR:O	1:A:763:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:LEU:O	2:B:545:PRO:HD2	2.12	0.49
1:C:360:PRO:HB2	1:C:363:ASP:HB2	1.94	0.49
1:C:485:VAL:O	1:C:485:VAL:HG22	2.12	0.49
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.95	0.49
1:E:296:ILE:O	1:E:300:LEU:HB2	2.12	0.49
1:A:72:SER:HA	1:A:439:GLY:O	2.13	0.49
1:A:730:LEU:C	1:A:730:LEU:HD22	2.38	0.49
1:C:156:VAL:HG23	1:C:337:MET:HE1	1.95	0.49
1:C:174:LEU:O	1:C:177:THR:HB	2.13	0.49
1:C:240:MET:O	1:C:240:MET:HE3	2.12	0.49
1:C:374:PRO:O	1:C:404:THR:HG23	2.11	0.49
2:D:505:ARG:HG3	2:D:505:ARG:NH1	2.28	0.49
1:E:211:PHE:N	1:E:211:PHE:CD2	2.80	0.49
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.12	0.49
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.37	0.49
2:F:517:THR:C	2:F:519:ALA:N	2.69	0.49
2:D:476:ALA:HA	2:D:582:LEU:HD23	1.93	0.49
2:D:495:ASN:OD1	2:D:495:ASN:N	2.45	0.49
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.95	0.49
1:C:315:GLU:C	1:C:319:LEU:HB2	2.37	0.49
1:E:46:ILE:N	1:E:46:ILE:HD12	2.28	0.49
1:E:760:ARG:O	1:E:761:PRO:C	2.56	0.49
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.76	0.48
1:A:619:MET:HE1	1:A:633:ILE:HD12	1.94	0.48
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.47	0.48
1:C:638:PRO:O	1:C:640:GLY:N	2.46	0.48
1:C:733:ILE:HG21	1:C:743:ILE:HD12	1.95	0.48
1:E:349:GLN:O	1:E:370:LYS:HA	2.12	0.48
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.48	0.48
1:C:543:GLN:O	1:C:546:GLU:N	2.46	0.48
1:C:734:GLN:N	1:C:734:GLN:HE21	2.11	0.48
1:E:4:PHE:HD1	1:E:8:GLN:OE1	1.95	0.48
1:E:289:MET:HE2	1:E:289:MET:HA	1.95	0.48
1:E:381:TYR:OH	1:E:481:MET:HG3	2.13	0.48
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.78	0.48
1:C:704:GLN:O	1:C:707:PRO:HD2	2.13	0.48
1:C:828:MET:HE2	2:D:576:ARG:HE	1.78	0.48
1:E:385:MET:HE2	1:E:460:ASP:HA	1.94	0.48
1:A:144:ARG:NH2	1:A:791:GLN:O	2.46	0.48
1:A:568:GLU:HB3	1:A:721:ASP:OD2	2.13	0.48
1:A:619:MET:HE1	1:A:633:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.95	0.48
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.94	0.48
1:E:179:ALA:O	1:E:183:GLU:HB2	2.13	0.48
1:E:341:HIS:O	1:E:342:LEU:C	2.57	0.48
1:E:500:ASP:O	1:E:503:LYS:HB2	2.14	0.48
1:A:10:ARG:NH2	1:A:449:PRO:HD3	2.28	0.48
1:A:388:THR:HG21	1:A:395:TYR:CG	2.48	0.48
1:A:591:GLU:OE2	1:A:685:ARG:NH1	2.46	0.48
1:A:730:LEU:C	1:A:730:LEU:CD2	2.87	0.48
1:C:258:THR:HG22	1:C:260:LYS:N	2.26	0.48
1:E:69:THR:O	1:E:389:SER:N	2.44	0.48
1:E:699:DDE:HAB1	3:E:843:APR:O3A	2.14	0.48
2:F:457:ALA:HB2	2:F:558:TRP:CE3	2.49	0.48
2:F:552:LEU:N	2:F:552:LEU:CD1	2.75	0.48
1:A:106:PRO:CG	1:A:114:GLU:HG3	2.43	0.48
1:A:262:THR:HG22	1:A:267:LYS:O	2.14	0.48
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.62	0.48
1:C:524:GLU:C	1:C:526:GLY:H	2.21	0.48
1:C:706:ILE:HB	2:D:493:ILE:HD12	1.95	0.48
1:C:759:GLN:OE1	1:C:766:PHE:HE2	1.96	0.48
1:E:43:ALA:O	1:E:77:LEU:HA	2.14	0.48
1:E:699:DDE:HAD2	1:E:699:DDE:HAA3	1.77	0.48
2:F:517:THR:C	2:F:519:ALA:H	2.21	0.48
1:A:132:ILE:HD12	1:A:162:ARG:HD3	1.94	0.48
1:A:669:TRP:HZ2	2:B:490:ARG:NH1	2.11	0.48
2:B:446:ALA:O	2:B:447:ALA:C	2.56	0.48
1:C:507:GLY:HA2	1:C:510:ARG:HD2	1.95	0.48
1:E:396:ALA:HB3	1:E:456:LEU:HB2	1.95	0.48
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.44	0.48
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.77	0.48
1:C:106:PRO:CG	1:C:114:GLU:HG3	2.44	0.48
1:C:581:ASN:N	1:C:704:GLN:OE1	2.43	0.48
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.28	0.48
2:D:493:ILE:O	2:D:493:ILE:HG22	2.13	0.48
1:E:749:LYS:HG3	1:E:750:LYS:CD	2.44	0.48
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.95	0.48
1:A:118:ALA:O	1:A:122:THR:HG23	2.13	0.48
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.43	0.48
1:A:380:LEU:C	1:A:380:LEU:HD23	2.39	0.48
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.25	0.48
1:A:669:TRP:HZ2	2:B:490:ARG:HH12	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLN:O	1:C:228:ARG:HG3	2.14	0.48
1:C:637:GLY:HA2	1:C:638:PRO:O	2.13	0.48
1:A:466:THR:CG2	1:A:467:GLY:N	2.76	0.48
1:C:208:THR:HG22	1:C:341:HIS:CG	2.49	0.48
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.29	0.48
2:D:465:ILE:H	2:D:465:ILE:CD1	2.25	0.48
1:E:552:VAL:HG13	1:E:553:PRO:N	2.28	0.48
1:E:699:DDE:HAC1	3:E:843:APR:H5'1	1.96	0.48
1:A:385:MET:HE2	1:A:460:ASP:HA	1.94	0.47
2:B:453:GLY:O	2:B:456:ARG:HD3	2.13	0.47
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.27	0.47
2:D:482:ALA:O	2:D:496:GLY:N	2.47	0.47
1:E:319:LEU:O	1:E:323:VAL:HG23	2.14	0.47
1:E:536:LEU:O	1:E:537:HIS:C	2.56	0.47
2:B:477:LEU:HB2	2:B:551:ARG:HD2	1.96	0.47
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.78	0.47
1:C:504:LEU:C	1:C:506:GLU:N	2.72	0.47
1:C:697:ALA:HA	1:C:700:ARG:CZ	2.44	0.47
1:E:727:PRO:HG2	1:E:774:VAL:HB	1.95	0.47
1:E:749:LYS:O	1:E:750:LYS:HD2	2.14	0.47
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.96	0.47
2:B:502:TYR:HB2	2:B:565:VAL:O	2.14	0.47
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.97	0.47
1:E:167:LEU:HD12	1:E:167:LEU:N	2.29	0.47
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.12	0.47
1:E:490:GLN:HA	1:E:531:ALA:HA	1.97	0.47
1:A:91:GLN:O	1:A:93:THR:HG23	2.15	0.47
2:B:507:SER:C	2:B:509:PRO:HD2	2.39	0.47
1:C:509:LYS:O	1:C:513:LYS:HE3	2.14	0.47
2:D:552:LEU:N	2:D:552:LEU:HD12	2.29	0.47
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.45	0.47
1:E:647:ILE:HB	1:E:687:ASN:ND2	2.30	0.47
1:A:149:GLU:HA	1:A:355:GLN:NE2	2.27	0.47
1:A:823:ARG:NH1	1:A:831:GLU:O	2.46	0.47
1:C:275:MET:HE2	1:C:276:PHE:CZ	2.49	0.47
2:D:447:ALA:O	2:D:448:GLN:C	2.57	0.47
1:E:241:MET:HA	1:E:244:LEU:HD12	1.96	0.47
1:E:545:LEU:O	1:E:550:ALA:HB3	2.15	0.47
1:E:633:ILE:HD13	1:E:645:LEU:HD22	1.96	0.47
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.49	0.47
1:A:806:SER:HB2	1:A:813:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:LEU:O	1:C:442:VAL:HA	2.14	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
2:F:571:ILE:CD1	2:F:587:ILE:HD13	2.44	0.47
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.30	0.47
1:A:401:PHE:CD2	1:A:478:MET:HE1	2.48	0.47
1:A:677:PHE:N	1:A:677:PHE:CD2	2.82	0.47
1:A:750:LYS:O	1:A:751:ARG:HB2	2.15	0.47
1:C:311:GLU:CA	1:C:314:LEU:HD13	2.40	0.47
1:C:454:ILE:HG13	1:C:455:GLY:N	2.27	0.47
1:C:627:VAL:CG2	1:C:631:ARG:NH2	2.77	0.47
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.15	0.47
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.97	0.47
1:E:488:VAL:HG23	1:E:489:VAL:HG23	1.96	0.47
1:A:16:VAL:CG1	1:A:345:PRO:HB2	2.45	0.47
1:C:100:ILE:HD13	1:C:338:ILE:HG21	1.96	0.47
1:C:129:VAL:HG13	1:C:134:GLY:C	2.40	0.47
1:C:504:LEU:O	1:C:506:GLU:N	2.47	0.47
2:D:566:VAL:HG12	2:D:567:ILE:N	2.30	0.47
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.50	0.47
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.49	0.47
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.15	0.47
1:A:488:VAL:HG23	1:A:489:VAL:HG23	1.96	0.47
2:B:523:ALA:O	2:B:524:ALA:C	2.56	0.47
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.50	0.47
1:E:528:HIS:C	1:E:529:ILE:HD13	2.40	0.47
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.95	0.47
1:E:89:ILE:C	1:E:91:GLN:N	2.71	0.47
1:E:500:ASP:CG	1:E:552:VAL:HG21	2.40	0.47
1:A:485:VAL:O	1:A:485:VAL:HG22	2.15	0.46
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.96	0.46
1:C:256:LYS:HA	1:C:256:LYS:CE	2.44	0.46
2:D:530:LEU:HD23	2:D:604:PRO:HD3	1.96	0.46
1:A:26:ALA:O	1:A:32:LYS:HD2	2.16	0.46
2:B:405:GLY:HA2	1:C:627:VAL:CG1	2.44	0.46
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.15	0.46
2:F:505:ARG:C	2:F:507:SER:H	2.23	0.46
1:A:103:ILE:HD13	1:A:121:VAL:HG23	1.97	0.46
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.45	0.46
1:A:511:LEU:HD22	1:A:545:LEU:HD13	1.96	0.46
1:C:385:MET:SD	1:C:396:ALA:HA	2.55	0.46
1:C:494:GLU:OE1	1:C:494:GLU:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:SER:O	1:E:98:PHE:N	2.47	0.46
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.80	0.46
2:F:443:PHE:CE2	2:F:445:GLU:HB2	2.50	0.46
2:F:446:ALA:O	2:F:447:ALA:C	2.59	0.46
1:A:685:ARG:NE	1:A:687:ASN:HD21	2.13	0.46
1:C:2:VAL:CG2	1:C:3:ALA:H	2.21	0.46
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.97	0.46
2:D:551:ARG:NH1	2:D:551:ARG:HG3	2.31	0.46
1:E:71:LYS:O	1:E:386:VAL:HG21	2.15	0.46
1:E:600:ALA:HB1	1:E:606:ILE:HG12	1.97	0.46
1:E:649:GLN:OE1	1:E:687:ASN:HB3	2.16	0.46
1:E:732:GLU:N	1:E:795:GLN:O	2.48	0.46
1:E:749:LYS:C	1:E:750:LYS:HD2	2.41	0.46
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.46	0.46
1:A:824:LYS:HE2	1:A:830:GLU:OE2	2.15	0.46
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.49	0.46
1:E:169:VAL:CG2	1:E:173:ASP:HB2	2.45	0.46
1:E:244:LEU:O	1:E:273:PHE:HB2	2.16	0.46
1:E:410:LYS:HA	1:E:430:ALA:HA	1.97	0.46
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.81	0.46
1:E:804:LEU:N	1:E:804:LEU:HD23	2.30	0.46
1:A:338:ILE:O	1:A:342:LEU:HB2	2.16	0.46
1:A:565:GLU:O	1:A:681:MET:HA	2.16	0.46
2:B:563:ARG:HG3	2:B:563:ARG:NH1	2.31	0.46
1:C:231:LYS:HD3	1:C:232:LYS:H	1.80	0.46
2:D:507:SER:C	2:D:509:PRO:HD2	2.41	0.46
1:E:237:LYS:O	1:E:241:MET:HG2	2.15	0.46
1:E:411:VAL:CG1	1:E:412:ARG:N	2.78	0.46
1:E:461:GLN:NE2	1:E:462:PHE:CE2	2.84	0.46
1:A:345:PRO:O	1:A:349:GLN:HG3	2.15	0.46
1:C:545:LEU:HA	1:C:549:HIS:HB2	1.98	0.46
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.98	0.46
2:D:465:ILE:HD13	2:D:465:ILE:N	2.29	0.46
1:E:111:PHE:O	1:E:112:SER:C	2.57	0.46
1:A:185:VAL:O	1:A:189:VAL:HG23	2.16	0.46
1:A:222:ILE:HD11	1:A:273:PHE:HE1	1.80	0.46
1:A:550:ALA:C	1:A:552:VAL:H	2.24	0.46
1:A:735:CYS:SG	1:A:739:ALA:HB3	2.56	0.46
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.51	0.46
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.97	0.46
1:E:374:PRO:O	1:E:404:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:THR:C	1:E:469:LEU:HD12	2.41	0.46
2:F:520:ALA:HA	2:F:521:PRO:HD2	1.61	0.46
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.96	0.46
1:A:230:ALA:O	1:A:235:VAL:HG22	2.16	0.46
2:B:417:TRP:NE1	2:B:568:PRO:HB2	2.31	0.46
2:B:435:VAL:HG11	2:B:508:LEU:HD11	1.97	0.46
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.16	0.46
2:D:476:ALA:CA	2:D:582:LEU:HD23	2.46	0.46
2:D:538:ARG:HA	2:D:538:ARG:HD2	1.64	0.46
2:D:577:ASN:ND2	2:D:577:ASN:O	2.48	0.46
1:E:129:VAL:HG13	1:E:135:VAL:HA	1.98	0.46
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.78	0.46
1:E:528:HIS:O	1:E:529:ILE:HD13	2.16	0.46
1:E:685:ARG:HE	1:E:687:ASN:ND2	2.11	0.46
1:A:220:PHE:CD1	1:A:220:PHE:C	2.94	0.46
1:A:563:TYR:O	1:A:564:ARG:HD2	2.15	0.46
1:C:16:VAL:C	1:C:18:ASN:N	2.72	0.46
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.98	0.46
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.97	0.46
1:C:742:GLY:O	1:C:745:SER:HB3	2.16	0.46
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.46
1:E:728:VAL:HB	1:E:800:HIS:HD2	1.79	0.46
1:E:771:TYR:CE1	1:E:799:ASP:OD1	2.69	0.46
1:C:626:ASP:O	1:C:627:VAL:C	2.58	0.45
2:D:517:THR:HG21	2:D:548:GLU:N	2.31	0.45
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.31	0.45
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.52	0.45
1:E:202:VAL:HG23	1:E:202:VAL:O	2.16	0.45
1:A:180:ARG:O	1:A:183:GLU:HB3	2.16	0.45
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.51	0.45
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.87	0.45
1:C:406:LYS:HB3	1:C:447:ASP:CB	2.47	0.45
1:C:506:GLU:O	1:C:510:ARG:HG3	2.16	0.45
1:E:129:VAL:HG12	1:E:130:ASP:H	1.81	0.45
1:E:360:PRO:C	1:E:362:ASP:H	2.23	0.45
1:E:654:GLN:O	1:E:655:TYR:HB2	2.16	0.45
2:F:437:VAL:HG11	2:F:511:PHE:CE2	2.51	0.45
1:A:619:MET:HE3	1:A:630:ALA:HB1	1.98	0.45
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.51	0.45
1:C:459:ILE:O	1:C:462:PHE:N	2.48	0.45
1:C:690:ASP:OD1	1:C:691:VAL:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:SER:O	1:E:115:VAL:HB	2.17	0.45
1:E:239:LYS:O	1:E:239:LYS:HG2	2.16	0.45
1:E:619:MET:HE3	1:E:630:ALA:HB1	1.98	0.45
2:F:500:ARG:O	2:F:566:VAL:HG13	2.16	0.45
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.46	0.45
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.97	0.45
1:A:400:VAL:O	1:A:450:ALA:HA	2.16	0.45
1:A:673:GLU:HG2	1:A:678:GLY:O	2.17	0.45
1:A:736:PRO:O	1:A:740:VAL:HG23	2.15	0.45
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.51	0.45
2:B:577:ASN:C	2:B:577:ASN:HD22	2.24	0.45
1:C:108:HIS:HD2	1:C:110:ASP:H	1.63	0.45
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.32	0.45
1:C:404:THR:CG2	1:C:449:PRO:HA	2.25	0.45
1:E:150:ARG:NH1	1:E:355:GLN:HB2	2.31	0.45
1:A:734:GLN:HE21	1:A:734:GLN:CA	2.26	0.45
1:C:111:PHE:HB3	1:C:114:GLU:HG2	1.99	0.45
1:C:335:LEU:O	1:C:339:VAL:HG23	2.16	0.45
2:D:427:ARG:O	2:D:430:GLU:N	2.48	0.45
2:D:577:ASN:C	2:D:577:ASN:HD22	2.25	0.45
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.45
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.81	0.45
1:E:536:LEU:O	1:E:539:GLU:HB3	2.17	0.45
1:A:2:VAL:CG2	1:A:3:ALA:N	2.78	0.45
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.98	0.45
2:D:448:GLN:O	2:D:449:SER:C	2.60	0.45
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.14	0.45
1:E:454:ILE:CG1	1:E:455:GLY:N	2.79	0.45
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.50	0.45
1:A:73:THR:OG1	1:A:386:VAL:HG11	2.17	0.45
1:A:160:VAL:HG23	1:A:212:GLY:O	2.17	0.45
1:C:840:ASP:CG	1:C:842:LEU:HD13	2.41	0.45
1:E:594:ASP:HB2	1:E:597:VAL:HG23	1.99	0.45
1:A:360:PRO:HD2	1:A:363:ASP:HB2	1.99	0.45
2:B:514:THR:OG1	2:B:515:SER:N	2.50	0.45
1:C:183:GLU:O	1:C:187:VAL:HG23	2.17	0.45
1:C:228:ARG:C	1:C:230:ALA:H	2.24	0.45
1:C:249:PHE:CD2	1:C:249:PHE:N	2.85	0.45
1:C:611:ASP:O	1:C:612:PHE:C	2.60	0.45
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.81	0.45
1:E:391:LYS:CG	1:E:392:GLY:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:797:VAL:HG22	1:E:798:PHE:N	2.31	0.45
2:F:450:ILE:O	2:F:454:GLY:HA2	2.16	0.45
1:A:654:GLN:O	1:A:655:TYR:HB2	2.17	0.45
1:C:24:VAL:O	1:C:24:VAL:HG12	2.17	0.45
1:E:132:ILE:HD12	1:E:132:ILE:H	1.81	0.45
1:E:495:VAL:CG1	1:E:554:LEU:HD23	2.46	0.45
2:F:420:GLU:CD	2:F:420:GLU:N	2.75	0.45
1:A:186:ASN:CG	1:A:201:GLN:HG2	2.42	0.45
1:C:22:MET:HA	1:C:122:THR:HB	1.98	0.45
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.32	0.45
1:E:731:VAL:O	1:E:731:VAL:HG13	2.16	0.45
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.56	0.45
1:A:94:ASP:OD1	1:A:94:ASP:C	2.60	0.44
1:A:249:PHE:CD2	1:A:249:PHE:N	2.85	0.44
1:A:594:ASP:O	1:A:595:GLU:C	2.60	0.44
1:C:82:SER:O	1:C:86:VAL:HG23	2.17	0.44
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.47	0.44
1:C:243:ARG:HH12	1:C:257:TRP:CD1	2.35	0.44
1:E:13:MET:SD	1:E:436:LEU:HD21	2.58	0.44
1:A:758:GLU:CG	1:A:767:THR:HG23	2.46	0.44
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.99	0.44
1:C:809:LEU:O	1:C:811:PRO:HD3	2.17	0.44
1:E:68:ILE:HG21	1:E:395:TYR:OH	2.16	0.44
1:E:189:VAL:HG11	1:E:201:GLN:HA	1.99	0.44
1:E:739:ALA:O	1:E:788:THR:HG22	2.17	0.44
1:E:792:ALA:O	1:E:794:PRO:HD3	2.17	0.44
2:F:400:PHE:CD1	2:F:429:LEU:CD2	3.00	0.44
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.99	0.44
2:B:450:ILE:O	2:B:454:GLY:HA2	2.17	0.44
1:C:4:PHE:HD1	1:C:8:GLN:OE1	2.00	0.44
1:C:253:LYS:HG3	1:C:253:LYS:O	2.17	0.44
1:C:792:ALA:O	1:C:794:PRO:HD3	2.17	0.44
2:D:451:VAL:O	2:D:451:VAL:CG1	2.64	0.44
1:E:3:ALA:HA	1:E:46:ILE:O	2.17	0.44
1:E:39:LEU:HD21	1:E:77:LEU:CG	2.47	0.44
1:E:325:ARG:HG2	1:E:325:ARG:HH11	1.81	0.44
1:A:16:VAL:C	1:A:18:ASN:N	2.75	0.44
1:A:228:ARG:C	1:A:230:ALA:N	2.76	0.44
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.98	0.44
1:A:319:LEU:O	1:A:320:LEU:C	2.61	0.44
1:A:429:LYS:HG2	1:A:462:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.81	0.44
1:C:391:LYS:HE3	1:C:393:ARG:HG3	1.99	0.44
1:E:22:MET:HA	1:E:122:THR:HB	1.98	0.44
1:E:466:THR:HG22	1:E:467:GLY:N	2.32	0.44
1:E:533:THR:H	1:E:537:HIS:CD2	2.36	0.44
1:E:606:ILE:HD12	1:E:619:MET:HG2	2.00	0.44
1:E:759:GLN:HG2	1:E:760:ARG:N	2.32	0.44
2:F:507:SER:C	2:F:509:PRO:HD2	2.42	0.44
1:A:112:SER:HB3	1:A:794:PRO:O	2.17	0.44
2:B:507:SER:C	2:B:509:PRO:CD	2.90	0.44
1:C:111:PHE:O	1:C:112:SER:C	2.59	0.44
1:C:254:THR:O	1:C:255:LYS:C	2.61	0.44
1:C:317:LYS:HA	1:C:317:LYS:HD2	1.66	0.44
1:C:836:GLN:HE21	1:C:836:GLN:N	2.03	0.44
1:E:25:ILE:HD12	1:E:142:VAL:HG12	1.99	0.44
1:E:314:LEU:C	1:E:319:LEU:HB2	2.42	0.44
1:E:690:ASP:O	1:E:691:VAL:HG23	2.18	0.44
1:E:711:ARG:O	1:E:712:ALA:C	2.59	0.44
1:A:117:ALA:HA	1:A:481:MET:SD	2.58	0.44
1:A:655:TYR:O	1:A:656:LEU:C	2.61	0.44
1:C:158:ASN:CG	1:C:159:LYS:H	2.26	0.44
1:C:391:LYS:HE3	1:C:393:ARG:CG	2.48	0.44
1:C:760:ARG:O	1:C:761:PRO:C	2.61	0.44
1:E:699:DDE:CAB	3:E:843:APR:H5R1	2.47	0.44
1:E:733:ILE:HD13	1:E:743:ILE:HD12	2.00	0.44
1:A:296:ILE:N	1:A:297:PRO:HD2	2.32	0.44
1:A:580:PRO:HB2	1:A:704:GLN:HE22	1.83	0.44
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.98	0.44
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.53	0.44
1:C:336:GLU:HG2	1:C:340:LEU:HD12	2.00	0.44
1:E:39:LEU:HD21	1:E:77:LEU:HD23	2.00	0.44
1:E:171:LYS:HZ3	1:E:283:ARG:HH21	1.65	0.44
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.48	0.44
1:A:731:VAL:HG23	1:A:731:VAL:O	2.18	0.44
2:B:442:THR:OG1	2:B:443:PHE:N	2.51	0.44
1:C:200:VAL:O	1:C:200:VAL:HG13	2.17	0.44
1:C:222:ILE:HG22	1:C:241:MET:HB2	2.00	0.44
1:E:699:DDE:HAC3	1:E:699:DDE:HAU2	1.82	0.44
2:F:444:LEU:O	2:F:445:GLU:C	2.59	0.44
2:F:471:ILE:HG21	2:F:501:VAL:HG21	2.00	0.44
1:A:143:LEU:O	1:A:144:ARG:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:O	1:A:352:ARG:HB2	2.18	0.44
1:A:494:GLU:HB3	1:A:555:LYS:HB3	2.00	0.44
2:B:484:ASP:OD2	2:B:494:ARG:N	2.51	0.44
1:C:129:VAL:HG12	1:C:130:ASP:N	2.33	0.44
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.53	0.44
1:E:490:GLN:HB3	1:E:531:ALA:CB	2.41	0.44
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.44
2:F:505:ARG:NH1	2:F:505:ARG:CG	2.79	0.44
1:A:45:ILE:HG12	1:A:76:SER:O	2.18	0.43
1:A:86:VAL:HG21	1:A:96:ASN:OD1	2.18	0.43
1:A:324:MET:HE2	1:A:324:MET:HA	2.00	0.43
1:A:705:ILE:O	1:A:706:ILE:C	2.59	0.43
1:E:296:ILE:N	1:E:297:PRO:HD2	2.33	0.43
1:E:311:GLU:HA	1:E:314:LEU:CD1	2.47	0.43
1:E:381:TYR:OH	1:E:481:MET:HE2	2.17	0.43
2:D:490:ARG:O	2:D:492:ARG:N	2.52	0.43
1:E:485:VAL:HG22	1:E:485:VAL:O	2.18	0.43
1:E:648:ASP:OD1	1:E:648:ASP:C	2.61	0.43
2:F:558:TRP:O	2:F:559:PRO:C	2.58	0.43
1:A:262:THR:HA	1:A:267:LYS:O	2.18	0.43
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.47	0.43
1:A:634:TRP:CE3	1:A:660:LYS:HG3	2.53	0.43
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.72	0.43
1:C:408:GLY:O	1:C:409:GLN:C	2.59	0.43
2:D:432:ARG:HA	2:D:432:ARG:NE	2.33	0.43
1:E:46:ILE:HD12	1:E:46:ILE:H	1.81	0.43
1:E:564:ARG:HD3	1:E:801:TRP:CH2	2.53	0.43
1:A:390:ASP:O	1:A:391:LYS:HB3	2.18	0.43
1:A:667:PHE:CZ	1:A:671:THR:HG21	2.53	0.43
1:C:283:ARG:HB3	1:C:299:LEU:HD21	2.00	0.43
2:D:451:VAL:O	2:D:451:VAL:HG12	2.17	0.43
1:E:536:LEU:CD1	1:E:540:ILE:HD11	2.48	0.43
1:E:620:ALA:HA	1:E:625:TRP:O	2.19	0.43
1:A:719:LEU:HD21	1:A:835:TRP:CE2	2.54	0.43
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.53	0.43
1:C:509:LYS:O	1:C:513:LYS:HG3	2.18	0.43
2:F:583:ASP:HA	2:F:584:PRO:HD2	1.89	0.43
2:D:490:ARG:O	2:D:490:ARG:HG3	2.19	0.43
1:E:21:ASN:ND2	1:E:345:PRO:CG	2.82	0.43
1:E:25:ILE:CG1	1:E:125:ALA:HB1	2.48	0.43
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:LYS:O	1:E:616:ALA:HB3	2.18	0.43
1:E:659:ILE:O	1:E:663:VAL:HG23	2.18	0.43
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.00	0.43
2:F:426:HIS:O	2:F:429:LEU:N	2.48	0.43
1:A:378:LEU:HD22	1:A:409:GLN:NE2	2.30	0.43
1:C:221:THR:O	1:C:222:ILE:C	2.61	0.43
1:C:380:LEU:HB3	1:C:469:LEU:HB2	2.01	0.43
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.53	0.43
2:D:488:ASP:OD1	2:D:489:ALA:N	2.51	0.43
1:E:215:LEU:HD23	1:E:216:HIS:CE1	2.53	0.43
1:E:314:LEU:CD1	1:E:322:VAL:HG21	2.48	0.43
1:E:406:LYS:HB3	1:E:447:ASP:HB3	2.00	0.43
1:A:335:LEU:O	1:A:339:VAL:HG23	2.19	0.43
1:A:607:ASN:O	1:A:615:ARG:HD3	2.19	0.43
1:E:303:LEU:O	1:E:304:GLU:CB	2.67	0.43
1:A:29:ASP:O	1:A:159:LYS:NZ	2.36	0.43
1:A:45:ILE:HB	1:A:76:SER:HB2	2.01	0.43
1:A:569:SER:O	1:A:592:PRO:HD3	2.18	0.43
1:A:581:ASN:O	1:A:582:LYS:CB	2.63	0.43
1:C:203:TYR:HB2	1:C:206:ARG:HB2	1.99	0.43
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.18	0.43
1:C:804:LEU:HD23	1:C:804:LEU:N	2.34	0.43
1:E:158:ASN:HA	1:E:212:GLY:O	2.19	0.43
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.53	0.43
1:E:699:DDE:HAB1	3:E:843:APR:H5'2	1.99	0.43
1:E:754:VAL:HA	1:E:770:ALA:HB2	2.01	0.43
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.40	0.43
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.49	0.43
2:B:438:GLY:HA3	2:B:471:ILE:HD12	2.01	0.43
1:C:192:TYR:HA	1:C:763:THR:HG21	2.01	0.43
1:C:581:ASN:HB3	1:C:583:HIS:HB2	2.01	0.43
1:A:108:HIS:CD2	1:A:110:ASP:OD2	2.72	0.42
1:A:406:LYS:O	1:A:409:GLN:HB3	2.19	0.42
1:A:522:MET:HE3	1:A:526:GLY:O	2.19	0.42
1:C:26:ALA:CB	1:C:128:VAL:HB	2.48	0.42
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.85	0.42
2:D:448:GLN:HE21	2:D:448:GLN:HB2	1.68	0.42
1:E:143:LEU:O	1:E:144:ARG:C	2.61	0.42
1:E:145:GLN:O	1:E:146:ALA:C	2.61	0.42
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.54	0.42
1:E:289:MET:HE1	1:E:317:LYS:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:O	1:A:36:THR:C	2.63	0.42
1:A:91:GLN:O	1:A:92:LYS:C	2.62	0.42
1:A:164:LEU:N	1:A:164:LEU:HD23	2.33	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.01	0.42
1:A:411:VAL:CG1	1:A:412:ARG:N	2.81	0.42
1:A:550:ALA:C	1:A:552:VAL:N	2.77	0.42
1:C:217:GLY:HA3	1:C:325:ARG:NH1	2.34	0.42
1:C:497:ASN:ND2	1:C:497:ASN:N	2.66	0.42
1:E:493:VAL:HG22	1:E:556:ILE:HD12	2.00	0.42
1:E:690:ASP:OD1	1:E:691:VAL:N	2.46	0.42
1:E:699:DDE:HAU3	1:E:699:DDE:HAB2	1.71	0.42
2:F:450:ILE:O	2:F:454:GLY:N	2.52	0.42
1:A:321:LYS:HZ2	1:A:325:ARG:HH11	1.68	0.42
1:A:363:ASP:O	1:A:367:ILE:HG13	2.19	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.81	0.42
1:C:237:LYS:O	1:C:241:MET:HG2	2.19	0.42
1:C:308:LYS:HB2	1:C:311:GLU:OE1	2.19	0.42
1:C:411:VAL:CG1	1:C:412:ARG:N	2.82	0.42
1:E:506:GLU:O	1:E:510:ARG:HG2	2.19	0.42
2:F:484:ASP:OD2	2:F:494:ARG:CG	2.66	0.42
1:A:37:ASP:O	1:A:40:VAL:N	2.52	0.42
1:C:253:LYS:HA	1:C:253:LYS:CE	2.28	0.42
1:C:718:LEU:HD12	1:C:718:LEU:HA	1.91	0.42
1:C:810:ASP:CG	1:C:812:THR:HG22	2.43	0.42
1:E:380:LEU:C	1:E:380:LEU:HD23	2.45	0.42
1:E:580:PRO:O	1:E:581:ASN:C	2.61	0.42
1:E:682:ARG:O	1:E:683:SER:HB2	2.20	0.42
1:A:42:ARG:HG2	1:A:331:ALA:HB1	2.01	0.42
1:C:19:VAL:HG12	1:C:20:ARG:N	2.35	0.42
1:C:218:TRP:CA	1:C:330:ALA:HB2	2.50	0.42
1:C:220:PHE:HB3	1:C:328:LEU:HD13	2.01	0.42
1:C:589:LYS:HE3	1:C:689:LEU:HD11	2.01	0.42
1:C:733:ILE:HG21	1:C:743:ILE:HD11	2.00	0.42
1:E:307:LEU:HB2	1:E:312:LYS:HD3	2.00	0.42
2:F:495:ASN:OD1	2:F:495:ASN:N	2.52	0.42
2:F:498:LEU:HD23	2:F:498:LEU:HA	1.72	0.42
1:A:200:VAL:O	1:A:200:VAL:CG1	2.67	0.42
1:A:279:ASP:O	1:A:280:PRO:C	2.60	0.42
1:A:682:ARG:O	1:A:683:SER:HB2	2.18	0.42
1:C:353:ALA:HB3	1:C:370:LYS:HG3	2.02	0.42
1:C:534:GLY:O	1:C:535:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:474:ASP:OD1	2:D:475:PRO:HD2	2.19	0.42
2:D:524:ALA:O	2:D:528:GLU:HG3	2.19	0.42
1:E:12:LEU:HG	1:E:99:LEU:HB2	2.02	0.42
1:A:390:ASP:O	1:A:391:LYS:CB	2.66	0.42
1:A:542:LEU:HD13	1:A:556:ILE:HG21	2.01	0.42
1:A:620:ALA:HA	1:A:625:TRP:O	2.19	0.42
1:A:810:ASP:O	1:A:816:GLY:HA3	2.20	0.42
1:C:260:LYS:C	1:C:262:THR:H	2.26	0.42
2:D:530:LEU:HA	2:D:604:PRO:HG3	2.01	0.42
2:D:563:ARG:HA	2:D:563:ARG:HD2	1.86	0.42
1:E:89:ILE:HG23	1:E:340:LEU:O	2.19	0.42
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.49	0.42
1:E:493:VAL:HG12	1:E:494:GLU:N	2.34	0.42
2:F:426:HIS:CE1	2:F:594:ILE:HB	2.55	0.42
1:A:145:GLN:OE1	1:A:734:GLN:HG2	2.20	0.42
1:A:503:LYS:HB2	1:A:552:VAL:HG21	2.02	0.42
2:B:460:GLN:CB	2:B:467:ARG:HD3	2.49	0.42
1:C:727:PRO:HG2	1:C:774:VAL:HB	2.01	0.42
1:E:10:ARG:HD2	1:E:10:ARG:O	2.20	0.42
1:E:459:ILE:HD12	1:E:459:ILE:N	2.35	0.42
1:E:486:SER:HA	1:E:487:PRO:HD3	1.80	0.42
1:E:578:LYS:HA	1:E:584:ASN:O	2.20	0.42
1:A:380:LEU:HD23	1:A:381:TYR:N	2.35	0.42
1:A:381:TYR:OH	1:A:481:MET:HE2	2.20	0.42
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.02	0.42
2:B:511:PHE:CE1	2:B:560:LEU:HD11	2.55	0.42
1:C:13:MET:HB3	1:C:452:ASN:ND2	2.35	0.42
1:C:146:ALA:O	1:C:151:ILE:HG12	2.19	0.42
2:D:471:ILE:HG13	2:D:554:THR:HB	2.01	0.42
2:F:531:ILE:HG22	2:F:533:HIS:N	2.34	0.42
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.84	0.42
1:A:149:GLU:O	1:A:150:ARG:HB2	2.20	0.42
1:A:192:TYR:HA	1:A:763:THR:CG2	2.50	0.42
1:A:644:ASN:HD22	1:A:684:VAL:N	2.14	0.42
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.50	0.42
1:C:706:ILE:HB	1:C:707:PRO:HD3	2.01	0.42
1:C:799:ASP:OD1	1:C:800:HIS:CD2	2.70	0.42
1:E:39:LEU:CD2	1:E:77:LEU:CD2	2.97	0.42
1:E:606:ILE:HD12	1:E:619:MET:CG	2.50	0.42
1:E:677:PHE:CD2	1:E:677:PHE:N	2.88	0.42
2:F:456:ARG:HH21	2:F:458:ARG:NH2	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:PHE:CD2	1:C:717:PHE:C	2.98	0.41
1:E:156:VAL:CG2	1:E:337:MET:HE1	2.49	0.41
1:E:306:VAL:O	1:E:306:VAL:HG23	2.20	0.41
1:E:406:LYS:O	1:E:409:GLN:HB3	2.18	0.41
2:F:540:ASP:OD2	2:F:540:ASP:N	2.51	0.41
1:A:89:ILE:CG2	1:A:91:GLN:HG2	2.50	0.41
1:A:387:PRO:HG3	1:A:394:PHE:CE1	2.55	0.41
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.03	0.41
1:C:131:THR:HG21	1:C:163:ALA:HB2	2.00	0.41
1:C:391:LYS:C	1:C:393:ARG:H	2.28	0.41
1:C:646:VAL:HG13	1:C:688:ILE:HD13	2.02	0.41
1:C:709:MET:HE3	1:C:713:THR:OG1	2.20	0.41
1:C:712:ALA:O	1:C:715:ALA:HB3	2.20	0.41
1:C:729:PHE:O	1:C:771:TYR:HA	2.20	0.41
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.40	0.41
2:D:484:ASP:OD2	2:D:494:ARG:CG	2.69	0.41
2:D:576:ARG:HG3	2:D:576:ARG:HH11	1.85	0.41
1:E:143:LEU:O	1:E:147:LEU:HG	2.20	0.41
1:E:274:ASN:O	1:E:279:ASP:HB2	2.19	0.41
1:E:558:PRO:CB	1:E:559:PRO:HD2	2.49	0.41
1:E:677:PHE:HB3	1:E:819:VAL:HG13	2.01	0.41
2:F:424:GLN:O	2:F:425:ALA:C	2.64	0.41
1:A:150:ARG:HG3	1:A:355:GLN:OE1	2.20	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.88	0.41
1:A:524:GLU:C	1:A:526:GLY:N	2.77	0.41
1:C:291:PHE:CE1	1:C:316:GLY:N	2.89	0.41
1:E:21:ASN:HD22	1:E:345:PRO:HG3	1.85	0.41
1:E:132:ILE:N	1:E:132:ILE:CD1	2.83	0.41
1:E:338:ILE:HA	1:E:342:LEU:HG	2.02	0.41
1:A:125:ALA:HB2	1:A:151:ILE:HG21	2.02	0.41
1:A:211:PHE:O	1:A:219:ALA:HA	2.19	0.41
1:A:380:LEU:HD13	1:A:456:LEU:HD11	2.01	0.41
1:A:626:ASP:C	1:A:628:THR:N	2.75	0.41
1:C:619:MET:HA	1:C:623:TYR:HD2	1.84	0.41
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.41	0.41
1:E:164:LEU:HD12	1:E:285:PHE:CE1	2.56	0.41
1:E:202:VAL:HB	1:E:209:VAL:CG2	2.50	0.41
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.35	0.41
1:E:823:ARG:HH12	1:E:828:MET:CB	2.33	0.41
2:F:474:ASP:O	2:F:475:PRO:C	2.62	0.41
1:A:27:HIS:HD2	1:A:29:ASP:N	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:PHE:N	1:A:677:PHE:HD2	2.18	0.41
1:A:739:ALA:C	1:A:741:GLY:N	2.74	0.41
2:B:522:GLU:H	2:B:522:GLU:CD	2.26	0.41
1:C:296:ILE:N	1:C:297:PRO:HD2	2.36	0.41
1:C:319:LEU:O	1:C:323:VAL:HG23	2.21	0.41
1:C:539:GLU:O	1:C:542:LEU:HB2	2.21	0.41
1:C:823:ARG:NH1	1:C:823:ARG:HG2	2.34	0.41
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.35	0.41
1:E:411:VAL:HG13	1:E:470:THR:O	2.20	0.41
1:E:663:VAL:HG13	1:E:709:MET:SD	2.61	0.41
1:E:807:ASP:OD2	1:E:807:ASP:C	2.62	0.41
2:F:487:PRO:N	2:F:493:ILE:HD11	2.36	0.41
1:A:109:VAL:HG22	1:A:138:GLN:HG3	2.03	0.41
1:C:81:MET:O	1:C:96:ASN:HB3	2.21	0.41
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.97	0.41
1:C:530:VAL:O	1:C:538:LEU:HD11	2.20	0.41
1:E:730:LEU:C	1:E:730:LEU:CD2	2.93	0.41
2:F:476:ALA:N	2:F:582:LEU:HD23	2.35	0.41
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.50	0.41
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.88	0.41
1:E:336:GLU:HG2	1:E:340:LEU:HD12	2.01	0.41
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.51	0.41
1:A:270:GLU:OE1	1:A:275:MET:HG3	2.21	0.41
2:B:503:VAL:HG12	2:B:564:THR:HG22	2.02	0.41
1:C:3:ALA:HA	1:C:46:ILE:HG22	2.02	0.41
1:C:166:GLU:HB3	1:C:167:LEU:H	1.63	0.41
1:C:406:LYS:O	1:C:409:GLN:HB3	2.21	0.41
1:C:600:ALA:HB1	1:C:606:ILE:HG12	2.02	0.41
1:C:682:ARG:O	1:C:683:SER:HB2	2.20	0.41
1:E:307:LEU:HB2	1:E:312:LYS:CD	2.51	0.41
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.51	0.41
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.96	0.41
2:F:435:VAL:HG21	2:F:598:PRO:HG3	2.03	0.41
2:F:443:PHE:O	2:F:444:LEU:C	2.64	0.41
1:A:111:PHE:O	1:A:112:SER:C	2.64	0.41
1:A:153:PRO:HD2	1:A:200:VAL:CG1	2.51	0.41
1:A:192:TYR:HA	1:A:763:THR:HG21	2.03	0.41
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.85	0.41
1:A:522:MET:CE	1:A:526:GLY:O	2.68	0.41
1:C:18:ASN:ND2	1:C:98:PHE:CE1	2.89	0.41
1:C:124:GLY:HA3	1:C:342:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:PRO:HD2	1:C:200:VAL:HG13	2.03	0.41
1:C:627:VAL:HG22	1:C:631:ARG:CZ	2.50	0.41
1:E:195:GLU:H	1:E:195:GLU:HG3	1.66	0.41
1:E:218:TRP:HA	1:E:328:LEU:O	2.21	0.41
1:E:357:TYR:CE2	1:E:359:GLY:HA3	2.56	0.41
1:E:406:LYS:O	1:E:407:SER:C	2.64	0.41
1:E:515:ASP:HA	1:E:516:PRO:HD3	1.80	0.41
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.55	0.41
1:E:731:VAL:CG2	1:E:796:MET:HB3	2.51	0.41
2:F:523:ALA:O	2:F:524:ALA:C	2.62	0.41
2:F:558:TRP:HA	2:F:561:ALA:HB3	2.02	0.41
1:A:4:PHE:CE2	1:A:45:ILE:HD12	2.55	0.41
1:A:167:LEU:HD12	1:A:167:LEU:N	2.36	0.41
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.56	0.41
1:A:600:ALA:HB1	1:A:606:ILE:HG13	2.03	0.41
2:B:484:ASP:CG	2:B:494:ARG:HE	2.29	0.41
2:B:535:LEU:HB3	2:B:536:PRO:HA	2.03	0.41
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.51	0.41
1:C:490:GLN:C	1:C:491:VAL:HG13	2.46	0.41
1:C:612:PHE:HA	1:C:615:ARG:NH2	2.36	0.41
2:D:498:LEU:HD23	2:D:498:LEU:HA	1.72	0.41
1:E:77:LEU:HD22	1:E:100:ILE:HG22	2.03	0.41
1:E:524:GLU:C	1:E:526:GLY:H	2.29	0.41
2:F:410:SER:OG	2:F:412:ARG:HB2	2.21	0.41
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.56	0.41
1:A:344:SER:C	1:A:346:VAL:H	2.29	0.40
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.86	0.40
1:C:413:ILE:HD13	1:C:459:ILE:HG23	2.03	0.40
1:C:548:ASP:O	1:C:549:HIS:C	2.64	0.40
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.86	0.40
1:A:524:GLU:C	1:A:526:GLY:H	2.28	0.40
1:A:549:HIS:CD2	1:A:549:HIS:H	2.38	0.40
1:A:824:LYS:O	1:A:825:ARG:C	2.64	0.40
2:B:448:GLN:HE21	2:B:448:GLN:HB2	1.63	0.40
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.52	0.40
1:C:16:VAL:C	1:C:18:ASN:H	2.29	0.40
1:C:400:VAL:O	1:C:451:GLY:N	2.39	0.40
1:C:490:GLN:O	1:C:491:VAL:CG1	2.68	0.40
1:C:536:LEU:O	1:C:537:HIS:C	2.64	0.40
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.56	0.40
1:E:155:VAL:HB	1:E:209:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:505:ARG:O	2:F:507:SER:N	2.54	0.40
1:A:13:MET:HB3	1:A:452:ASN:ND2	2.37	0.40
1:A:129:VAL:HG13	1:A:134:GLY:C	2.46	0.40
1:A:231:LYS:O	1:A:233:PHE:N	2.55	0.40
1:A:254:THR:O	1:A:255:LYS:HB2	2.21	0.40
1:A:504:LEU:HD13	1:A:554:LEU:HD21	2.02	0.40
2:B:420:GLU:H	2:B:420:GLU:CD	2.28	0.40
2:B:531:ILE:HD12	2:B:533:HIS:CE1	2.56	0.40
1:E:68:ILE:HD12	1:E:390:ASP:CB	2.27	0.40
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.85	0.40
1:E:414:GLN:HB3	1:E:418:TYR:CD2	2.56	0.40
1:E:498:ALA:O	1:E:499:ASN:C	2.65	0.40
1:E:601:ILE:HG12	1:E:606:ILE:HB	2.04	0.40
2:B:492:ARG:O	2:B:492:ARG:HG2	2.21	0.40
1:C:536:LEU:O	1:C:540:ILE:HG12	2.22	0.40
2:D:583:ASP:O	2:D:584:PRO:C	2.62	0.40
1:E:27:HIS:CD2	1:E:28:VAL:N	2.89	0.40
1:E:158:ASN:O	1:E:159:LYS:HB2	2.21	0.40
1:E:188:ILE:HG23	1:E:192:TYR:CE2	2.57	0.40
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.03	0.40
1:E:617:ARG:HA	1:E:617:ARG:NE	2.37	0.40
2:F:528:GLU:OE2	2:F:535:LEU:N	2.42	0.40
2:F:566:VAL:HG12	2:F:567:ILE:N	2.37	0.40
1:A:212:GLY:HA2	1:A:218:TRP:CZ3	2.57	0.40
1:A:581:ASN:ND2	1:A:699:DDE:O	2.55	0.40
1:C:73:THR:O	1:C:73:THR:HG22	2.21	0.40
1:C:156:VAL:CG2	1:C:337:MET:HE1	2.51	0.40
1:C:284:LEU:HD23	1:C:299:LEU:HG	2.03	0.40
1:C:636:PHE:CE1	1:C:645:LEU:HD21	2.56	0.40
1:C:638:PRO:HG3	1:C:671:THR:C	2.47	0.40
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.86	0.40
1:E:149:GLU:O	1:E:150:ARG:HB2	2.21	0.40
1:E:581:ASN:ND2	1:E:699:DDE:O	2.53	0.40
1:E:595:GLU:OE2	1:E:682:ARG:NH1	2.49	0.40
2:F:429:LEU:HD13	2:F:502:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	818/842 (97%)	732 (90%)	74 (9%)	12 (2%)	8	30
1	C	818/842 (97%)	711 (87%)	87 (11%)	20 (2%)	4	20
1	E	818/842 (97%)	707 (86%)	97 (12%)	14 (2%)	7	27
2	B	205/207 (99%)	179 (87%)	24 (12%)	2 (1%)	12	39
2	D	205/207 (99%)	176 (86%)	24 (12%)	5 (2%)	4	20
2	F	205/207 (99%)	175 (85%)	27 (13%)	3 (2%)	8	30
All	All	3069/3147 (98%)	2680 (87%)	333 (11%)	56 (2%)	6	26

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	C	235	VAL
1	C	460	ASP
1	C	639	ASP
1	C	761	PRO
1	E	112	SER
1	E	761	PRO
1	A	309	GLY
1	A	460	ASP
1	A	498	ALA
1	A	761	PRO
2	B	518	LEU
1	C	309	GLY
2	D	491	GLY
1	E	304	GLU
1	E	390	ASP
1	E	428	ILE
1	E	479	LYS
1	E	621	ASP
2	F	506	SER

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Mol	Chain	Res	Type
1	A	479	LYS
2	B	506	SER
1	C	112	SER
1	C	314	LEU
1	C	479	LYS
1	C	582	LYS
2	D	405	GLY
1	E	233	PHE
2	F	577	ASN
1	A	111	PHE
1	A	215	LEU
1	A	390	ASP
1	A	610	ASP
1	C	329	PRO
1	C	390	ASP
1	C	446	ASP
2	D	447	ALA
1	E	302	LYS
1	E	582	LYS
1	E	743	ILE
1	A	287	ALA
1	A	391	LYS
1	C	166	GLU
1	C	266	GLY
1	C	505	VAL
1	E	446	ASP
1	E	460	ASP
1	C	292	LYS
1	C	558	PRO
1	C	677	PHE
1	E	90	LYS
1	C	491	VAL
1	C	743	ILE
2	D	454	GLY
2	D	604	PRO
2	F	493	ILE

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	699/714 (98%)	663 (95%)	36 (5%)	21	49
1	C	699/714 (98%)	640 (92%)	59 (8%)	10	33
1	E	699/714 (98%)	666 (95%)	33 (5%)	23	52
2	B	161/162 (99%)	145 (90%)	16 (10%)	7	27
2	D	161/162 (99%)	143 (89%)	18 (11%)	6	22
2	F	161/162 (99%)	144 (89%)	17 (11%)	6	24
All	All	2580/2628 (98%)	2401 (93%)	179 (7%)	14	40

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	28	VAL
1	A	46	ILE
1	A	81	MET
1	A	83	ASP
1	A	94	ASP
1	A	112	SER
1	A	138	GLN
1	A	152	LYS
1	A	154	VAL
1	A	195	GLU
1	A	200	VAL
1	A	236	ASP
1	A	262	THR
1	A	275	MET
1	A	308	LYS
1	A	347	THR
1	A	352	ARG
1	A	460	ASP
1	A	489	VAL
1	A	597	VAL
1	A	599	LEU
1	A	625	TRP
1	A	677	PHE
1	A	698	ILE
1	A	710	ARG
1	A	718	LEU

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Mol	Chain	Res	Type
1	A	724	ILE
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	761	PRO
1	A	767	THR
1	A	775	ASN
1	A	836	GLN
1	A	842	LEU
2	B	412	ARG
2	B	422	LEU
2	B	467	ARG
2	B	471	ILE
2	B	488	ASP
2	B	492	ARG
2	B	494	ARG
2	B	495	ASN
2	B	499	LEU
2	B	518	LEU
2	B	540	ASP
2	B	547	GLU
2	B	551	ARG
2	B	559	PRO
2	B	560	LEU
2	B	602	SER
1	C	14	ASP
1	C	23	SER
1	C	28	VAL
1	C	36	THR
1	C	46	ILE
1	C	81	MET
1	C	83	ASP
1	C	94	ASP
1	C	105	SER
1	C	154	VAL
1	C	159	LYS
1	C	164	LEU
1	C	172	GLU
1	C	183	GLU
1	C	195	GLU
1	C	200	VAL
1	C	231	LYS

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Mol	Chain	Res	Type
1	C	235	VAL
1	C	242	ASP
1	C	253	LYS
1	C	300	LEU
1	C	320	LEU
1	C	324	MET
1	C	347	THR
1	C	352	ARG
1	C	432	GLN
1	C	460	ASP
1	C	461	GLN
1	C	480	VAL
1	C	489	VAL
1	C	494	GLU
1	C	495	VAL
1	C	497	ASN
1	C	500	ASP
1	C	524	GLU
1	C	528	HIS
1	C	543	GLN
1	C	544	ASP
1	C	552	VAL
1	C	556	ILE
1	C	597	VAL
1	C	599	LEU
1	C	609	ARG
1	C	625	TRP
1	C	677	PHE
1	C	718	LEU
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	757	GLU
1	C	761	PRO
1	C	767	THR
1	C	775	ASN
1	C	796	MET
1	C	804	LEU
1	C	813	SER
1	C	820	LEU
1	C	836	GLN
1	C	837	GLU

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Mol	Chain	Res	Type
2	D	403	ASP
2	D	411	THR
2	D	422	LEU
2	D	427	ARG
2	D	465	ILE
2	D	467	ARG
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	509	PRO
2	D	538	ARG
2	D	540	ASP
2	D	547	GLU
2	D	551	ARG
2	D	560	LEU
2	D	568	PRO
2	D	602	SER
2	D	604	PRO
1	E	36	THR
1	E	46	ILE
1	E	77	LEU
1	E	94	ASP
1	E	161	ASP
1	E	186	ASN
1	E	211	PHE
1	E	216	HIS
1	E	262	THR
1	E	263	ASP
1	E	275	MET
1	E	300	LEU
1	E	313	ASP
1	E	347	THR
1	E	460	ASP
1	E	473	GLU
1	E	489	VAL
1	E	552	VAL
1	E	599	LEU
1	E	625	TRP
1	E	627	VAL
1	E	677	PHE
1	E	698	ILE
1	E	710	ARG

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Mol	Chain	Res	Type
1	E	718	LEU
1	E	730	LEU
1	E	734	GLN
1	E	761	PRO
1	E	767	THR
1	E	786	GLN
1	E	823	ARG
1	E	836	GLN
1	E	837	GLU
2	F	411	THR
2	F	422	LEU
2	F	427	ARG
2	F	437	VAL
2	F	467	ARG
2	F	498	LEU
2	F	499	LEU
2	F	505	ARG
2	F	513	ARG
2	F	514	THR
2	F	531	ILE
2	F	538	ARG
2	F	540	ASP
2	F	548	GLU
2	F	552	LEU
2	F	560	LEU
2	F	604	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	91	GLN
1	A	108	HIS
1	A	138	GLN
1	A	201	GLN
1	A	355	GLN
1	A	409	GLN
1	A	414	GLN
1	A	452	ASN
1	A	537	HIS
1	A	549	HIS
1	A	581	ASN

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Mol	Chain	Res	Type
1	A	583	HIS
1	A	584	ASN
1	A	644	ASN
1	A	654	GLN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	748	ASN
1	A	753	GLN
1	A	795	GLN
1	A	800	HIS
1	A	836	GLN
2	B	424	GLN
2	B	428	GLN
2	B	448	GLN
2	B	495	ASN
2	B	577	ASN
1	C	21	ASN
1	C	27	HIS
1	C	91	GLN
1	C	101	ASN
1	C	138	GLN
1	C	201	GLN
1	C	251	ASN
1	C	259	ASN
1	C	274	ASN
1	C	414	GLN
1	C	452	ASN
1	C	497	ASN
1	C	499	ASN
1	C	528	HIS
1	C	537	HIS
1	C	547	HIS
1	C	549	HIS
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	753	GLN

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Mol	Chain	Res	Type
1	C	759	GLN
1	C	800	HIS
1	C	836	GLN
2	D	448	GLN
2	D	460	GLN
2	D	577	ASN
2	D	592	GLN
1	E	21	ASN
1	E	27	HIS
1	E	91	GLN
1	E	138	GLN
1	E	201	GLN
1	E	259	ASN
1	E	371	ASN
1	E	414	GLN
1	E	528	HIS
1	E	537	HIS
1	E	549	HIS
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	748	ASN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN
2	F	448	GLN
2	F	460	GLN
2	F	577	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	DDE	E	699	1,3	18,20,21	1.96	5 (27%)	17,28,30	3.04	6 (35%)
1	DDE	A	699	1	9,10,21	0.61	0	8,12,30	1.05	0
1	DDE	C	699	1	9,10,21	0.98	1 (11%)	8,12,30	1.07	0

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
1	DDE	E	699	1,3	-	2/20/21/23	0/1/1/1
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1
1	DDE	C	699	1	-	1/5/6/23	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	OAG-CBI	5.22	1.33	1.23
1	E	699	DDE	CAT-CE1	3.32	1.55	1.49
1	E	699	DDE	CG-ND1	-2.81	1.33	1.38
1	E	699	DDE	CAC-NCB	2.49	1.59	1.50
1	C	699	DDE	CB-CA	2.24	1.58	1.53
1	E	699	DDE	CD2-CG	-2.18	1.31	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	699	DDE	CAU-CAT-CE1	9.74	150.71	114.38
1	E	699	DDE	OAG-CBI-NAD	4.64	131.24	123.04
1	E	699	DDE	CD2-NE2-CE1	-3.27	104.81	107.55
1	E	699	DDE	CB-CG-CD2	2.50	134.44	129.33
1	E	699	DDE	CA-CB-CG	-2.44	107.75	113.77
1	E	699	DDE	CG-CD2-NE2	2.06	109.68	106.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	699	DDE	O-C-CA-CB
1	C	699	DDE	O-C-CA-CB
1	E	699	DDE	OAG-CBI-CBW-NCB
1	E	699	DDE	CE1-CAT-CAU-CBW

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	699	DDE	11	0
1	A	699	DDE	1	0
1	C	699	DDE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
3	APR	E	843	1	38,38,39	2.60	12 (31%)	53,58,60	1.48	7 (13%)

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
3	APR	E	843	1	1/1/9/10	4/22/51/54	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	843	APR	PB-O3A	11.97	1.72	1.59
3	E	843	APR	C2-N1	4.35	1.41	1.33
3	E	843	APR	PA-O3A	3.44	1.63	1.59
3	E	843	APR	C3'-C4'	2.94	1.60	1.53
3	E	843	APR	C5-C4	2.85	1.44	1.39
3	E	843	APR	O2'-C2'	2.61	1.49	1.43
3	E	843	APR	C1'-N9	2.40	1.53	1.46
3	E	843	APR	C8-N7	2.39	1.36	1.31
3	E	843	APR	C4-N3	2.34	1.38	1.34
3	E	843	APR	C4-N9	2.33	1.42	1.37
3	E	843	APR	O4D-C4D	2.28	1.48	1.44
3	E	843	APR	O4D-C1D	2.14	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	843	APR	O2D-C2D-C3D	-4.84	101.89	111.43
3	E	843	APR	C1D-C2D-C3D	3.59	107.37	101.63
3	E	843	APR	C1D-O4D-C4D	3.46	115.71	108.06
3	E	843	APR	O4D-C1D-C2D	-2.95	100.68	105.76
3	E	843	APR	O2A-PA-O3A	2.74	114.67	107.27
3	E	843	APR	O4'-C1'-N9	2.72	113.31	108.09
3	E	843	APR	O3A-PB-O1B	2.54	118.35	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	843	APR	C1D

All (4) torsion outliers are listed below:

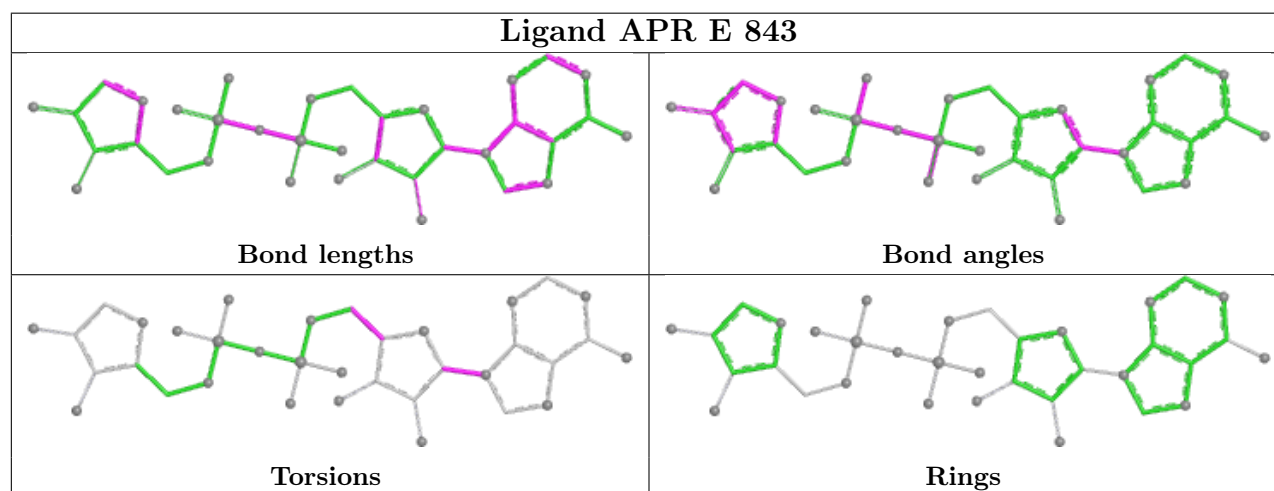
Mol	Chain	Res	Type	Atoms
3	E	843	APR	O4'-C1'-N9-C4
3	E	843	APR	O4'-C1'-N9-C8
3	E	843	APR	O4'-C4'-C5'-O5'
3	E	843	APR	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	843	APR	6	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	822/842 (97%)	-0.10	1 (0%) 92 86	5, 48, 81, 101	0
1	C	822/842 (97%)	0.29	21 (2%) 57 34	11, 64, 123, 135	0
1	E	822/842 (97%)	1.00	132 (16%) 4 2	7, 106, 129, 147	0
2	B	207/207 (100%)	-0.57	1 (0%) 87 72	5, 22, 55, 71	0
2	D	207/207 (100%)	-0.44	2 (0%) 79 59	5, 25, 64, 78	0
2	F	207/207 (100%)	-0.42	1 (0%) 87 72	7, 27, 64, 79	0
All	All	3087/3147 (98%)	0.22	158 (5%) 33 17	5, 54, 123, 147	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	126	LEU	6.4
1	E	338	ILE	5.4
1	E	146	ALA	5.3
1	E	154	VAL	5.3
1	E	273	PHE	5.1
1	E	339	VAL	5.1
1	E	200	VAL	5.1
1	E	175	TYR	4.8
1	E	343	PRO	4.8
1	E	335	LEU	4.7
1	E	189	VAL	4.7
1	E	197	LEU	4.5
1	E	780	PHE	4.5
1	E	196	VAL	4.4
1	E	277	ILE	4.3
1	E	334	LEU	4.1
1	E	127	VAL	4.1
1	E	342	LEU	3.9
1	C	281	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	155	VAL	3.9
1	E	99	LEU	3.8
1	E	245	TRP	3.8
1	E	143	LEU	3.7
1	E	348	ALA	3.7
1	C	507	GLY	3.5
1	E	207	GLY	3.5
1	E	746	VAL	3.5
1	E	781	THR	3.5
1	E	110	ASP	3.5
1	E	364	ALA	3.5
1	C	504	LEU	3.5
1	E	205	ALA	3.5
1	E	747	LEU	3.4
1	E	210	ALA	3.3
1	E	151	ILE	3.3
1	C	505	VAL	3.3
1	E	92	LYS	3.3
1	E	789	GLY	3.2
1	E	784	LEU	3.2
1	C	552	VAL	3.2
1	E	770	ALA	3.1
1	E	501	LEU	3.1
1	C	270	GLU	3.1
1	C	251	ASN	3.1
1	C	216	HIS	3.1
1	E	765	LEU	3.1
1	E	269	LEU	3.0
1	E	349	GLN	3.0
1	E	777	SER	3.0
1	E	163	ALA	3.0
1	E	194	ASP	3.0
1	E	36	THR	3.0
1	E	222	ILE	3.0
1	E	104	ASP	2.9
1	E	498	ALA	2.9
1	E	790	GLY	2.9
1	E	21	ASN	2.9
1	E	193	ALA	2.9
1	E	368	ALA	2.9
1	E	167	LEU	2.9
2	D	485	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	179	ALA	2.9
1	E	23	SER	2.8
1	E	174	LEU	2.8
1	E	201	GLN	2.8
1	E	347	THR	2.8
1	E	24	VAL	2.7
1	E	17	THR	2.7
1	E	346	VAL	2.7
1	C	553	PRO	2.7
1	E	541	CYS	2.7
1	E	796	MET	2.7
1	E	356	LEU	2.7
1	E	743	ILE	2.7
1	E	188	ILE	2.6
2	F	485	GLN	2.6
1	E	209	VAL	2.6
1	E	86	VAL	2.6
1	E	109	VAL	2.6
1	E	268	PRO	2.6
1	E	542	LEU	2.6
1	E	476	HIS	2.6
1	E	535	GLU	2.6
1	E	87	LYS	2.6
1	E	259	ASN	2.5
1	E	731	VAL	2.5
1	E	276	PHE	2.5
1	E	35	LEU	2.5
1	E	202	VAL	2.5
1	E	241	MET	2.5
1	E	73	THR	2.5
1	E	139	THR	2.5
1	E	89	ILE	2.5
1	C	493	VAL	2.5
1	C	233	PHE	2.4
1	E	123	ASP	2.4
1	A	309	GLY	2.4
1	E	787	ALA	2.4
1	C	255	LYS	2.4
1	E	190	SER	2.4
1	E	128	VAL	2.4
1	E	204	PRO	2.4
1	E	526	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	475	ALA	2.3
1	E	536	LEU	2.3
1	E	153	PRO	2.3
1	C	235	VAL	2.3
1	E	185	VAL	2.3
1	E	33	SER	2.3
1	E	131	THR	2.3
1	E	81	MET	2.3
1	C	320	LEU	2.3
1	E	340	LEU	2.3
1	E	184	SER	2.3
1	E	39	LEU	2.3
1	E	98	PHE	2.3
1	E	199	ASP	2.3
1	E	164	LEU	2.3
1	E	113	SER	2.3
1	E	187	VAL	2.2
1	E	754	VAL	2.2
1	E	280	PRO	2.2
2	D	548	GLU	2.2
1	C	234	GLY	2.2
1	E	147	LEU	2.2
1	E	337	MET	2.2
1	E	235	VAL	2.2
1	E	281	ILE	2.2
1	C	500	ASP	2.2
1	E	523	SER	2.2
1	E	525	SER	2.2
1	E	278	LEU	2.2
1	C	551	GLY	2.2
1	E	160	VAL	2.1
1	C	501	LEU	2.1
1	E	737	GLU	2.1
1	E	67	GLY	2.1
1	E	134	GLY	2.1
1	E	366	CYS	2.1
1	E	484	SER	2.1
1	E	182	VAL	2.1
1	C	300	LEU	2.1
1	E	351	TYR	2.1
1	E	519	LEU	2.1
1	E	752	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	783	GLU	2.1
1	E	25	ILE	2.1
1	E	216	HIS	2.1
1	E	240	MET	2.1
1	E	517	CYS	2.1
1	E	763	THR	2.1
1	E	553	PRO	2.1
1	E	740	VAL	2.0
1	E	208	THR	2.0
1	C	267	LYS	2.0
1	E	20	ARG	2.0
1	C	165	LEU	2.0
2	B	518	LEU	2.0

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

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
1	DDE	C	699	10/21	0.69	0.15	44,52,55,56	0
1	DDE	A	699	10/21	0.81	0.12	37,41,46,47	0
1	DDE	E	699	20/21	0.84	0.17	48,68,80,81	0

6.3 Carbohydrates ⓘ

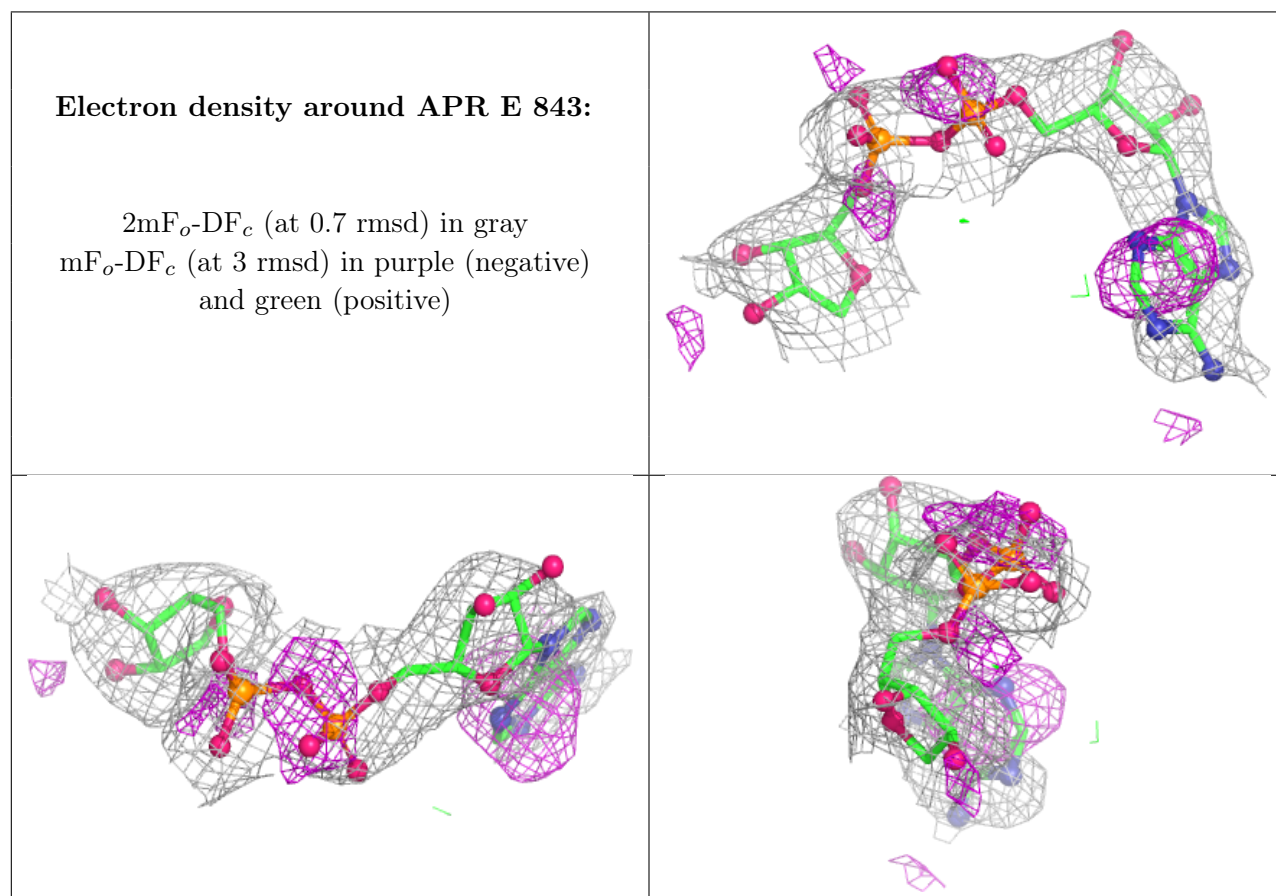
There are no oligosaccharides in this entry.

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
3	APR	E	843	35/36	0.76	0.15	64,71,85,86	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.