



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:36 AM UTC

PDB ID : 1ZM9 / pdb_00001zm9
Title : Structure of eEF2-ETA in complex with PJ34
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 : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

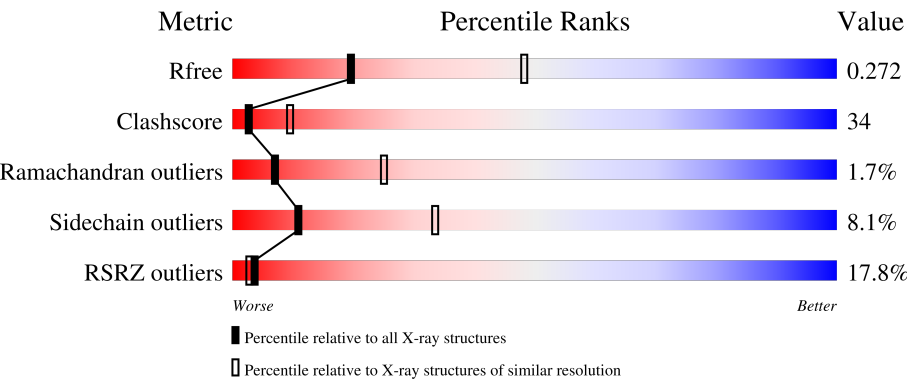
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	6% 51% 41% 5% .
1	C	842	16% 40% 49% 8% ..
1	E	842	41% 46% 47% 5% .
2	B	207	3% 52% 41% 6%
2	D	207	3% 55% 37% 7%

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Mol	Chain	Length	Quality of chain
2	F	207	3% 56% 36% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24042 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
			6405	4075	1093	1207	30			

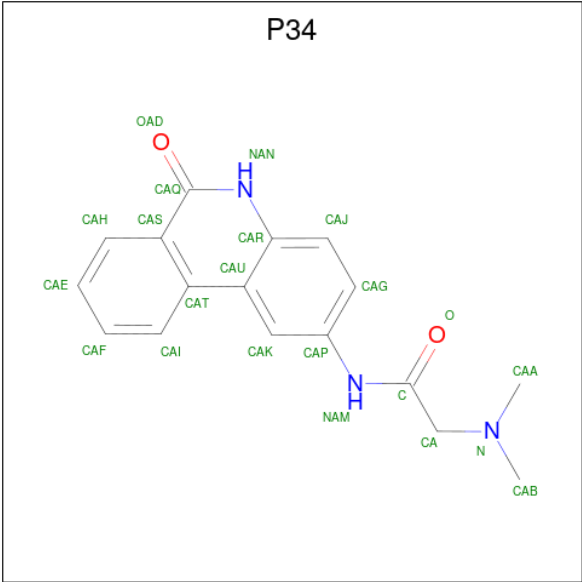
There are 3 discrepancies between the modelled and reference sequences:

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
			1587	1001	283	303			
2	D	207	Total	C	N	O	0	0	0
			1587	1001	283	303			
2	F	207	Total	C	N	O	0	0	0
			1587	1001	283	303			

- Molecule 3 is N 2 ,N 2 -DIMETHYL-N 1 -(6-OXO-5,6-DIHYDROPHENANTHRIDIN-2-Y L)GLYCINAMIDE (CCD ID: P34) (formula: C₁₇H₁₇N₃O₂).

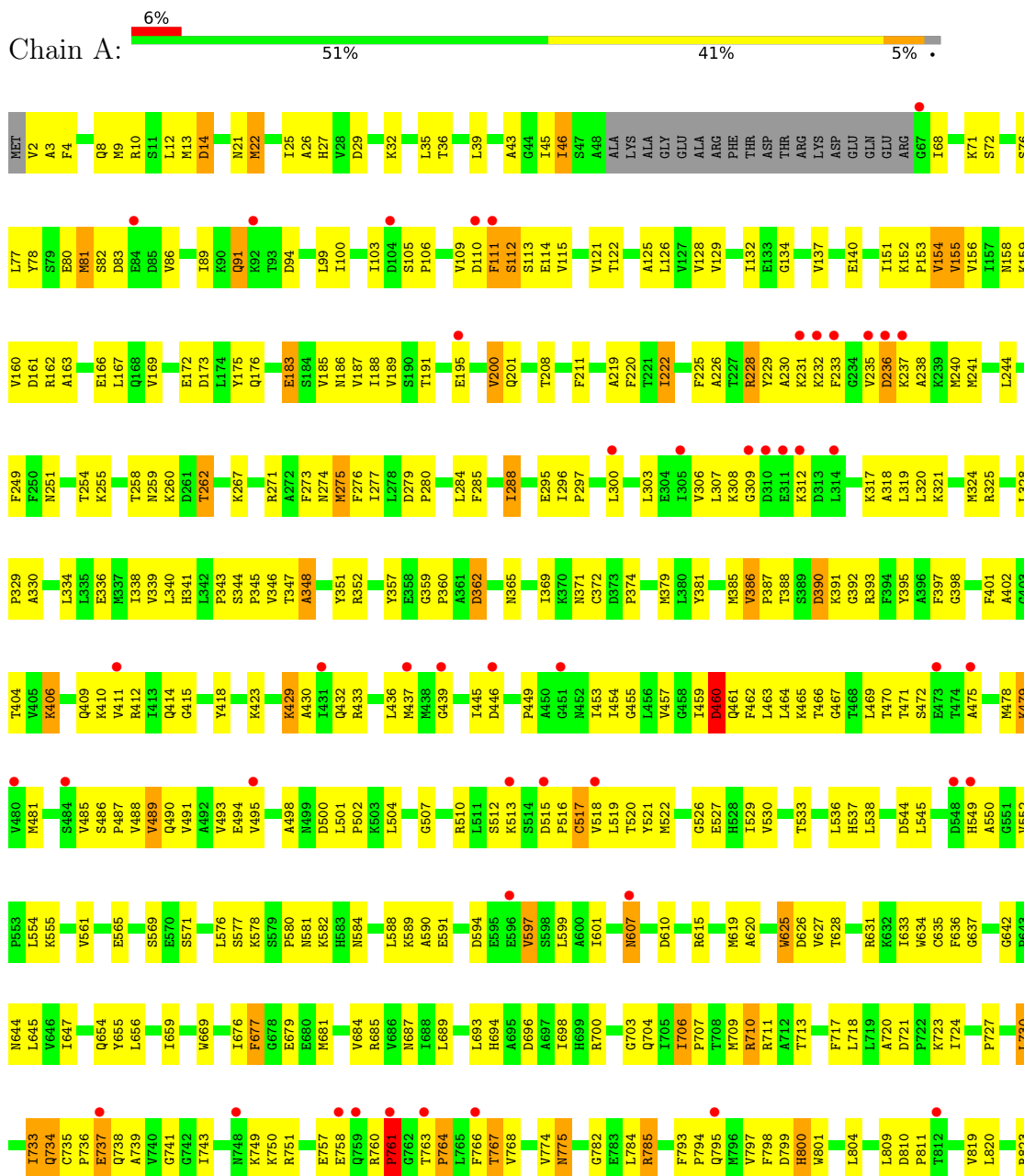


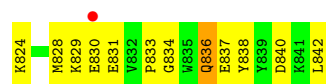
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			22	17	3	2		
3	D	1	Total	C	N	O	0	0
			22	17	3	2		
3	F	1	Total	C	N	O	0	0
			22	17	3	2		

3 Residue-property plots

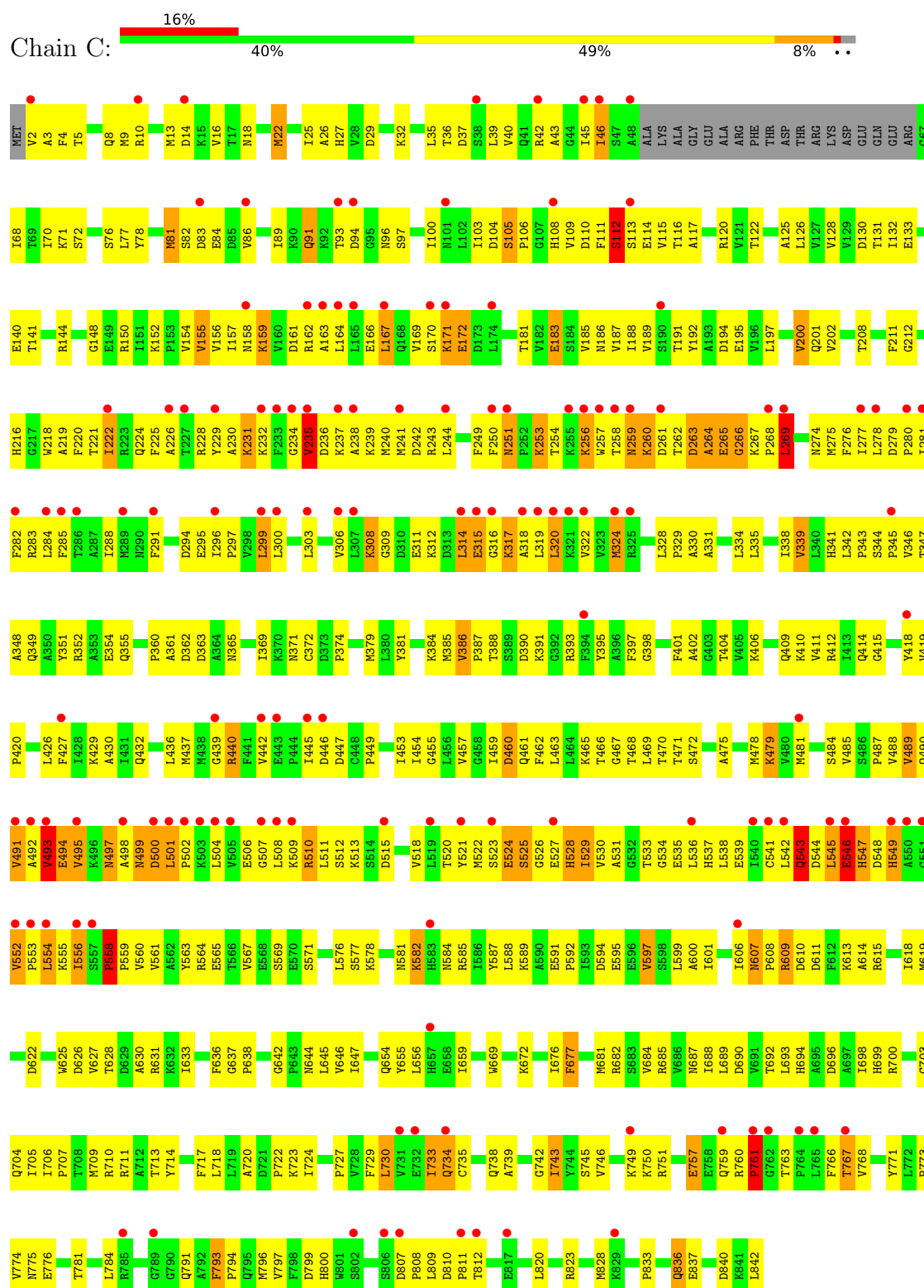
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

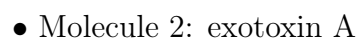


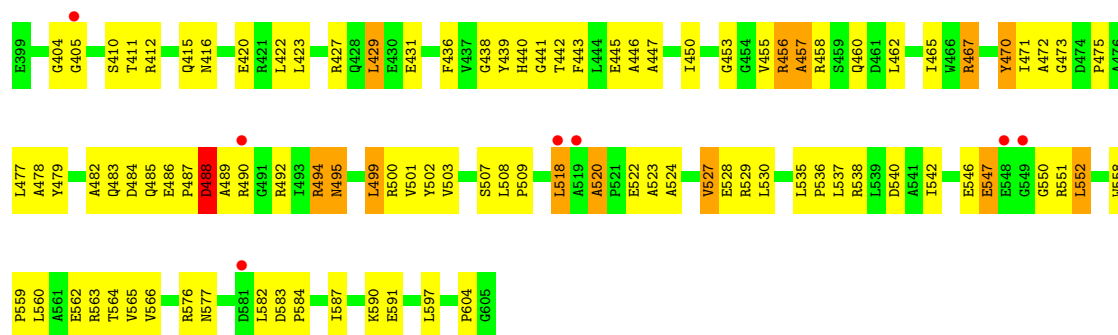


● Molecule 1: Elongation factor 2

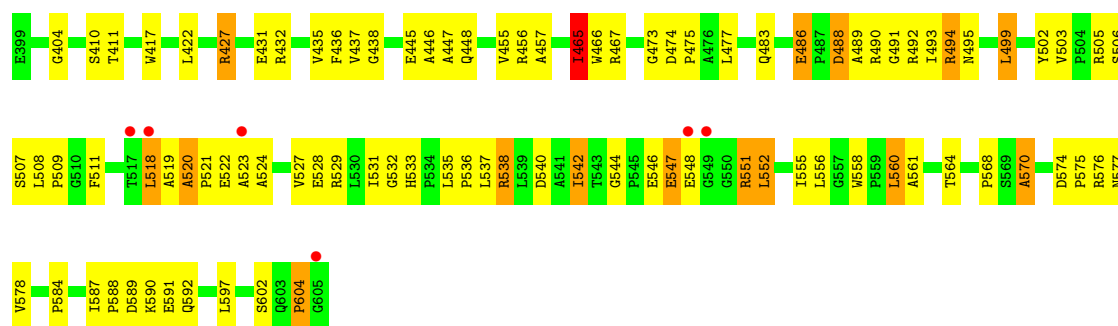


● Molecule 1: Elongation factor 2

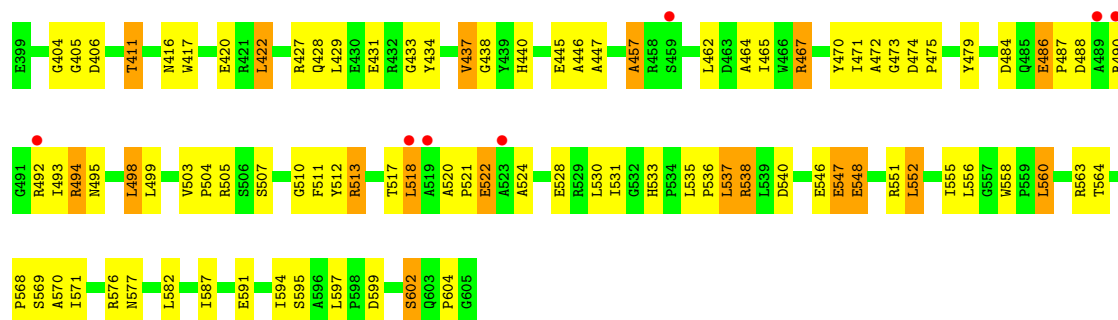




• Molecule 2: exotoxin A



• 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	330.84Å 68.74Å 191.46Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 99.2 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.274 0.254 , 0.272	Depositor DCC
R_{free} test set	2056 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.0	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	0.89	EDS
Total number of atoms	24042	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 31.59 % 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 1.0789e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P34, 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	0.65	1/6517 (0.0%)	1.02	24/8823 (0.3%)
1	C	0.67	1/6517 (0.0%)	1.10	39/8823 (0.4%)
1	E	0.59	0/6517	1.01	20/8823 (0.2%)
2	B	0.69	0/1626	1.15	11/2216 (0.5%)
2	D	0.71	0/1626	1.15	10/2216 (0.5%)
2	F	0.65	0/1626	1.12	10/2216 (0.5%)
All	All	0.64	2/24429 (0.0%)	1.06	114/33117 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	556	ILE	CA-C	7.59	1.62	1.52
1	A	706	ILE	CA-CB	-6.90	1.50	1.54

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	543	GLN	OE1-CD-NE2	-9.62	112.98	122.60
2	F	518	LEU	N-CA-C	9.40	125.94	111.56
1	C	547	HIS	N-CA-C	9.32	121.53	111.36
1	C	554	LEU	N-CA-C	9.05	122.03	109.18
1	A	236	ASP	N-CA-C	-9.00	94.52	109.46
1	C	314	LEU	N-CA-C	8.94	121.86	110.24
1	C	315	GLU	N-CA-C	8.32	120.74	108.60
2	D	520	ALA	N-CA-C	8.21	119.57	110.13
2	F	438	GLY	N-CA-C	8.19	121.58	110.69
1	C	260	LYS	N-CA-C	-7.92	100.08	110.53
1	C	471	THR	N-CA-C	-7.85	105.67	114.62
1	E	471	THR	N-CA-C	-7.84	105.68	114.62
2	B	488	ASP	N-CA-C	-7.73	100.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	498	ALA	N-CA-C	7.54	123.09	111.56
1	C	22	MET	N-CA-C	7.50	119.43	108.86
2	D	518	LEU	N-CA-C	7.48	126.73	110.80
1	A	471	THR	N-CA-C	-7.20	106.42	114.62
2	B	411	THR	N-CA-C	-7.18	103.78	112.54
1	C	607	ASN	CA-C-N	7.17	127.17	119.28
1	C	607	ASN	C-N-CA	7.17	127.17	119.28
1	C	510	ARG	N-CA-C	-7.10	104.24	113.12
1	C	543	GLN	CG-CD-NE2	6.94	126.81	116.40
1	E	552	VAL	CA-C-N	6.86	127.26	119.92
1	E	552	VAL	C-N-CA	6.86	127.26	119.92
1	E	554	LEU	N-CA-C	6.81	119.53	109.24
1	C	386	VAL	CA-C-N	6.81	127.18	119.83
1	C	386	VAL	C-N-CA	6.81	127.18	119.83
2	B	587	ILE	N-CA-C	-6.81	102.78	108.63
1	C	498	ALA	N-CA-C	6.72	125.12	110.80
1	C	115	VAL	N-CA-C	-6.71	104.23	110.53
1	A	154	VAL	N-CA-C	-6.65	99.16	108.27
1	C	558	PRO	N-CA-C	6.62	118.78	110.70
2	B	457	ALA	N-CA-C	-6.62	102.27	110.41
1	A	22	MET	N-CA-C	6.54	118.09	108.86
2	B	465	ILE	N-CA-C	6.54	121.06	112.76
1	A	115	VAL	N-CA-C	-6.52	104.40	110.53
1	A	415	GLY	CA-C-N	6.43	126.65	119.32
1	A	415	GLY	C-N-CA	6.43	126.65	119.32
1	C	155	VAL	N-CA-C	6.24	118.64	108.97
2	F	537	LEU	N-CA-C	-6.24	102.30	110.53
1	C	259	ASN	N-CA-C	-6.23	106.65	114.56
2	B	527	VAL	N-CA-C	-6.18	104.72	110.53
1	E	115	VAL	N-CA-C	-6.14	104.76	110.53
1	C	251	ASN	CA-C-N	6.13	126.67	120.04
1	C	251	ASN	C-N-CA	6.13	126.67	120.04
1	A	155	VAL	N-CA-C	6.10	118.57	109.17
1	E	733	ILE	N-CA-C	6.10	116.90	108.12
1	E	793	PHE	CA-C-N	6.05	126.01	119.78
1	E	793	PHE	C-N-CA	6.05	126.01	119.78
2	F	411	THR	N-CA-C	-5.97	104.85	111.71
1	C	339	VAL	N-CA-C	5.96	116.14	110.53
1	E	348	ALA	N-CA-C	5.94	117.84	111.36
1	A	348	ALA	N-CA-C	5.93	117.82	111.36
2	D	486	GLU	CA-C-N	5.88	127.19	119.84
2	D	486	GLU	C-N-CA	5.88	127.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	415	GLY	CA-C-N	5.85	125.32	119.24
1	E	415	GLY	C-N-CA	5.85	125.32	119.24
2	B	429	LEU	N-CA-C	-5.82	105.02	111.36
1	A	386	VAL	CA-C-N	5.82	126.11	119.83
1	A	386	VAL	C-N-CA	5.82	126.11	119.83
1	A	733	ILE	N-CA-C	5.76	116.42	108.12
1	C	552	VAL	CA-C-N	5.74	125.65	119.85
1	C	552	VAL	C-N-CA	5.74	125.65	119.85
1	C	793	PHE	CA-C-N	5.73	126.05	119.92
1	C	793	PHE	C-N-CA	5.73	126.05	119.92
2	B	520	ALA	N-CA-C	5.71	116.17	109.60
2	D	492	ARG	N-CA-C	5.67	118.87	110.48
2	D	438	GLY	N-CA-C	5.64	119.23	110.88
2	F	517	THR	N-CA-C	-5.64	103.26	110.53
1	C	415	GLY	CA-C-N	5.61	125.72	119.32
1	C	415	GLY	C-N-CA	5.61	125.72	119.32
2	D	537	LEU	N-CA-C	-5.59	102.62	110.50
2	F	486	GLU	CA-C-N	5.56	126.79	119.84
2	F	486	GLU	C-N-CA	5.56	126.79	119.84
2	F	457	ALA	N-CA-C	-5.54	103.39	110.53
1	E	288	ILE	N-CA-C	5.54	116.27	110.62
1	C	386	VAL	N-CA-C	5.52	113.91	107.89
2	F	465	ILE	N-CA-C	5.52	119.84	111.89
1	E	386	VAL	N-CA-C	5.50	113.89	107.89
2	D	465	ILE	N-CA-C	5.44	118.73	111.44
1	C	104	ASP	N-CA-C	5.44	118.17	110.50
2	D	570	ALA	N-CA-C	-5.44	106.32	113.17
1	C	169	VAL	N-CA-C	5.41	115.78	107.77
1	E	386	VAL	CA-C-N	5.34	125.60	119.83
1	E	386	VAL	C-N-CA	5.34	125.60	119.83
1	A	721	ASP	CA-C-N	5.33	125.24	119.85
1	A	721	ASP	C-N-CA	5.33	125.24	119.85
2	D	519	ALA	N-CA-C	5.32	122.14	110.80
1	A	607	ASN	CA-C-N	5.32	125.13	119.28
1	A	607	ASN	C-N-CA	5.32	125.13	119.28
1	E	558	PRO	CA-C-N	5.25	125.01	119.76
1	E	558	PRO	C-N-CA	5.25	125.01	119.76
2	B	591	GLU	N-CA-C	-5.25	105.61	112.23
1	E	622	ASP	N-CA-C	5.24	119.30	113.01
2	B	443	PHE	N-CA-C	5.24	118.23	110.48
1	A	800	HIS	N-CA-C	5.21	116.21	108.60
1	A	288	ILE	N-CA-C	5.19	115.81	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	622	ASP	N-CA-C	5.19	119.24	113.01
1	C	263	ASP	N-CA-C	-5.17	102.53	110.14
1	C	269	LEU	N-CA-C	5.16	117.31	108.90
1	C	171	LYS	N-CA-C	-5.13	105.37	110.97
1	C	308	LYS	N-CA-C	5.13	117.52	107.57
1	A	517	CYS	N-CA-C	5.12	119.22	112.92
1	A	834	GLY	N-CA-C	-5.12	104.61	112.85
1	A	339	VAL	CB-CA-C	-5.09	105.35	112.02
1	A	810	ASP	CA-C-N	5.07	126.18	119.84
1	A	810	ASP	C-N-CA	5.07	126.18	119.84
2	F	595	SER	N-CA-C	5.07	118.77	112.59
2	B	478	ALA	N-CA-C	-5.06	105.67	111.14
1	C	545	LEU	CA-C-N	-5.06	111.88	121.54
1	C	545	LEU	C-N-CA	-5.06	111.88	121.54
1	C	733	ILE	N-CA-C	5.05	115.39	108.12
1	E	155	VAL	N-CA-C	5.02	117.06	109.12
1	A	386	VAL	N-CA-C	5.01	113.35	107.89

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	361	0
1	C	6405	0	6472	536	0
1	E	6405	0	6472	469	0
2	B	1587	0	1539	95	0
2	D	1587	0	1539	93	0
2	F	1587	0	1539	85	0
3	B	22	0	17	0	0
3	D	22	0	17	0	0
3	F	22	0	17	1	0
All	All	24042	0	24084	1615	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 34.

All (1615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:VAL:HG22	1:E:553:PRO:CD	1.53	1.37
1:E:552:VAL:CG2	1:E:553:PRO:HD3	1.65	1.27
1:C:546:GLU:HA	1:C:554:LEU:CD1	1.71	1.18
1:C:500:ASP:OD2	1:C:552:VAL:HG11	1.44	1.18
1:A:828:MET:HE2	2:B:576:ARG:NE	1.59	1.17
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.26	1.15
1:A:828:MET:HE2	2:B:576:ARG:HE	1.02	1.11
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.26	1.09
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.34	1.09
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.16	1.08
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.35	1.08
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.33	1.07
1:C:545:LEU:O	1:C:546:GLU:O	1.72	1.07
1:E:556:ILE:HG22	1:E:557:SER:H	1.21	1.06
1:C:256:LYS:HE2	1:C:256:LYS:CA	1.84	1.05
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.32	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.39	1.04
2:B:546:GLU:HG3	2:B:547:GLU:HG3	1.31	1.03
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.37	1.02
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.42	1.02
1:A:10:ARG:HD3	1:A:445:ILE:HD11	1.40	1.02
2:D:531:ILE:HD11	2:D:533:HIS:O	1.59	1.00
1:E:786:GLN:N	1:E:786:GLN:OE1	1.95	1.00
1:C:256:LYS:HA	1:C:256:LYS:CE	1.92	0.99
2:B:488:ASP:OD2	2:B:490:ARG:HG2	1.62	0.99
1:A:533:THR:H	1:A:537:HIS:CD2	1.81	0.99
2:B:477:LEU:HD13	2:B:551:ARG:NH1	1.78	0.98
1:A:694:HIS:HD2	1:A:696:ASP:H	1.12	0.98
1:C:256:LYS:HE2	1:C:256:LYS:HA	0.98	0.97
1:A:27:HIS:HD2	1:A:29:ASP:H	1.09	0.97
2:B:490:ARG:HD2	2:B:492:ARG:HD2	1.47	0.96
1:C:2:VAL:HG22	1:C:3:ALA:H	1.28	0.96
1:C:166:GLU:C	1:C:167:LEU:HD12	1.90	0.96
1:A:819:VAL:O	1:A:823:ARG:HG3	1.63	0.96
1:A:533:THR:H	1:A:537:HIS:HD2	1.00	0.95
1:E:27:HIS:HD2	1:E:29:ASP:H	1.12	0.95
2:D:527:VAL:O	2:D:531:ILE:HG23	1.66	0.94
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.03	0.94

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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	0.94
1:E:546:GLU:HB2	1:E:554:LEU:HD12	1.46	0.94
1:A:429:LYS:HE3	1:A:430:ALA:H	1.31	0.94
1:C:546:GLU:HA	1:C:554:LEU:HD12	1.50	0.93
2:B:490:ARG:CD	2:B:492:ARG:HD2	1.97	0.93
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.03	0.92
1:E:404:THR:HG22	1:E:449:PRO:HA	1.51	0.92
1:E:495:VAL:CG1	1:E:554:LEU:HD23	1.99	0.92
1:C:42:ARG:HG3	1:C:331:ALA:CB	1.98	0.92
1:E:828:MET:HE2	2:F:576:ARG:HE	1.33	0.92
1:C:511:LEU:HA	1:C:549:HIS:CE1	2.05	0.91
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.00	0.91
1:C:265:GLU:HG3	1:C:266:GLY:H	1.32	0.91
1:C:523:SER:OG	1:C:527:GLU:HB2	1.69	0.91
1:A:578:LYS:HE3	1:A:840:ASP:OD1	1.69	0.90
1:A:45:ILE:HD12	1:A:76:SER:HB3	1.54	0.90
1:A:404:THR:HG22	1:A:449:PRO:HA	1.52	0.90
1:C:759:GLN:HB3	1:C:766:PHE:CE2	2.05	0.90
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.55	0.89
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.72	0.88
1:C:2:VAL:HG22	1:C:3:ALA:N	1.84	0.88
1:C:234:GLY:O	1:C:235:VAL:HG23	1.72	0.88
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.54	0.88
1:C:536:LEU:HD12	1:C:537:HIS:N	1.88	0.88
1:C:404:THR:HG22	1:C:449:PRO:HA	1.53	0.88
1:C:4:PHE:HD1	1:C:8:GLN:OE1	1.57	0.88
1:C:694:HIS:HD2	1:C:696:ASP:H	1.19	0.87
2:D:520:ALA:HB3	2:D:522:GLU:OE2	1.75	0.87
1:E:289:MET:HE1	1:E:316:GLY:C	1.99	0.87
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.55	0.87
1:E:91:GLN:HE22	1:E:344:SER:H	1.18	0.87
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.05	0.86
1:A:833:PRO:HB3	1:A:837:GLU:OE1	1.76	0.85
2:D:556:LEU:HD22	2:D:560:LEU:HD13	1.58	0.84
1:C:546:GLU:HA	1:C:554:LEU:HD11	1.58	0.84
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.59	0.84
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.08	0.83
1:C:546:GLU:CA	1:C:554:LEU:CD1	2.55	0.83
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.59	0.83
1:C:27:HIS:HD2	1:C:29:ASP:H	1.22	0.83
1:C:157:ILE:CD1	1:C:181:THR:HG21	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:VAL:HG22	1:E:553:PRO:HD3	0.86	0.83
2:F:488:ASP:CG	2:F:492:ARG:HB2	2.03	0.83
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.44	0.83
1:C:546:GLU:CA	1:C:554:LEU:HD12	2.07	0.83
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.77	0.82
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.60	0.82
1:A:533:THR:N	1:A:537:HIS:HD2	1.77	0.82
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.10	0.82
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.62	0.81
1:E:495:VAL:HG12	1:E:554:LEU:CD2	2.09	0.81
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.63	0.81
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.60	0.81
1:A:828:MET:CE	2:B:576:ARG:HE	1.91	0.81
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.62	0.81
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.81
1:C:2:VAL:CG2	1:C:3:ALA:H	1.94	0.81
1:E:27:HIS:CD2	1:E:29:ASP:H	1.98	0.81
1:A:27:HIS:CD2	1:A:29:ASP:H	1.96	0.80
1:C:638:PRO:HB3	1:C:672:LYS:HG2	1.61	0.80
1:E:694:HIS:O	1:E:700:ARG:HD3	1.82	0.80
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.50	0.80
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.63	0.80
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.16	0.80
1:C:511:LEU:CA	1:C:549:HIS:CE1	2.64	0.80
1:C:836:GLN:H	1:C:836:GLN:HE21	1.28	0.80
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.64	0.80
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.12	0.79
1:E:300:LEU:HG	1:E:305:ILE:HB	1.65	0.79
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.64	0.79
1:C:311:GLU:HA	1:C:314:LEU:HD13	1.64	0.79
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.47	0.79
2:B:427:ARG:O	2:B:431:GLU:HG3	1.83	0.79
1:C:157:ILE:HD11	1:C:181:THR:HG21	1.65	0.79
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.12	0.79
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.63	0.78
1:E:615:ARG:HG2	1:E:619:MET:HE2	1.65	0.78
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.45	0.78
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.19	0.78
1:C:494:GLU:O	1:C:555:LYS:HB3	1.84	0.78
2:F:513:ARG:HB2	2:F:513:ARG:HH11	1.49	0.78
1:E:237:LYS:HA	1:E:240:MET:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.65	0.78
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.66	0.78
1:A:230:ALA:O	1:A:235:VAL:HG22	1.83	0.77
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.60	0.77
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.14	0.77
1:E:412:ARG:HH11	1:E:412:ARG:HG2	1.50	0.77
1:E:552:VAL:CG2	1:E:553:PRO:CD	2.42	0.77
1:E:734:GLN:N	1:E:734:GLN:HE21	1.81	0.77
1:A:644:ASN:HD22	1:A:684:VAL:HB	1.49	0.77
1:C:311:GLU:HA	1:C:314:LEU:CD1	2.15	0.77
1:E:836:GLN:H	1:E:836:GLN:HE21	1.28	0.77
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.66	0.76
1:E:141:THR:HA	1:E:144:ARG:NH2	2.00	0.76
1:E:556:ILE:HG22	1:E:557:SER:N	2.00	0.76
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.68	0.76
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.68	0.76
1:C:836:GLN:H	1:C:836:GLN:NE2	1.84	0.76
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.15	0.76
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.66	0.75
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.16	0.75
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.69	0.75
1:E:736:PRO:HB2	1:E:738:GLN:CG	2.16	0.75
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.67	0.75
1:A:321:LYS:O	1:A:325:ARG:HG3	1.87	0.75
1:C:117:ALA:N	1:C:481:MET:HE1	2.01	0.75
1:C:191:THR:O	1:C:763:THR:HG22	1.86	0.75
2:D:455:VAL:O	2:D:456:ARG:HG2	1.87	0.75
1:C:545:LEU:O	1:C:546:GLU:C	2.24	0.75
2:D:427:ARG:O	2:D:431:GLU:HG3	1.86	0.75
1:E:74:ALA:O	1:E:439:GLY:HA2	1.86	0.75
2:B:552:LEU:N	2:B:552:LEU:HD12	2.01	0.74
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.87	0.74
1:C:166:GLU:HB3	1:C:167:LEU:CD1	2.17	0.74
1:E:338:ILE:O	1:E:342:LEU:HB2	1.87	0.74
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.22	0.74
1:A:544:ASP:O	1:A:549:HIS:HD2	1.71	0.74
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.68	0.74
1:A:615:ARG:HG2	1:A:619:MET:HE2	1.68	0.74
1:E:186:ASN:CG	1:E:201:GLN:HE21	1.96	0.74
1:E:500:ASP:O	1:E:503:LYS:HB2	1.87	0.74
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LYS:HE3	1:C:393:ARG:HG3	1.70	0.73
1:C:584:ASN:ND2	1:C:694:HIS:H	1.86	0.73
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.70	0.73
1:E:786:GLN:OE1	1:E:786:GLN:CA	2.36	0.73
1:E:836:GLN:H	1:E:836:GLN:NE2	1.85	0.73
2:B:438:GLY:HA3	2:B:471:ILE:HD13	1.70	0.73
1:C:454:ILE:HG13	1:C:455:GLY:H	1.54	0.73
1:E:591:GLU:O	1:E:685:ARG:HB3	1.89	0.73
2:B:439:TYR:CE2	2:B:475:PRO:HD3	2.24	0.73
1:C:552:VAL:HB	1:C:553:PRO:CD	2.18	0.73
1:C:291:PHE:HE1	1:C:315:GLU:CB	1.97	0.72
1:A:251:ASN:HB3	1:A:254:THR:OG1	1.89	0.72
1:A:258:THR:HG22	1:A:259:ASN:N	2.03	0.72
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.71	0.72
1:C:533:THR:H	1:C:537:HIS:CD2	2.08	0.72
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.54	0.72
2:B:477:LEU:HD13	2:B:551:ARG:HH12	1.53	0.72
2:F:488:ASP:OD2	2:F:492:ARG:HD3	1.89	0.72
1:E:26:ALA:CB	1:E:128:VAL:HB	2.19	0.72
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.71	0.72
1:E:503:LYS:CB	1:E:551:GLY:HA3	2.17	0.72
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.71	0.72
1:C:494:GLU:OE1	1:C:494:GLU:HA	1.87	0.72
1:C:509:LYS:N	1:C:509:LYS:HD2	2.05	0.72
1:C:533:THR:H	1:C:537:HIS:HD2	1.37	0.71
2:F:522:GLU:CD	2:F:522:GLU:H	1.97	0.71
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.25	0.71
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.71	0.71
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.20	0.71
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.06	0.71
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.73	0.71
1:C:584:ASN:HD21	1:C:694:HIS:H	1.38	0.71
1:A:694:HIS:CD2	1:A:696:ASP:H	2.03	0.71
1:C:251:ASN:OD1	1:C:269:LEU:HD11	1.91	0.71
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.71	0.71
1:E:508:LEU:HD22	1:E:520:THR:HB	1.72	0.71
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.71	0.71
1:C:265:GLU:HG3	1:C:266:GLY:N	1.99	0.70
1:E:185:VAL:O	1:E:189:VAL:HG23	1.91	0.70
1:A:836:GLN:H	1:A:836:GLN:HE21	1.37	0.70
2:B:552:LEU:HD12	2:B:552:LEU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.72	0.70
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.06	0.70
1:C:509:LYS:O	1:C:513:LYS:HE3	1.91	0.70
1:E:331:ALA:O	1:E:335:LEU:HG	1.90	0.70
1:C:258:THR:HG22	1:C:260:LYS:H	1.56	0.70
1:E:226:ALA:O	1:E:230:ALA:HB2	1.92	0.70
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.74	0.70
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.73	0.70
1:C:546:GLU:HA	1:C:554:LEU:CG	2.22	0.70
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.74	0.70
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.92	0.70
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.72	0.70
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.21	0.70
1:E:556:ILE:CG2	1:E:557:SER:H	2.04	0.70
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.72	0.70
1:E:454:ILE:HG13	1:E:455:GLY:H	1.55	0.70
1:A:820:LEU:HD11	1:A:830:GLU:HG2	1.74	0.69
1:A:391:LYS:HB3	1:A:393:ARG:HG2	1.74	0.69
1:A:410:LYS:HA	1:A:430:ALA:HA	1.74	0.69
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.73	0.69
1:C:694:HIS:O	1:C:700:ARG:HD3	1.92	0.69
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.14	0.69
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.91	0.69
1:C:511:LEU:HD13	1:C:549:HIS:CD2	2.27	0.69
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.73	0.69
1:C:511:LEU:HD22	1:C:545:LEU:HD13	1.73	0.69
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.73	0.69
1:A:429:LYS:HE3	1:A:430:ALA:N	2.07	0.69
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.23	0.69
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.28	0.69
1:E:142:VAL:O	1:E:145:GLN:HB2	1.92	0.69
1:C:538:LEU:O	1:C:542:LEU:HG	1.93	0.69
1:E:89:ILE:C	1:E:91:GLN:H	2.01	0.69
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.56	0.69
1:A:669:TRP:HZ2	2:B:490:ARG:CD	2.06	0.69
1:C:615:ARG:HG2	1:C:619:MET:HE2	1.74	0.69
1:C:511:LEU:HA	1:C:549:HIS:NE2	2.06	0.68
1:A:757:GLU:HG3	1:A:768:VAL:HG22	1.75	0.68
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.29	0.68
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.74	0.68
1:E:528:HIS:C	1:E:529:ILE:HD13	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.08	0.68
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.94	0.68
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.28	0.68
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.09	0.68
1:C:694:HIS:CD2	1:C:696:ASP:H	2.09	0.68
1:A:591:GLU:O	1:A:685:ARG:HB3	1.94	0.68
1:A:824:LYS:HE3	1:A:830:GLU:OE2	1.94	0.68
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.29	0.67
1:E:546:GLU:CB	1:E:554:LEU:HD12	2.23	0.67
1:C:3:ALA:HA	1:C:46:ILE:O	1.94	0.67
1:E:785:ARG:NH2	1:E:786:GLN:HE22	1.93	0.67
1:C:497:ASN:HD22	1:C:497:ASN:N	1.91	0.67
2:D:552:LEU:N	2:D:552:LEU:HD12	2.10	0.67
1:E:334:LEU:O	1:E:338:ILE:HG12	1.95	0.67
1:A:571:SER:HB2	1:A:589:LYS:HG2	1.74	0.67
1:C:530:VAL:O	1:C:530:VAL:HG12	1.95	0.67
2:D:417:TRP:CZ2	2:D:568:PRO:HD2	2.29	0.67
1:A:694:HIS:O	1:A:700:ARG:HD3	1.95	0.67
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.16	0.67
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.77	0.67
1:C:497:ASN:N	1:C:497:ASN:ND2	2.42	0.67
1:C:501:LEU:C	1:C:501:LEU:HD23	2.19	0.67
1:C:588:LEU:C	1:C:588:LEU:HD12	2.19	0.67
1:E:91:GLN:NE2	1:E:344:SER:H	1.91	0.67
1:E:694:HIS:CD2	1:E:696:ASP:H	2.02	0.67
1:A:258:THR:HG22	1:A:259:ASN:H	1.58	0.67
1:C:543:GLN:HG2	1:C:544:ASP:N	2.08	0.67
1:E:710:ARG:HG3	1:E:710:ARG:HH11	1.60	0.67
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.76	0.67
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.77	0.67
1:C:354:GLU:OE2	1:C:361:ALA:HB1	1.95	0.67
1:C:591:GLU:O	1:C:685:ARG:HB3	1.94	0.67
1:C:488:VAL:HG23	1:C:489:VAL:HG22	1.77	0.67
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.24	0.67
1:A:836:GLN:H	1:A:836:GLN:NE2	1.92	0.66
2:D:465:ILE:HD13	2:D:465:ILE:H	1.59	0.66
1:A:285:PHE:HE2	1:A:324:MET:SD	2.18	0.66
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.10	0.66
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.77	0.66
1:C:530:VAL:O	1:C:538:LEU:CD1	2.44	0.66
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.30	0.66
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.76	0.66
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.77	0.66
1:C:311:GLU:O	1:C:314:LEU:HD13	1.96	0.66
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.77	0.66
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.30	0.66
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.64	0.66
1:C:253:LYS:HA	1:C:253:LYS:CE	2.21	0.66
1:C:578:LYS:HE3	1:C:840:ASP:OD1	1.95	0.66
1:A:27:HIS:HD2	1:A:29:ASP:N	1.89	0.66
1:A:429:LYS:HG3	1:A:430:ALA:H	1.59	0.66
1:C:132:ILE:HG23	1:C:133:GLU:N	2.11	0.66
1:C:72:SER:HA	1:C:439:GLY:O	1.96	0.66
1:C:759:GLN:HB3	1:C:766:PHE:CD2	2.31	0.66
1:E:495:VAL:CG1	1:E:554:LEU:CD2	2.71	0.65
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.77	0.65
1:C:454:ILE:HG13	1:C:455:GLY:N	2.12	0.65
1:A:324:MET:HE2	1:A:324:MET:HA	1.78	0.65
1:C:226:ALA:O	1:C:230:ALA:HB2	1.96	0.65
1:C:493:VAL:HG21	1:C:545:LEU:HD21	1.77	0.65
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.76	0.65
1:A:734:GLN:HE21	1:A:734:GLN:N	1.95	0.65
1:C:231:LYS:HG2	1:C:232:LYS:N	2.10	0.65
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.27	0.65
2:F:537:LEU:O	2:F:538:ARG:HD3	1.96	0.65
1:E:578:LYS:HE3	1:E:840:ASP:OD1	1.96	0.65
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.31	0.65
1:A:3:ALA:HA	1:A:46:ILE:O	1.96	0.65
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.31	0.65
1:C:492:ALA:HA	1:C:528:HIS:O	1.96	0.65
2:D:523:ALA:O	2:D:527:VAL:HG23	1.96	0.65
1:E:258:THR:HG22	1:E:259:ASN:H	1.61	0.65
1:C:183:GLU:O	1:C:187:VAL:HG23	1.97	0.65
2:F:420:GLU:CD	2:F:420:GLU:H	2.05	0.65
2:F:548:GLU:HG2	2:F:548:GLU:O	1.96	0.65
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.27	0.65
1:C:490:GLN:O	1:C:491:VAL:HG13	1.97	0.65
1:C:609:ARG:HG3	1:C:609:ARG:HH11	1.62	0.64
1:C:167:LEU:HD12	1:C:167:LEU:N	2.11	0.64
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.36	0.64
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.79	0.64
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.80	0.64
1:A:429:LYS:HG3	1:A:430:ALA:N	2.12	0.64
1:C:27:HIS:CD2	1:C:29:ASP:H	2.10	0.64
1:C:157:ILE:HD11	1:C:181:THR:CG2	2.26	0.64
1:C:275:MET:HE2	1:C:276:PHE:CE1	2.32	0.64
1:E:275:MET:HE2	1:E:276:PHE:CE1	2.33	0.64
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.31	0.64
1:C:384:LYS:HB2	1:C:465:LYS:HE3	1.78	0.64
1:C:275:MET:HE2	1:C:276:PHE:CZ	2.32	0.64
1:C:507:GLY:HA2	1:C:510:ARG:HD2	1.79	0.64
1:C:541:CYS:O	1:C:545:LEU:HB2	1.98	0.64
2:F:556:LEU:HD22	2:F:560:LEU:CD1	2.26	0.64
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.80	0.64
1:E:454:ILE:HG13	1:E:455:GLY:N	2.12	0.64
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.79	0.64
1:E:162:ARG:O	1:E:166:GLU:HB2	1.98	0.64
2:B:455:VAL:C	2:B:456:ARG:HD2	2.23	0.64
1:A:581:ASN:O	1:A:582:LYS:HB2	1.98	0.63
1:C:828:MET:HE2	2:D:576:ARG:HE	1.62	0.63
2:F:504:PRO:HD3	2:F:563:ARG:O	1.98	0.63
1:C:265:GLU:OE2	1:C:267:LYS:HE3	1.97	0.63
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.79	0.63
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.78	0.63
1:E:781:THR:O	1:E:785:ARG:HG3	1.97	0.63
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.80	0.63
1:E:528:HIS:O	1:E:529:ILE:HD13	1.99	0.63
1:C:529:ILE:N	1:C:529:ILE:HD12	2.14	0.63
1:C:192:TYR:HA	1:C:763:THR:HG21	1.79	0.63
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.14	0.63
1:C:609:ARG:HG3	1:C:609:ARG:NH1	2.13	0.63
1:A:454:ILE:HG13	1:A:455:GLY:H	1.64	0.63
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.13	0.63
2:B:537:LEU:O	2:B:538:ARG:HD3	1.98	0.63
1:E:588:LEU:C	1:E:588:LEU:HD12	2.23	0.63
2:B:495:ASN:N	2:B:495:ASN:HD22	1.96	0.63
1:E:710:ARG:HG3	1:E:710:ARG:NH1	2.14	0.62
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.80	0.62
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.81	0.62
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.34	0.62
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.81	0.62
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.65	0.62
1:E:500:ASP:CB	1:E:552:VAL:HG11	2.29	0.62
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.63	0.62
1:C:607:ASN:HB3	1:C:610:ASP:CG	2.24	0.62
1:E:584:ASN:ND2	1:E:694:HIS:H	1.97	0.62
1:A:504:LEU:HD13	1:A:554:LEU:HD21	1.82	0.62
1:C:311:GLU:CA	1:C:314:LEU:HD13	2.29	0.62
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.81	0.62
2:B:410:SER:OG	2:B:412:ARG:HB3	1.99	0.62
2:F:493:ILE:O	2:F:493:ILE:HG22	2.00	0.62
2:F:552:LEU:HD12	2:F:552:LEU:N	2.15	0.62
1:A:735:CYS:SG	1:A:739:ALA:HB3	2.40	0.62
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.30	0.62
1:E:321:LYS:O	1:E:325:ARG:HG3	1.99	0.62
1:A:619:MET:HE1	1:A:633:ILE:CD1	2.30	0.62
1:A:809:LEU:O	1:A:811:PRO:HD3	2.00	0.62
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.82	0.61
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.63	0.61
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.14	0.61
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.81	0.61
1:C:311:GLU:OE2	1:C:322:VAL:HG11	2.01	0.61
2:D:455:VAL:O	2:D:456:ARG:CG	2.48	0.61
1:A:2:VAL:HG22	1:A:3:ALA:N	2.15	0.61
2:B:477:LEU:HD13	2:B:551:ARG:HH11	1.65	0.61
1:C:103:ILE:HD12	1:C:122:THR:HG22	1.81	0.61
1:E:508:LEU:HD22	1:E:520:THR:CG2	2.31	0.61
1:E:607:ASN:HB3	1:E:610:ASP:OD2	1.99	0.61
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.35	0.61
1:E:81:MET:O	1:E:96:ASN:HB3	2.00	0.61
1:E:410:LYS:HA	1:E:430:ALA:HA	1.82	0.61
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.83	0.61
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.66	0.61
1:C:749:LYS:O	1:C:750:LYS:HD2	2.00	0.61
1:E:495:VAL:HA	1:E:554:LEU:HA	1.81	0.61
1:A:162:ARG:O	1:A:166:GLU:HB2	2.00	0.61
1:A:669:TRP:CZ2	2:B:490:ARG:HD2	2.36	0.61
1:C:296:ILE:CD1	1:C:319:LEU:HD21	2.29	0.61
1:C:344:SER:C	1:C:346:VAL:H	2.09	0.61
1:C:243:ARG:HH12	1:C:257:TRP:CD1	2.19	0.60
1:C:563:TYR:O	1:C:564:ARG:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.30	0.60
1:C:810:ASP:OD1	1:C:812:THR:HG22	2.01	0.60
1:A:565:GLU:CD	1:A:676:ILE:HB	2.26	0.60
1:A:584:ASN:ND2	1:A:694:HIS:H	1.99	0.60
1:A:737:GLU:CG	1:A:766:PHE:CE2	2.82	0.60
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.84	0.60
2:D:417:TRP:CH2	2:D:568:PRO:HD2	2.35	0.60
1:A:158:ASN:ND2	1:A:159:LYS:HG2	2.16	0.60
1:C:192:TYR:HA	1:C:763:THR:CG2	2.31	0.60
1:C:506:GLU:O	1:C:510:ARG:HG3	2.01	0.60
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.36	0.60
2:F:537:LEU:O	2:F:538:ARG:CD	2.49	0.60
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.82	0.60
1:C:410:LYS:HE2	1:C:430:ALA:HB2	1.83	0.60
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.31	0.60
1:A:550:ALA:O	1:A:552:VAL:HG23	2.01	0.60
1:C:491:VAL:O	1:C:529:ILE:HA	2.02	0.60
1:C:734:GLN:N	1:C:734:GLN:HE21	1.98	0.60
1:E:694:HIS:HD2	1:E:696:ASP:N	1.93	0.59
1:A:183:GLU:O	1:A:187:VAL:HG23	2.03	0.59
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.36	0.59
1:E:167:LEU:HD12	1:E:167:LEU:H	1.66	0.59
1:C:258:THR:HG22	1:C:259:ASN:N	2.18	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.32	0.59
1:E:412:ARG:HH12	1:E:428:ILE:HD11	1.67	0.59
1:A:381:TYR:O	1:A:398:GLY:HA3	2.02	0.59
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.85	0.59
1:E:258:THR:HG22	1:E:259:ASN:N	2.18	0.59
1:E:749:LYS:O	1:E:750:LYS:HD2	2.02	0.59
1:C:251:ASN:H	1:C:251:ASN:HD22	1.50	0.59
2:F:556:LEU:HD22	2:F:560:LEU:HD13	1.84	0.59
1:E:493:VAL:HG12	1:E:494:GLU:N	2.17	0.59
1:C:535:GLU:O	1:C:539:GLU:HG3	2.03	0.59
1:E:500:ASP:HA	1:E:503:LYS:HD2	1.83	0.59
1:A:454:ILE:HG13	1:A:455:GLY:N	2.17	0.59
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.84	0.59
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.85	0.59
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.83	0.59
1:C:258:THR:HG22	1:C:259:ASN:H	1.68	0.59
1:C:569:SER:O	1:C:720:ALA:HB1	2.02	0.59
1:E:619:MET:HE1	1:E:633:ILE:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.37	0.59
2:B:457:ALA:O	2:B:458:ARG:HG3	2.03	0.59
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.43	0.58
1:E:584:ASN:HD21	1:E:694:HIS:H	1.49	0.58
1:E:591:GLU:HG2	1:E:685:ARG:HG2	1.84	0.58
1:A:240:MET:O	1:A:244:LEU:HG	2.03	0.58
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.68	0.58
1:E:147:LEU:HD12	1:E:192:TYR:HB2	1.86	0.58
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.33	0.58
1:A:466:THR:HG22	1:A:467:GLY:N	2.19	0.58
1:E:91:GLN:HE22	1:E:344:SER:N	1.95	0.58
1:A:501:LEU:C	1:A:501:LEU:HD23	2.28	0.58
2:F:487:PRO:HA	2:F:492:ARG:O	2.02	0.58
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.84	0.58
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.34	0.58
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.02	0.58
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.18	0.58
1:C:412:ARG:HG2	1:C:412:ARG:HH11	1.68	0.58
1:C:611:ASP:OD2	1:C:613:LYS:HB2	2.04	0.58
1:E:581:ASN:O	1:E:582:LYS:HB2	2.02	0.58
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.29	0.58
1:C:45:ILE:HD11	1:C:78:TYR:N	2.19	0.58
1:C:511:LEU:CD1	1:C:549:HIS:NE2	2.67	0.58
1:C:45:ILE:HG12	1:C:76:SER:O	2.04	0.58
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.34	0.58
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.67	0.58
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.39	0.58
1:E:289:MET:HE2	1:E:289:MET:HA	1.86	0.58
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.86	0.58
1:C:410:LYS:HA	1:C:430:ALA:HA	1.84	0.58
1:C:544:ASP:O	1:C:549:HIS:N	2.37	0.58
1:C:609:ARG:HH11	1:C:609:ARG:CG	2.17	0.58
2:D:508:LEU:N	2:D:509:PRO:CD	2.67	0.58
1:E:69:THR:OG1	1:E:389:SER:HB3	2.04	0.58
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.33	0.58
1:A:588:LEU:HD12	1:A:588:LEU:C	2.28	0.58
1:C:132:ILE:HG23	1:C:133:GLU:H	1.68	0.58
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.13	0.58
2:D:546:GLU:HG3	2:D:547:GLU:CG	2.22	0.57
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.37	0.57
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG12	1:A:412:ARG:N	2.18	0.57
1:C:543:GLN:CG	1:C:544:ASP:N	2.67	0.57
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.85	0.57
1:A:169:VAL:HG22	1:A:173:ASP:HB2	1.86	0.57
1:A:275:MET:HE2	1:A:276:PHE:CE1	2.39	0.57
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.04	0.57
1:A:737:GLU:CG	1:A:766:PHE:HE2	2.14	0.57
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.40	0.57
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.85	0.57
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.68	0.57
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.39	0.57
1:C:581:ASN:O	1:C:582:LYS:HB2	2.03	0.57
1:C:619:MET:HE1	1:C:633:ILE:CD1	2.34	0.57
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.21	0.57
1:E:508:LEU:HD22	1:E:520:THR:CB	2.35	0.57
2:F:445:GLU:OE1	2:F:494:ARG:NH2	2.37	0.57
1:A:669:TRP:CZ2	2:B:490:ARG:CD	2.87	0.57
1:C:91:GLN:O	1:C:93:THR:HG23	2.04	0.57
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.69	0.57
1:A:72:SER:HA	1:A:439:GLY:O	2.05	0.57
1:A:175:TYR:HD2	1:A:176:GLN:HE21	1.53	0.57
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.32	0.57
1:C:263:ASP:O	1:C:265:GLU:N	2.35	0.57
1:C:426:LEU:O	1:C:427:PHE:CD1	2.58	0.57
1:E:569:SER:O	1:E:720:ALA:HB1	2.05	0.57
1:A:584:ASN:HD21	1:A:694:HIS:H	1.52	0.57
1:C:565:GLU:CD	1:C:676:ILE:HB	2.30	0.57
2:D:465:ILE:HG12	2:D:466:TRP:CD1	2.39	0.57
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.19	0.57
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.35	0.57
1:E:303:LEU:O	1:E:304:GLU:HB2	2.05	0.57
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.86	0.57
1:C:167:LEU:CD1	1:C:167:LEU:N	2.68	0.56
1:C:200:VAL:O	1:C:200:VAL:HG13	2.05	0.56
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.40	0.56
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.70	0.56
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.86	0.56
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.35	0.56
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.70	0.56
1:A:429:LYS:CE	1:A:430:ALA:H	2.12	0.56
1:A:619:MET:HE1	1:A:633:ILE:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.40	0.56
1:E:186:ASN:OD1	1:E:186:ASN:C	2.48	0.56
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.21	0.56
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.87	0.56
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.38	0.56
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.87	0.56
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.87	0.56
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.05	0.56
1:A:710:ARG:HG3	1:A:710:ARG:NH1	2.21	0.56
1:C:345:PRO:O	1:C:349:GLN:HG3	2.05	0.56
2:F:582:LEU:HD21	2:F:587:ILE:HD11	1.88	0.56
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.41	0.56
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.87	0.56
1:E:279:ASP:O	1:E:283:ARG:HG2	2.06	0.56
1:A:631:ARG:NH2	2:F:406:ASP:OD2	2.38	0.56
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.36	0.56
1:C:571:SER:HB2	1:C:589:LYS:CG	2.35	0.56
1:E:43:ALA:HB1	1:E:78:TYR:O	2.06	0.56
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.87	0.56
1:C:529:ILE:HG22	1:C:530:VAL:N	2.20	0.56
1:C:750:LYS:O	1:C:751:ARG:HB2	2.05	0.56
1:E:132:ILE:HD12	1:E:132:ILE:N	2.20	0.56
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.56
1:C:4:PHE:CD1	1:C:8:GLN:OE1	2.48	0.56
1:C:348:ALA:O	1:C:352:ARG:HB2	2.05	0.56
1:C:494:GLU:OE1	1:C:494:GLU:CA	2.53	0.56
2:D:576:ARG:HG3	2:D:576:ARG:HH11	1.70	0.56
1:A:522:MET:HE3	1:A:526:GLY:O	2.06	0.56
1:C:222:ILE:HG22	1:C:241:MET:HB2	1.88	0.56
2:B:546:GLU:HG3	2:B:547:GLU:CG	2.22	0.56
2:B:563:ARG:HG3	2:B:563:ARG:HH11	1.71	0.56
1:C:234:GLY:O	1:C:235:VAL:CG2	2.50	0.56
1:C:381:TYR:O	1:C:398:GLY:HA3	2.05	0.56
1:C:478:MET:O	1:C:479:LYS:C	2.49	0.56
1:C:499:ASN:O	1:C:502:PRO:HD2	2.05	0.56
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.70	0.56
1:C:669:TRP:CD1	1:C:669:TRP:C	2.83	0.56
1:A:385:MET:HE2	1:A:460:ASP:HA	1.86	0.55
2:B:455:VAL:O	2:B:456:ARG:HD2	2.06	0.55
1:C:412:ARG:HG2	1:C:412:ARG:NH1	2.21	0.55
1:C:511:LEU:HD13	1:C:549:HIS:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:GLU:OE1	1:E:186:ASN:ND2	2.39	0.55
1:E:200:VAL:HG22	1:E:200:VAL:O	2.06	0.55
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.88	0.55
1:C:208:THR:HG22	1:C:341:HIS:CG	2.41	0.55
1:C:545:LEU:HA	1:C:549:HIS:HB2	1.88	0.55
1:E:493:VAL:CG1	1:E:494:GLU:N	2.69	0.55
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.88	0.55
1:C:637:GLY:O	1:C:642:GLY:HA3	2.06	0.55
1:A:401:PHE:CD2	1:A:478:MET:HE1	2.41	0.55
1:A:758:GLU:O	1:A:766:PHE:HD1	1.89	0.55
1:C:253:LYS:HE3	1:C:253:LYS:CA	2.22	0.55
1:C:546:GLU:HA	1:C:554:LEU:HG	1.89	0.55
1:C:646:VAL:HG13	1:C:688:ILE:CD1	2.36	0.55
1:A:45:ILE:HB	1:A:76:SER:HB2	1.87	0.55
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.89	0.55
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.88	0.55
2:B:471:ILE:HG21	2:B:501:VAL:HG21	1.88	0.55
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.87	0.55
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.36	0.55
1:C:243:ARG:HH12	1:C:257:TRP:CG	2.22	0.55
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.47	0.55
1:E:809:LEU:O	1:E:811:PRO:HD3	2.06	0.55
1:A:191:THR:O	1:A:763:THR:HG22	2.07	0.55
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.88	0.55
1:A:277:ILE:O	1:A:280:PRO:HD2	2.07	0.55
1:C:239:LYS:O	1:C:243:ARG:HG3	2.07	0.55
1:C:291:PHE:CE1	1:C:315:GLU:OE1	2.60	0.55
1:C:522:MET:HA	1:C:527:GLU:O	2.06	0.55
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.89	0.55
1:A:109:VAL:CG1	1:A:793:PHE:HE1	2.20	0.55
1:A:348:ALA:O	1:A:352:ARG:HB2	2.07	0.55
2:D:520:ALA:HB1	2:D:521:PRO:CD	2.36	0.55
1:E:348:ALA:O	1:E:352:ARG:HB2	2.07	0.55
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.88	0.55
1:A:344:SER:C	1:A:346:VAL:H	2.14	0.55
1:C:250:PHE:HB3	1:C:275:MET:HE1	1.87	0.55
1:C:311:GLU:OE2	1:C:322:VAL:CG1	2.54	0.55
1:C:619:MET:HE1	1:C:633:ILE:HD11	1.88	0.55
2:D:432:ARG:CZ	2:D:432:ARG:HA	2.37	0.55
1:E:385:MET:HE2	1:E:460:ASP:HA	1.89	0.55
1:E:432:GLN:HB2	1:E:457:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:LEU:N	1:C:549:HIS:CE1	2.75	0.55
1:C:524:GLU:C	1:C:526:GLY:H	2.15	0.55
1:C:552:VAL:HB	1:C:553:PRO:HD3	1.88	0.55
1:E:391:LYS:HG3	1:E:392:GLY:H	1.72	0.55
1:E:749:LYS:O	1:E:749:LYS:HG3	2.06	0.55
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.89	0.55
1:C:591:GLU:HG2	1:C:685:ARG:HG2	1.88	0.55
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.15	0.55
1:E:494:GLU:OE1	1:E:494:GLU:HA	2.07	0.55
1:A:365:ASN:O	1:A:369:ILE:HG12	2.07	0.54
1:E:240:MET:O	1:E:244:LEU:HG	2.06	0.54
1:E:786:GLN:N	1:E:786:GLN:CD	2.65	0.54
1:A:186:ASN:CG	1:A:201:GLN:HG2	2.32	0.54
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.22	0.54
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.36	0.54
1:C:411:VAL:HG12	1:C:412:ARG:N	2.22	0.54
1:C:581:ASN:HD21	1:C:704:GLN:HG3	1.71	0.54
1:E:709:MET:HE3	1:E:713:THR:OG1	2.07	0.54
2:B:522:GLU:CD	2:B:522:GLU:H	2.14	0.54
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.72	0.54
2:D:465:ILE:H	2:D:465:ILE:CD1	2.21	0.54
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.06	0.54
1:E:146:ALA:HA	1:E:151:ILE:HD12	1.89	0.54
1:A:478:MET:O	1:A:479:LYS:C	2.50	0.54
1:C:251:ASN:H	1:C:251:ASN:ND2	2.06	0.54
1:E:522:MET:HB2	2:F:490:ARG:HH12	1.71	0.54
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.90	0.54
1:A:391:LYS:HG3	1:A:392:GLY:H	1.72	0.54
2:D:574:ASP:OD1	2:D:575:PRO:HD2	2.07	0.54
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.43	0.54
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.43	0.54
1:C:243:ARG:HH11	1:C:257:TRP:CG	2.24	0.54
1:C:285:PHE:HE2	1:C:324:MET:SD	2.31	0.54
2:D:518:LEU:HD11	2:D:542:ILE:HD13	1.89	0.54
2:D:527:VAL:CG1	2:D:542:ILE:HD12	2.37	0.54
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.76	0.54
1:E:619:MET:HE1	1:E:633:ILE:HD11	1.90	0.54
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.38	0.54
1:C:565:GLU:OE1	1:C:676:ILE:HG12	2.07	0.54
1:E:39:LEU:CD1	1:E:334:LEU:HD12	2.37	0.54
1:E:545:LEU:O	1:E:550:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.48	0.54
1:E:740:VAL:HG21	1:E:766:PHE:HD1	1.72	0.54
1:C:226:ALA:CB	1:C:241:MET:HB3	2.38	0.54
2:D:507:SER:C	2:D:509:PRO:HD2	2.33	0.54
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.88	0.54
1:A:155:VAL:HG12	1:A:156:VAL:N	2.22	0.54
1:E:26:ALA:O	1:E:32:LYS:HD2	2.07	0.54
1:A:100:ILE:HD13	1:A:338:ILE:HG21	1.90	0.54
1:A:110:ASP:C	1:A:112:SER:H	2.16	0.54
1:A:799:ASP:OD1	1:A:800:HIS:HD2	1.91	0.54
1:C:459:ILE:HG21	1:C:463:LEU:HD12	1.89	0.54
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.38	0.54
1:E:114:GLU:O	1:E:117:ALA:HB3	2.08	0.54
1:E:556:ILE:N	1:E:556:ILE:HD12	2.23	0.54
1:C:311:GLU:C	1:C:314:LEU:HD13	2.34	0.53
1:C:530:VAL:O	1:C:538:LEU:HD11	2.08	0.53
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.35	0.53
1:E:284:LEU:HD11	1:E:303:LEU:CD1	2.37	0.53
1:E:524:GLU:HG3	1:E:669:TRP:CZ3	2.43	0.53
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.89	0.53
1:E:626:ASP:C	1:E:628:THR:N	2.63	0.53
1:A:25:ILE:CD1	1:A:125:ALA:HB1	2.38	0.53
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.89	0.53
1:A:155:VAL:CG1	1:A:156:VAL:N	2.72	0.53
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.89	0.53
1:C:200:VAL:O	1:C:200:VAL:CG1	2.56	0.53
1:E:39:LEU:HD11	1:E:334:LEU:HD12	1.89	0.53
1:E:501:LEU:HD23	1:E:501:LEU:C	2.33	0.53
2:B:546:GLU:CG	2:B:547:GLU:HG3	2.22	0.53
1:C:158:ASN:HD22	1:C:159:LYS:HG2	1.72	0.53
1:E:72:SER:HA	1:E:439:GLY:O	2.08	0.53
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.90	0.53
1:A:569:SER:O	1:A:720:ALA:HB1	2.08	0.53
1:C:43:ALA:HB1	1:C:78:TYR:O	2.07	0.53
1:E:411:VAL:HG12	1:E:412:ARG:N	2.22	0.53
1:E:693:LEU:HB3	1:E:700:ARG:HD2	1.91	0.53
1:A:200:VAL:O	1:A:200:VAL:HG13	2.08	0.53
1:A:644:ASN:ND2	1:A:684:VAL:HB	2.20	0.53
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.73	0.53
1:C:709:MET:HE3	1:C:713:THR:OG1	2.09	0.53
1:E:500:ASP:CG	1:E:552:VAL:HG11	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:HD2	1:A:176:GLN:NE2	2.07	0.53
1:C:148:GLY:HA2	1:C:760:ARG:HH22	1.70	0.53
1:C:263:ASP:OD1	1:C:264:ALA:N	2.42	0.53
1:E:289:MET:HE1	1:E:317:LYS:N	2.23	0.53
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.91	0.53
1:C:16:VAL:HG12	1:C:346:VAL:HG23	1.90	0.53
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.88	0.53
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.91	0.53
1:C:644:ASN:ND2	1:C:684:VAL:H	2.06	0.53
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.73	0.53
1:E:563:TYR:O	1:E:564:ARG:HD2	2.08	0.53
2:F:420:GLU:CD	2:F:420:GLU:N	2.67	0.53
1:A:507:GLY:HA2	1:A:510:ARG:HB2	1.89	0.53
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.24	0.53
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.89	0.53
1:A:306:VAL:HG23	1:A:306:VAL:O	2.09	0.53
2:B:490:ARG:HD2	2:B:492:ARG:CD	2.29	0.53
1:C:157:ILE:HD12	1:C:181:THR:HG21	1.89	0.53
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.91	0.53
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.44	0.53
2:F:429:LEU:O	2:F:434:TYR:HB2	2.09	0.53
1:A:43:ALA:HB1	1:A:78:TYR:O	2.10	0.52
1:A:71:LYS:HB3	1:A:386:VAL:HG23	1.90	0.52
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.89	0.52
2:B:440:HIS:O	2:B:499:LEU:HB2	2.09	0.52
2:B:462:LEU:O	2:B:467:ARG:NH2	2.42	0.52
2:B:484:ASP:OD2	2:B:494:ARG:HG2	2.09	0.52
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.08	0.52
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.45	0.52
2:F:462:LEU:O	2:F:467:ARG:NH2	2.42	0.52
1:A:230:ALA:O	1:A:235:VAL:CG2	2.57	0.52
1:A:750:LYS:O	1:A:751:ARG:HB2	2.09	0.52
1:C:410:LYS:HG3	1:C:429:LYS:C	2.35	0.52
2:D:584:PRO:HA	2:D:587:ILE:HD13	1.91	0.52
2:D:589:ASP:O	2:D:592:GLN:N	2.41	0.52
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.74	0.52
1:A:820:LEU:CD1	1:A:830:GLU:HG2	2.38	0.52
1:C:265:GLU:OE2	1:C:267:LYS:HG3	2.08	0.52
1:E:167:LEU:HD12	1:E:167:LEU:N	2.24	0.52
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.39	0.52
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.38	0.52
2:B:467:ARG:HG3	2:B:558:TRP:HD1	1.71	0.52
1:E:3:ALA:HA	1:E:46:ILE:O	2.09	0.52
1:E:707:PRO:O	1:E:711:ARG:HG3	2.10	0.52
1:A:681:MET:HE2	1:A:717:PHE:CD1	2.44	0.52
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.92	0.52
1:C:315:GLU:O	1:C:318:ALA:HB3	2.09	0.52
1:C:722:PRO:O	1:C:723:LYS:HD2	2.09	0.52
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.39	0.52
1:E:176:GLN:O	1:E:180:ARG:HG3	2.09	0.52
1:E:338:ILE:HA	1:E:342:LEU:HG	1.90	0.52
1:E:491:VAL:O	1:E:529:ILE:HG23	2.10	0.52
1:C:126:LEU:HD11	1:C:156:VAL:HG21	1.91	0.52
1:C:231:LYS:CG	1:C:232:LYS:N	2.72	0.52
1:C:539:GLU:HA	1:C:542:LEU:HD12	1.92	0.52
2:D:523:ALA:O	2:D:524:ALA:C	2.53	0.52
1:E:82:SER:O	1:E:86:VAL:HG23	2.09	0.52
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.92	0.52
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.91	0.52
1:C:710:ARG:NH1	1:C:714:TYR:CE2	2.78	0.52
1:E:9:MET:O	1:E:12:LEU:HB3	2.10	0.52
1:E:482:LYS:HB3	1:E:797:VAL:HG21	1.92	0.52
2:B:490:ARG:NE	2:B:492:ARG:HD2	2.24	0.52
1:C:525:SER:OG	1:C:527:GLU:HG2	2.10	0.52
1:A:707:PRO:O	1:A:711:ARG:HG3	2.10	0.52
1:E:80:GLU:HA	1:E:96:ASN:O	2.10	0.52
2:F:518:LEU:HD22	2:F:518:LEU:N	2.24	0.52
1:A:208:THR:HG22	1:A:341:HIS:CG	2.44	0.52
1:C:390:ASP:O	1:C:391:LYS:HB2	2.10	0.52
1:C:525:SER:OG	1:C:527:GLU:CG	2.58	0.52
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.44	0.52
1:C:284:LEU:O	1:C:288:ILE:HB	2.10	0.51
2:D:531:ILE:CD1	2:D:533:HIS:O	2.45	0.51
1:E:103:ILE:HD12	1:E:103:ILE:N	2.24	0.51
1:A:411:VAL:HG13	1:A:470:THR:O	2.11	0.51
1:E:284:LEU:HD23	1:E:299:LEU:CD2	2.40	0.51
2:F:520:ALA:HB1	2:F:522:GLU:OE2	2.10	0.51
1:C:371:ASN:O	1:C:372:CYS:C	2.53	0.51
1:C:542:LEU:O	1:C:545:LEU:HB3	2.10	0.51
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.91	0.51
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:CG	1:A:430:ALA:H	2.24	0.51
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.24	0.51
1:C:638:PRO:HB3	1:C:672:LYS:CG	2.37	0.51
2:D:520:ALA:HB3	2:D:522:GLU:CD	2.33	0.51
1:E:179:ALA:O	1:E:183:GLU:HB2	2.10	0.51
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.25	0.51
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.09	0.51
1:A:749:LYS:O	1:A:750:LYS:HD2	2.10	0.51
2:B:420:GLU:H	2:B:420:GLU:CD	2.19	0.51
1:C:117:ALA:CA	1:C:481:MET:HE1	2.40	0.51
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.10	0.51
1:C:521:TYR:O	1:C:529:ILE:HD12	2.11	0.51
1:C:546:GLU:N	1:C:554:LEU:HD12	2.26	0.51
1:A:284:LEU:HD11	1:A:303:LEU:CD1	2.41	0.51
2:B:450:ILE:HG23	2:B:455:VAL:HG23	1.91	0.51
2:B:507:SER:C	2:B:509:PRO:HD2	2.35	0.51
1:C:45:ILE:HG12	1:C:76:SER:C	2.36	0.51
1:C:521:TYR:CD1	1:C:529:ILE:HD13	2.46	0.51
1:C:589:LYS:HE3	1:C:689:LEU:HD11	1.92	0.51
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.58	0.51
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.76	0.51
1:C:256:LYS:HD3	1:C:257:TRP:H	1.75	0.51
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.93	0.51
1:E:254:THR:O	1:E:256:LYS:HG3	2.11	0.51
2:F:513:ARG:HH11	2:F:513:ARG:CB	2.21	0.51
2:B:453:GLY:O	2:B:456:ARG:HD3	2.11	0.51
1:C:262:THR:OG1	1:C:263:ASP:N	2.44	0.51
1:C:365:ASN:O	1:C:369:ILE:HG12	2.11	0.51
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.41	0.51
1:E:597:VAL:O	1:E:601:ILE:HG13	2.10	0.51
1:A:824:LYS:HE3	1:A:830:GLU:CD	2.35	0.50
1:C:314:LEU:O	1:C:319:LEU:HD13	2.11	0.50
2:D:505:ARG:C	2:D:507:SER:H	2.19	0.50
1:E:12:LEU:HG	1:E:99:LEU:HB2	1.93	0.50
1:E:536:LEU:O	1:E:539:GLU:N	2.44	0.50
1:E:620:ALA:HA	1:E:625:TRP:O	2.10	0.50
1:C:156:VAL:HG21	1:C:334:LEU:HD22	1.94	0.50
1:C:116:THR:HB	1:C:481:MET:HE3	1.93	0.50
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.76	0.50
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.75	0.50
2:F:524:ALA:O	2:F:528:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CD1	1:A:220:PHE:C	2.90	0.50
1:A:229:TYR:CZ	1:A:276:PHE:HB3	2.46	0.50
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.46	0.50
1:C:42:ARG:HG3	1:C:331:ALA:HB1	1.88	0.50
1:C:543:GLN:HA	1:C:546:GLU:HG3	1.92	0.50
1:E:488:VAL:HG23	1:E:489:VAL:CG2	2.42	0.50
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.45	0.50
1:A:200:VAL:O	1:A:200:VAL:CG1	2.59	0.50
1:A:627:VAL:O	1:A:631:ARG:HG3	2.12	0.50
2:B:404:GLY:HA2	1:C:626:ASP:CG	2.36	0.50
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.93	0.50
1:C:644:ASN:HD22	1:C:684:VAL:H	1.58	0.50
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.11	0.50
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.27	0.50
1:E:36:THR:O	1:E:40:VAL:HG23	2.11	0.50
1:E:496:LYS:HG3	1:E:496:LYS:O	2.11	0.50
2:F:546:GLU:CG	2:F:547:GLU:HG3	2.24	0.50
1:A:404:THR:HG22	1:A:449:PRO:CA	2.35	0.50
1:C:315:GLU:HA	1:C:319:LEU:CB	2.19	0.50
1:C:404:THR:HG22	1:C:449:PRO:CA	2.36	0.50
1:C:823:ARG:NH2	1:C:833:PRO:HD3	2.26	0.50
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.93	0.50
1:A:565:GLU:O	1:A:681:MET:HA	2.11	0.50
1:C:70:ILE:N	1:C:440:ARG:O	2.39	0.50
1:C:235:VAL:CG1	1:C:236:ASP:N	2.75	0.50
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.93	0.50
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.47	0.50
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.93	0.50
1:C:100:ILE:HD13	1:C:338:ILE:HG21	1.93	0.50
1:C:840:ASP:OD1	1:C:842:LEU:HD13	2.10	0.50
1:E:404:THR:HG22	1:E:449:PRO:CA	2.35	0.50
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.47	0.50
1:C:523:SER:O	1:C:526:GLY:N	2.42	0.50
2:D:455:VAL:HG12	2:D:456:ARG:N	2.27	0.50
1:E:237:LYS:HA	1:E:240:MET:CB	2.36	0.50
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.42	0.50
1:E:545:LEU:O	1:E:550:ALA:CB	2.60	0.50
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.77	0.50
2:B:488:ASP:OD1	2:B:489:ALA:N	2.45	0.49
1:C:809:LEU:O	1:C:811:PRO:HD3	2.11	0.49
1:E:565:GLU:O	1:E:681:MET:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:TRP:HZ2	2:B:490:ARG:HD2	1.73	0.49
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.94	0.49
2:D:465:ILE:HD13	2:D:465:ILE:N	2.26	0.49
1:A:824:LYS:CE	1:A:830:GLU:OE2	2.58	0.49
1:C:294:ASP:OD1	1:C:295:GLU:N	2.45	0.49
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.38	0.49
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.47	0.49
2:F:522:GLU:OE1	2:F:522:GLU:N	2.44	0.49
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.94	0.49
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.94	0.49
1:A:485:VAL:O	1:A:485:VAL:HG22	2.12	0.49
1:A:491:VAL:HG13	1:A:538:LEU:HD21	1.95	0.49
1:C:45:ILE:HB	1:C:76:SER:HB2	1.95	0.49
1:C:231:LYS:CE	1:C:232:LYS:HG3	2.19	0.49
1:C:265:GLU:CG	1:C:266:GLY:H	2.14	0.49
1:C:291:PHE:CZ	1:C:316:GLY:CA	2.95	0.49
1:C:681:MET:HE2	1:C:717:PHE:CD1	2.47	0.49
1:E:466:THR:HG22	1:E:467:GLY:N	2.27	0.49
1:E:633:ILE:HG12	1:E:647:ILE:CD1	2.42	0.49
1:A:760:ARG:O	1:A:761:PRO:C	2.56	0.49
1:C:552:VAL:HB	1:C:553:PRO:HD2	1.92	0.49
1:C:614:ALA:O	1:C:618:ILE:HG12	2.11	0.49
2:D:436:PHE:HB2	2:D:502:TYR:CE2	2.47	0.49
2:D:455:VAL:C	2:D:456:ARG:HG2	2.37	0.49
1:E:325:ARG:HG2	1:E:325:ARG:HH11	1.77	0.49
1:E:401:PHE:CD2	1:E:478:MET:HE1	2.48	0.49
1:E:736:PRO:O	1:E:737:GLU:C	2.55	0.49
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.94	0.49
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.94	0.49
2:B:500:ARG:O	2:B:566:VAL:HG13	2.12	0.49
2:B:552:LEU:N	2:B:552:LEU:CD1	2.72	0.49
1:E:503:LYS:CG	1:E:551:GLY:HA3	2.42	0.49
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.78	0.49
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.42	0.49
1:A:21:ASN:ND2	1:A:345:PRO:HG3	2.27	0.49
1:A:571:SER:HB2	1:A:589:LYS:CG	2.40	0.49
1:A:703:GLY:HA3	2:B:485:GLN:O	2.13	0.49
1:C:152:LYS:HD2	1:C:200:VAL:HG22	1.94	0.49
1:C:546:GLU:CA	1:C:554:LEU:HD11	2.35	0.49
1:C:626:ASP:C	1:C:628:THR:N	2.70	0.49
1:E:734:GLN:N	1:E:734:GLN:NE2	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:734:GLN:HE21	1:E:734:GLN:H	1.59	0.49
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.38	0.49
1:A:22:MET:HA	1:A:122:THR:HB	1.95	0.49
1:A:258:THR:CG2	1:A:259:ASN:N	2.73	0.49
2:B:523:ALA:O	2:B:524:ALA:C	2.54	0.49
1:C:647:ILE:HG13	1:C:685:ARG:NE	2.28	0.49
1:C:698:ILE:HG23	1:C:699:DDE:N	2.28	0.49
1:E:491:VAL:O	1:E:529:ILE:CG2	2.61	0.49
1:E:565:GLU:CD	1:E:676:ILE:HB	2.38	0.49
1:E:681:MET:HE2	1:E:717:PHE:CD1	2.48	0.49
1:A:222:ILE:HD13	1:A:222:ILE:N	2.27	0.49
1:C:240:MET:O	1:C:244:LEU:HG	2.13	0.49
1:C:509:LYS:O	1:C:513:LYS:HG3	2.13	0.49
1:C:543:GLN:HG2	1:C:544:ASP:OD1	2.13	0.49
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.93	0.49
1:A:433:ARG:HB2	1:A:457:VAL:HB	1.95	0.49
1:A:549:HIS:CD2	1:A:549:HIS:H	2.29	0.49
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.27	0.49
1:C:277:ILE:HG22	1:C:278:LEU:N	2.27	0.49
1:C:410:LYS:HG3	1:C:429:LYS:O	2.12	0.49
2:F:505:ARG:HG3	2:F:505:ARG:HH11	1.78	0.49
1:C:344:SER:C	1:C:346:VAL:N	2.70	0.48
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.95	0.48
1:E:40:VAL:C	1:E:42:ARG:H	2.21	0.48
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.47	0.48
1:E:626:ASP:O	1:E:628:THR:N	2.46	0.48
1:E:736:PRO:HB3	1:E:738:GLN:CD	2.38	0.48
1:A:709:MET:HE3	1:A:713:THR:OG1	2.14	0.48
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.27	0.48
1:C:212:GLY:HA2	1:C:218:TRP:CZ3	2.48	0.48
1:C:216:HIS:CE1	1:C:317:LYS:NZ	2.82	0.48
1:C:401:PHE:CD2	1:C:478:MET:HE1	2.48	0.48
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.93	0.48
2:D:477:LEU:HD13	2:D:551:ARG:NH1	2.28	0.48
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.42	0.48
1:E:546:GLU:OE2	1:E:554:LEU:N	2.34	0.48
1:A:9:MET:O	1:A:13:MET:HG3	2.13	0.48
1:A:10:ARG:NH1	1:A:14:ASP:OD2	2.46	0.48
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.96	0.48
1:A:739:ALA:C	1:A:741:GLY:N	2.70	0.48
1:C:116:THR:HB	1:C:481:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.13	0.48
1:C:268:PRO:O	1:C:269:LEU:HD23	2.13	0.48
1:C:647:ILE:HB	1:C:687:ASN:ND2	2.27	0.48
2:D:457:ALA:HB2	2:D:558:TRP:CE3	2.49	0.48
2:D:511:PHE:CE1	2:D:560:LEU:HD11	2.49	0.48
1:E:278:LEU:O	1:E:282:PHE:HB2	2.13	0.48
1:E:736:PRO:CB	1:E:738:GLN:CD	2.87	0.48
2:F:479:TYR:CD2	2:F:582:LEU:HD13	2.48	0.48
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.94	0.48
1:A:388:THR:HG21	1:A:395:TYR:CG	2.48	0.48
1:C:110:ASP:C	1:C:112:SER:H	2.20	0.48
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.96	0.48
1:C:746:VAL:HA	1:C:749:LYS:HG2	1.96	0.48
1:E:527:GLU:HB3	1:E:529:ILE:HD11	1.95	0.48
2:F:530:LEU:HD21	2:F:602:SER:O	2.13	0.48
1:A:486:SER:O	1:A:488:VAL:HG13	2.13	0.48
1:C:459:ILE:CD1	1:C:469:LEU:HD21	2.44	0.48
1:E:22:MET:HA	1:E:122:THR:HB	1.94	0.48
1:A:262:THR:HG22	1:A:267:LYS:O	2.13	0.48
1:C:385:MET:H	1:C:465:LYS:HD2	1.78	0.48
1:E:711:ARG:HD2	2:F:577:ASN:HD21	1.79	0.48
1:A:520:THR:HA	1:A:529:ILE:O	2.13	0.48
1:A:550:ALA:C	1:A:552:VAL:N	2.71	0.48
1:A:819:VAL:O	1:A:823:ARG:CG	2.50	0.48
1:C:284:LEU:HD11	1:C:303:LEU:CD1	2.44	0.48
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.49	0.48
1:E:386:VAL:HG11	1:E:437:MET:CE	2.43	0.48
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.96	0.48
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.22	0.48
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.49	0.48
1:A:597:VAL:O	1:A:601:ILE:HG13	2.14	0.48
2:B:441:GLY:O	2:B:442:THR:HB	2.13	0.48
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.95	0.48
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.48	0.48
1:A:381:TYR:OH	1:A:481:MET:HE2	2.14	0.48
1:A:797:VAL:HG22	1:A:798:PHE:N	2.29	0.48
1:C:436:LEU:HD23	1:C:454:ILE:CD1	2.44	0.48
1:E:17:THR:HB	1:E:92:LYS:O	2.13	0.48
1:E:141:THR:HA	1:E:144:ARG:CZ	2.44	0.48
1:E:324:MET:HE2	1:E:324:MET:HA	1.96	0.48
1:E:381:TYR:O	1:E:398:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:VAL:HG13	1:E:470:THR:O	2.14	0.48
1:E:546:GLU:HG3	1:E:554:LEU:HG	1.95	0.48
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.37	0.48
1:A:232:LYS:HD2	1:A:232:LYS:O	2.14	0.48
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.49	0.48
1:A:763:THR:HB	1:A:764:PRO:HD2	1.96	0.48
1:C:155:VAL:HG12	1:C:156:VAL:N	2.27	0.48
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.96	0.48
1:E:381:TYR:OH	1:E:481:MET:HE2	2.14	0.48
2:B:477:LEU:CD1	2:B:551:ARG:NH1	2.65	0.47
1:C:711:ARG:HD2	2:D:577:ASN:HD21	1.79	0.47
1:E:183:GLU:O	1:E:187:VAL:HG23	2.14	0.47
1:E:508:LEU:CD2	1:E:520:THR:CG2	2.92	0.47
1:E:782:GLY:HA2	1:E:785:ARG:HE	1.79	0.47
1:A:158:ASN:HD22	1:A:159:LYS:HG2	1.78	0.47
1:A:336:GLU:HG2	1:A:340:LEU:HD12	1.96	0.47
1:A:411:VAL:CG1	1:A:412:ARG:N	2.77	0.47
1:A:423:LYS:HG2	1:A:423:LYS:O	2.14	0.47
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.94	0.47
1:C:70:ILE:O	1:C:440:ARG:HG3	2.14	0.47
1:C:261:ASP:O	1:C:269:LEU:N	2.46	0.47
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.95	0.47
2:F:484:ASP:OD2	2:F:494:ARG:N	2.44	0.47
1:A:429:LYS:CG	1:A:430:ALA:N	2.78	0.47
1:A:634:TRP:O	1:A:635:CYS:HB3	2.14	0.47
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.49	0.47
1:E:729:PHE:CZ	1:E:774:VAL:HG22	2.49	0.47
1:A:129:VAL:HG13	1:A:134:GLY:C	2.39	0.47
2:B:438:GLY:HA3	2:B:471:ILE:CD1	2.41	0.47
1:E:69:THR:O	1:E:389:SER:N	2.47	0.47
1:E:77:LEU:CB	1:E:100:ILE:HB	2.44	0.47
1:E:335:LEU:O	1:E:339:VAL:HG23	2.14	0.47
1:E:500:ASP:OD2	1:E:552:VAL:HG11	2.15	0.47
1:E:836:GLN:HE21	1:E:836:GLN:N	2.06	0.47
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.96	0.47
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.43	0.47
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.38	0.47
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.44	0.47
1:C:224:GLN:O	1:C:228:ARG:HG3	2.14	0.47
1:C:565:GLU:O	1:C:681:MET:HA	2.14	0.47
1:C:411:VAL:HG11	1:C:469:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.44	0.47
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.96	0.47
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.29	0.47
1:A:162:ARG:HG3	1:A:166:GLU:OE2	2.14	0.47
1:A:219:ALA:HB3	1:A:330:ALA:HA	1.97	0.47
1:A:676:ILE:O	1:A:677:PHE:HB3	2.15	0.47
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.95	0.47
1:C:110:ASP:OD1	1:C:781:THR:CG2	2.55	0.47
1:C:587:TYR:CD2	1:C:690:ASP:HB3	2.49	0.47
1:C:636:PHE:CD1	1:C:645:LEU:HD21	2.50	0.47
2:D:531:ILE:HG13	2:D:533:HIS:H	1.78	0.47
1:E:150:ARG:CZ	1:E:355:GLN:OE1	2.62	0.47
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.15	0.47
1:E:284:LEU:HD13	1:E:324:MET:HE1	1.96	0.47
1:E:786:GLN:CD	1:E:786:GLN:H	2.23	0.47
2:F:440:HIS:O	2:F:499:LEU:HB2	2.14	0.47
1:A:175:TYR:CD2	1:A:176:GLN:NE2	2.83	0.47
1:A:461:GLN:NE2	1:A:462:PHE:CE2	2.83	0.47
1:C:291:PHE:CZ	1:C:316:GLY:HA2	2.49	0.47
1:C:636:PHE:CE1	1:C:645:LEU:HD21	2.50	0.47
2:D:542:ILE:HG23	2:D:542:ILE:O	2.13	0.47
1:E:546:GLU:HG3	1:E:554:LEU:N	2.30	0.47
1:A:129:VAL:HG13	1:A:134:GLY:O	2.14	0.47
1:A:231:LYS:C	1:A:233:PHE:H	2.23	0.47
1:A:360:PRO:C	1:A:362:ASP:H	2.22	0.47
2:B:508:LEU:N	2:B:509:PRO:CD	2.78	0.47
1:C:155:VAL:CG1	1:C:156:VAL:N	2.77	0.47
1:C:244:LEU:HD22	1:C:277:ILE:CD1	2.45	0.47
1:C:262:THR:HA	1:C:267:LYS:O	2.14	0.47
1:C:360:PRO:C	1:C:362:ASP:H	2.22	0.47
1:C:454:ILE:CG1	1:C:455:GLY:H	2.26	0.47
1:C:459:ILE:HD11	1:C:469:LEU:HD21	1.96	0.47
1:A:676:ILE:HG22	1:A:677:PHE:CD2	2.50	0.47
2:B:524:ALA:O	2:B:528:GLU:HG3	2.15	0.47
1:C:82:SER:O	1:C:86:VAL:HG23	2.15	0.47
1:C:279:ASP:HB3	1:C:280:PRO:CD	2.43	0.47
1:C:306:VAL:HG23	1:C:306:VAL:O	2.14	0.47
1:C:490:GLN:O	1:C:491:VAL:CG1	2.62	0.47
1:C:729:PHE:O	1:C:771:TYR:HA	2.15	0.47
1:C:836:GLN:HE21	1:C:836:GLN:N	2.06	0.47
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:646:VAL:HG13	1:E:688:ILE:CD1	2.45	0.47
1:A:258:THR:HG22	1:A:260:LYS:HG2	1.95	0.46
1:A:386:VAL:HG11	1:A:437:MET:CE	2.45	0.46
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.97	0.46
2:B:563:ARG:HG3	2:B:563:ARG:NH1	2.30	0.46
1:C:130:ASP:OD2	1:C:132:ILE:HG22	2.15	0.46
1:E:626:ASP:O	1:E:627:VAL:C	2.57	0.46
2:D:446:ALA:O	2:D:447:ALA:C	2.56	0.46
1:E:4:PHE:CE2	1:E:45:ILE:HD12	2.50	0.46
2:F:488:ASP:OD2	2:F:492:ARG:CD	2.61	0.46
1:A:823:ARG:NH1	1:A:831:GLU:O	2.48	0.46
1:C:211:PHE:N	1:C:211:PHE:CD2	2.84	0.46
1:C:222:ILE:N	1:C:222:ILE:HD13	2.30	0.46
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.51	0.46
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.97	0.46
1:C:700:ARG:HE	1:C:700:ARG:HB2	1.42	0.46
1:E:581:ASN:ND2	1:E:699:DDE:O	2.49	0.46
1:A:296:ILE:N	1:A:297:PRO:HD2	2.30	0.46
1:A:512:SER:HA	1:A:518:VAL:CG1	2.46	0.46
1:A:619:MET:HE1	1:A:633:ILE:HD12	1.97	0.46
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.97	0.46
1:C:338:ILE:O	1:C:342:LEU:HB2	2.16	0.46
1:E:736:PRO:O	1:E:738:GLN:N	2.48	0.46
1:E:750:LYS:O	1:E:751:ARG:HB2	2.15	0.46
2:F:505:ARG:HG3	2:F:505:ARG:NH1	2.31	0.46
1:C:3:ALA:HA	1:C:46:ILE:HG22	1.98	0.46
1:C:523:SER:O	1:C:524:GLU:C	2.58	0.46
2:D:575:PRO:HG2	2:D:576:ARG:N	2.31	0.46
1:E:149:GLU:O	1:E:150:ARG:HB2	2.15	0.46
1:E:296:ILE:O	1:E:300:LEU:HB2	2.15	0.46
1:A:80:GLU:C	1:A:81:MET:HG2	2.40	0.46
1:A:249:PHE:CD2	1:A:249:PHE:N	2.83	0.46
2:B:415:GLN:O	2:B:416:ASN:HB2	2.16	0.46
2:B:577:ASN:C	2:B:577:ASN:HD22	2.23	0.46
1:C:317:LYS:HD2	1:C:317:LYS:HA	1.53	0.46
1:C:760:ARG:O	1:C:761:PRO:C	2.59	0.46
1:E:143:LEU:O	1:E:147:LEU:HG	2.15	0.46
1:E:237:LYS:O	1:E:241:MET:HG2	2.14	0.46
1:E:493:VAL:CG1	1:E:494:GLU:H	2.29	0.46
1:E:646:VAL:HG13	1:E:688:ILE:HD13	1.97	0.46
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:510:GLY:O	2:F:512:TYR:CD1	2.69	0.46
1:A:186:ASN:OD1	1:A:201:GLN:HG2	2.15	0.46
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.49	0.46
2:B:507:SER:C	2:B:509:PRO:CD	2.88	0.46
1:E:150:ARG:NH1	1:E:351:TYR:O	2.49	0.46
1:E:181:THR:O	1:E:185:VAL:HG23	2.16	0.46
1:E:500:ASP:OD1	1:E:503:LYS:HD2	2.16	0.46
1:E:552:VAL:CB	1:E:553:PRO:CD	2.93	0.46
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.81	0.46
1:A:2:VAL:CG2	1:A:3:ALA:N	2.79	0.46
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.95	0.46
1:C:335:LEU:O	1:C:339:VAL:HG23	2.16	0.46
1:C:497:ASN:HD22	1:C:497:ASN:H	1.60	0.46
1:C:552:VAL:CB	1:C:553:PRO:CD	2.84	0.46
1:C:707:PRO:O	1:C:711:ARG:HG3	2.16	0.46
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.31	0.46
1:E:74:ALA:O	1:E:439:GLY:CA	2.59	0.46
1:E:735:CYS:SG	1:E:736:PRO:HD2	2.56	0.46
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.96	0.46
1:A:371:ASN:O	1:A:372:CYS:C	2.58	0.46
1:A:694:HIS:HD2	1:A:696:ASP:N	1.95	0.46
1:A:700:ARG:HE	1:A:700:ARG:HB2	1.42	0.46
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.97	0.46
1:E:454:ILE:CG1	1:E:455:GLY:N	2.79	0.46
1:E:536:LEU:O	1:E:539:GLU:HB3	2.15	0.46
1:E:732:GLU:N	1:E:795:GLN:O	2.45	0.46
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.81	0.46
1:C:314:LEU:HD21	1:C:322:VAL:HG21	1.97	0.46
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.46	0.46
2:D:495:ASN:OD1	2:D:495:ASN:N	2.48	0.46
2:D:576:ARG:HG3	2:D:576:ARG:NH1	2.29	0.46
2:D:588:PRO:O	2:D:591:GLU:N	2.46	0.46
1:E:262:THR:HG21	1:E:266:GLY:HA2	1.97	0.46
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.64	0.45
1:E:32:LYS:NZ	1:E:106:PRO:O	2.49	0.45
1:E:202:VAL:HG23	1:E:202:VAL:O	2.16	0.45
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.97	0.45
1:A:240:MET:O	1:A:240:MET:HE3	2.16	0.45
2:B:495:ASN:N	2:B:495:ASN:ND2	2.60	0.45
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.16	0.45
1:C:685:ARG:NE	1:C:687:ASN:HD21	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.98	0.45
1:E:221:THR:HG21	1:E:336:GLU:OE1	2.15	0.45
1:E:433:ARG:HB3	1:E:457:VAL:HB	1.98	0.45
1:E:606:ILE:HD12	1:E:619:MET:CG	2.46	0.45
1:E:760:ARG:O	1:E:761:PRO:C	2.59	0.45
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.63	0.45
1:A:727:PRO:HB3	1:A:801:TRP:CZ3	2.51	0.45
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.97	0.45
2:B:546:GLU:HG2	2:B:550:GLY:HA3	1.99	0.45
2:D:552:LEU:N	2:D:552:LEU:CD1	2.78	0.45
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.85	0.45
1:C:186:ASN:OD1	1:C:202:VAL:N	2.48	0.45
1:E:109:VAL:HG12	1:E:109:VAL:O	2.16	0.45
1:E:276:PHE:C	1:E:277:ILE:HD13	2.41	0.45
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.51	0.45
1:C:228:ARG:C	1:C:230:ALA:H	2.25	0.45
1:C:411:VAL:CG1	1:C:412:ARG:N	2.80	0.45
1:C:454:ILE:CG1	1:C:455:GLY:N	2.79	0.45
1:C:523:SER:HG	1:C:527:GLU:HB2	1.76	0.45
2:D:518:LEU:N	2:D:518:LEU:HD22	2.31	0.45
2:D:518:LEU:HD22	2:D:518:LEU:H	1.81	0.45
1:E:360:PRO:C	1:E:362:ASP:H	2.24	0.45
1:E:823:ARG:NH1	1:E:823:ARG:HG2	2.30	0.45
1:E:840:ASP:OD1	1:E:842:LEU:HD13	2.15	0.45
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.46	0.45
1:C:705:ILE:HD12	1:C:705:ILE:N	2.31	0.45
1:E:414:GLN:HB3	1:E:418:TYR:CD2	2.51	0.45
2:F:457:ALA:HB2	2:F:558:TRP:CE3	2.52	0.45
1:A:167:LEU:HD12	1:A:167:LEU:N	2.32	0.45
1:A:317:LYS:O	1:A:318:ALA:C	2.59	0.45
1:C:249:PHE:N	1:C:249:PHE:CD2	2.85	0.45
1:C:253:LYS:HG3	1:C:253:LYS:O	2.17	0.45
1:C:374:PRO:O	1:C:404:THR:HG23	2.17	0.45
1:C:485:VAL:O	1:C:485:VAL:HG22	2.15	0.45
1:C:546:GLU:HB2	1:C:547:HIS:H	1.36	0.45
1:C:656:LEU:O	1:C:659:ILE:HG12	2.16	0.45
1:E:89:ILE:HG22	1:E:91:GLN:HB3	1.99	0.45
1:E:591:GLU:HG2	1:E:685:ARG:CG	2.45	0.45
1:A:620:ALA:HA	1:A:625:TRP:O	2.17	0.45
1:A:627:VAL:HG11	2:F:406:ASP:OD1	2.16	0.45
2:B:551:ARG:NH1	2:B:551:ARG:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:LYS:CD	1:C:257:TRP:H	2.29	0.45
1:C:294:ASP:OD1	1:C:295:GLU:HG3	2.17	0.45
1:C:296:ILE:N	1:C:297:PRO:HD2	2.32	0.45
1:C:588:LEU:HD12	1:C:588:LEU:O	2.17	0.45
2:D:447:ALA:O	2:D:448:GLN:C	2.60	0.45
1:E:274:ASN:O	1:E:279:ASP:HB2	2.16	0.45
1:E:505:VAL:O	1:E:505:VAL:HG12	2.17	0.45
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.45
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.52	0.45
1:A:228:ARG:C	1:A:230:ALA:H	2.24	0.45
1:A:231:LYS:C	1:A:233:PHE:N	2.75	0.45
1:A:258:THR:HG22	1:A:260:LYS:H	1.82	0.45
1:A:581:ASN:O	1:A:582:LYS:CB	2.65	0.45
1:A:607:ASN:HB3	1:A:610:ASP:OD2	2.17	0.45
1:C:152:LYS:CD	1:C:200:VAL:HG22	2.45	0.45
1:E:314:LEU:CD1	1:E:322:VAL:HG21	2.47	0.45
1:E:379:MET:SD	1:E:470:THR:HG22	2.57	0.45
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.52	0.45
2:F:552:LEU:HD12	2:F:552:LEU:H	1.80	0.45
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.81	0.45
1:A:626:ASP:C	1:A:628:THR:N	2.72	0.45
1:C:186:ASN:HB3	1:C:201:GLN:HE21	1.82	0.45
1:C:262:THR:CA	1:C:269:LEU:HG	2.47	0.45
1:C:288:ILE:HD13	1:C:319:LEU:HG	1.98	0.45
1:C:495:VAL:CG1	1:C:554:LEU:HD23	2.46	0.45
1:C:807:ASP:OD2	1:C:808:PRO:HD2	2.17	0.45
2:D:546:GLU:OE1	2:D:551:ARG:NH1	2.50	0.45
2:F:406:ASP:O	2:F:416:ASN:ND2	2.42	0.45
2:F:498:LEU:O	2:F:569:SER:HB3	2.17	0.45
1:A:840:ASP:OD1	1:A:842:LEU:HD13	2.17	0.44
1:C:588:LEU:C	1:C:588:LEU:CD1	2.87	0.44
2:D:437:VAL:HG11	2:D:511:PHE:CE2	2.51	0.44
2:D:474:ASP:O	2:D:475:PRO:C	2.57	0.44
1:E:495:VAL:HG12	1:E:553:PRO:O	2.16	0.44
1:E:536:LEU:O	1:E:537:HIS:C	2.59	0.44
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.80	0.44
1:A:607:ASN:HB3	1:A:610:ASP:CG	2.42	0.44
1:A:736:PRO:O	1:A:737:GLU:C	2.61	0.44
1:C:216:HIS:NE2	1:C:317:LYS:NZ	2.65	0.44
1:C:468:THR:C	1:C:469:LEU:HD12	2.42	0.44
1:C:522:MET:SD	1:C:528:HIS:HA	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:ILE:HB	1:C:687:ASN:HD22	1.83	0.44
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.99	0.44
1:E:218:TRP:HA	1:E:328:LEU:O	2.17	0.44
1:E:305:ILE:HG21	1:E:323:VAL:HG13	1.99	0.44
1:E:524:GLU:C	1:E:526:GLY:H	2.25	0.44
2:B:558:TRP:O	2:B:562:GLU:HG3	2.17	0.44
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.99	0.44
1:C:220:PHE:CD1	1:C:220:PHE:C	2.95	0.44
1:E:167:LEU:H	1:E:167:LEU:CD1	2.29	0.44
1:E:672:LYS:HG3	1:E:673:GLU:HG3	2.00	0.44
1:E:730:LEU:C	1:E:730:LEU:CD2	2.90	0.44
1:A:211:PHE:O	1:A:219:ALA:HA	2.17	0.44
1:C:42:ARG:HG3	1:C:331:ALA:HB2	1.93	0.44
1:C:391:LYS:HE3	1:C:393:ARG:CG	2.45	0.44
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.99	0.44
1:C:646:VAL:HG13	1:C:688:ILE:HD13	1.97	0.44
2:D:522:GLU:OE1	2:D:522:GLU:N	2.46	0.44
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.15	0.44
2:F:433:GLY:O	2:F:505:ARG:HB2	2.16	0.44
1:A:82:SER:O	1:A:86:VAL:HG23	2.17	0.44
1:A:226:ALA:CB	1:A:241:MET:HB3	2.47	0.44
1:C:411:VAL:HG13	1:C:470:THR:O	2.17	0.44
2:D:538:ARG:HD2	2:D:538:ARG:HA	1.63	0.44
1:E:371:ASN:O	1:E:372:CYS:C	2.60	0.44
1:E:594:ASP:HB2	1:E:597:VAL:HG23	1.99	0.44
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.82	0.44
1:E:736:PRO:C	1:E:738:GLN:N	2.76	0.44
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.48	0.44
2:B:410:SER:OG	2:B:412:ARG:CB	2.64	0.44
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.99	0.44
2:F:474:ASP:O	2:F:475:PRO:C	2.61	0.44
1:A:155:VAL:HG21	1:A:185:VAL:HG11	2.00	0.44
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.83	0.44
1:C:504:LEU:C	1:C:506:GLU:N	2.76	0.44
1:E:496:LYS:HB2	1:E:555:LYS:NZ	2.27	0.44
1:E:721:ASP:C	1:E:721:ASP:OD1	2.60	0.44
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.52	0.44
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.99	0.44
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.99	0.44
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.99	0.44
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:727:PRO:HG2	1:C:774:VAL:HB	2.00	0.44
1:C:729:PHE:CE2	1:C:796:MET:HE3	2.52	0.44
2:D:551:ARG:HG3	2:D:551:ARG:NH1	2.33	0.44
1:E:145:GLN:O	1:E:146:ALA:C	2.60	0.44
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.53	0.44
1:E:533:THR:H	1:E:537:HIS:CD2	2.35	0.44
1:E:619:MET:HE1	1:E:633:ILE:HD12	1.98	0.44
2:B:495:ASN:ND2	2:B:495:ASN:H	2.16	0.44
2:D:508:LEU:HD23	2:D:508:LEU:HA	1.74	0.44
2:D:518:LEU:HD21	2:D:544:GLY:HA3	2.00	0.44
1:E:9:MET:HE2	1:E:438:MET:SD	2.58	0.44
1:A:13:MET:SD	1:A:436:LEU:HD21	2.58	0.43
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.99	0.43
1:A:730:LEU:C	1:A:730:LEU:CD2	2.91	0.43
1:A:733:ILE:O	1:A:767:THR:HA	2.18	0.43
2:B:523:ALA:O	2:B:527:VAL:HG23	2.18	0.43
1:C:600:ALA:HB1	1:C:606:ILE:HG12	1.98	0.43
2:D:588:PRO:O	2:D:589:ASP:C	2.60	0.43
1:E:37:ASP:O	1:E:41:GLN:HG3	2.18	0.43
1:E:89:ILE:O	1:E:91:GLN:N	2.50	0.43
1:E:303:LEU:O	1:E:304:GLU:CB	2.66	0.43
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.52	0.43
1:A:45:ILE:HD12	1:A:76:SER:CB	2.38	0.43
1:A:211:PHE:CD2	1:A:211:PHE:N	2.86	0.43
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.49	0.43
1:C:5:THR:OG1	1:C:8:GLN:HG3	2.18	0.43
1:C:395:TYR:CE1	1:C:457:VAL:HG13	2.53	0.43
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.52	0.43
1:C:546:GLU:N	1:C:554:LEU:CD1	2.80	0.43
2:D:528:GLU:HA	2:D:531:ILE:HG12	2.00	0.43
2:D:575:PRO:HG2	2:D:576:ARG:H	1.82	0.43
2:D:589:ASP:O	2:D:590:LYS:C	2.60	0.43
1:E:500:ASP:CG	1:E:552:VAL:HB	2.43	0.43
2:F:427:ARG:CG	2:F:428:GLN:N	2.80	0.43
2:F:521:PRO:O	2:F:524:ALA:HB3	2.18	0.43
1:A:132:ILE:HD12	1:A:162:ARG:NE	2.33	0.43
1:A:494:GLU:HB3	1:A:555:LYS:HB3	1.99	0.43
1:A:495:VAL:HG13	1:A:504:LEU:HD22	2.00	0.43
2:B:446:ALA:O	2:B:447:ALA:C	2.60	0.43
2:B:470:TYR:CD1	2:B:470:TYR:N	2.86	0.43
1:C:141:THR:O	1:C:144:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ASN:C	1:C:501:LEU:H	2.25	0.43
1:A:237:LYS:O	1:A:238:ALA:C	2.60	0.43
1:A:823:ARG:NH1	1:A:829:LYS:O	2.51	0.43
2:D:547:GLU:O	2:D:548:GLU:C	2.61	0.43
2:D:552:LEU:HD12	2:D:552:LEU:H	1.83	0.43
1:E:360:PRO:HB2	1:E:363:ASP:HB2	2.00	0.43
1:E:411:VAL:CG1	1:E:412:ARG:N	2.81	0.43
1:E:495:VAL:HA	1:E:554:LEU:HD23	2.00	0.43
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.82	0.43
2:F:546:GLU:CG	2:F:547:GLU:N	2.81	0.43
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.99	0.43
1:C:291:PHE:HZ	1:C:316:GLY:CA	2.31	0.43
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.54	0.43
2:F:538:ARG:HA	2:F:538:ARG:HD2	1.60	0.43
2:F:546:GLU:OE1	2:F:551:ARG:N	2.46	0.43
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.83	0.43
1:C:132:ILE:CG2	1:C:133:GLU:N	2.79	0.43
1:E:508:LEU:HD21	1:E:530:VAL:CG2	2.48	0.43
1:E:700:ARG:O	1:E:705:ILE:HD13	2.17	0.43
2:F:427:ARG:O	2:F:431:GLU:HG3	2.19	0.43
1:A:693:LEU:HB3	1:A:700:ARG:HD2	2.01	0.43
1:A:711:ARG:NH1	1:A:838:TYR:HA	2.33	0.43
1:C:186:ASN:CB	1:C:201:GLN:HG2	2.49	0.43
1:C:360:PRO:HB2	1:C:363:ASP:HB2	2.00	0.43
1:C:607:ASN:HB3	1:C:610:ASP:OD2	2.18	0.43
1:E:13:MET:SD	1:E:436:LEU:HD21	2.58	0.43
1:E:79:SER:O	1:E:98:PHE:N	2.52	0.43
1:E:454:ILE:CG1	1:E:455:GLY:H	2.26	0.43
1:E:740:VAL:O	1:E:740:VAL:HG12	2.18	0.43
1:A:273:PHE:HD1	1:A:277:ILE:HD12	1.81	0.43
1:C:385:MET:HE2	1:C:460:ASP:HA	2.00	0.43
1:E:220:PHE:HB3	1:E:328:LEU:HD13	2.00	0.43
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.18	0.43
1:E:429:LYS:HG3	1:E:462:PHE:CE1	2.54	0.43
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.53	0.43
1:E:690:ASP:OD1	1:E:691:VAL:N	2.50	0.43
2:F:505:ARG:C	2:F:507:SER:H	2.27	0.43
1:A:488:VAL:HG23	1:A:489:VAL:HG23	2.00	0.43
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.89	0.43
1:A:727:PRO:HG2	1:A:774:VAL:HB	2.00	0.43
2:B:457:ALA:C	2:B:458:ARG:HG3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:MET:O	1:C:13:MET:HG3	2.19	0.43
1:C:194:ASP:HB2	1:C:197:LEU:HG	2.01	0.43
1:E:129:VAL:HG12	1:E:130:ASP:N	2.33	0.43
1:E:711:ARG:HD2	2:F:577:ASN:ND2	2.33	0.43
1:A:228:ARG:C	1:A:230:ALA:N	2.76	0.43
1:A:466:THR:CG2	1:A:467:GLY:N	2.82	0.43
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.48	0.43
1:C:534:GLY:O	1:C:535:GLU:C	2.62	0.43
1:C:595:GLU:OE2	1:C:682:ARG:NH1	2.51	0.43
1:C:606:ILE:HD12	1:C:619:MET:CG	2.49	0.43
1:E:118:ALA:O	1:E:122:THR:HG23	2.19	0.43
1:E:189:VAL:O	1:E:193:ALA:CB	2.67	0.43
1:E:600:ALA:HB1	1:E:606:ILE:HG12	1.99	0.43
2:F:446:ALA:O	2:F:447:ALA:C	2.62	0.43
1:A:26:ALA:CB	1:A:128:VAL:HB	2.48	0.42
1:C:22:MET:HA	1:C:122:THR:HB	2.00	0.42
1:C:277:ILE:O	1:C:281:ILE:HD12	2.18	0.42
1:C:490:GLN:C	1:C:491:VAL:HG13	2.44	0.42
1:A:103:ILE:HD13	1:A:121:VAL:HG23	2.00	0.42
1:C:91:GLN:HE22	1:C:343:PRO:HA	1.84	0.42
1:C:521:TYR:CE2	1:C:529:ILE:HB	2.54	0.42
2:D:577:ASN:O	2:D:578:VAL:C	2.60	0.42
1:E:490:GLN:O	1:E:491:VAL:HG13	2.19	0.42
1:E:626:ASP:C	1:E:628:THR:H	2.26	0.42
2:B:552:LEU:H	2:B:552:LEU:CD1	2.26	0.42
1:C:161:ASP:CG	1:C:162:ARG:N	2.77	0.42
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.72	0.42
1:C:637:GLY:C	1:C:642:GLY:HA3	2.43	0.42
2:D:435:VAL:HB	2:D:505:ARG:HH11	1.84	0.42
2:D:505:ARG:C	2:D:507:SER:N	2.78	0.42
1:E:522:MET:HB2	2:F:490:ARG:NH1	2.34	0.42
1:E:553:PRO:C	1:E:554:LEU:HG	2.44	0.42
1:E:705:ILE:N	1:E:705:ILE:HD12	2.35	0.42
1:E:722:PRO:O	1:E:723:LYS:HD2	2.19	0.42
2:F:510:GLY:O	2:F:512:TYR:CE1	2.72	0.42
1:A:580:PRO:HD2	1:A:704:GLN:OE1	2.19	0.42
1:A:824:LYS:CE	1:A:830:GLU:CD	2.92	0.42
1:C:536:LEU:CD1	1:C:537:HIS:N	2.73	0.42
2:D:518:LEU:HD21	2:D:544:GLY:CA	2.49	0.42
1:E:211:PHE:CD2	1:E:211:PHE:N	2.87	0.42
1:E:418:TYR:HB3	1:E:477:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:778:PHE:N	1:E:778:PHE:CD2	2.87	0.42
2:F:464:ALA:O	2:F:467:ARG:HB3	2.19	0.42
2:F:498:LEU:HD23	2:F:498:LEU:HA	1.74	0.42
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.55	0.42
2:B:439:TYR:O	2:B:471:ILE:HB	2.20	0.42
1:C:742:GLY:O	1:C:745:SER:HB3	2.20	0.42
2:D:503:VAL:HG12	2:D:564:THR:HG22	2.01	0.42
1:E:43:ALA:O	1:E:77:LEU:HA	2.19	0.42
1:E:68:ILE:HG23	1:E:390:ASP:HB2	2.01	0.42
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.55	0.42
1:E:406:LYS:HB3	1:E:447:ASP:HB3	2.01	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
1:A:4:PHE:HD1	1:A:8:GLN:CD	2.28	0.42
1:A:167:LEU:HD12	1:A:167:LEU:H	1.83	0.42
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.55	0.42
1:A:518:VAL:HG22	1:A:519:LEU:N	2.35	0.42
1:A:676:ILE:HG22	1:A:677:PHE:HD2	1.85	0.42
1:C:108:HIS:HD2	1:C:110:ASP:H	1.66	0.42
1:C:131:THR:HG21	1:C:163:ALA:HB2	2.01	0.42
1:C:150:ARG:HG3	1:C:355:GLN:OE1	2.19	0.42
1:C:501:LEU:C	1:C:501:LEU:CD2	2.90	0.42
2:D:455:VAL:O	2:D:456:ARG:CD	2.68	0.42
2:D:531:ILE:HG13	2:D:532:GLY:N	2.33	0.42
2:D:561:ALA:HA	2:D:564:THR:HG23	2.01	0.42
1:E:235:VAL:HG11	1:E:239:LYS:HD3	2.02	0.42
1:E:295:GLU:O	1:E:296:ILE:C	2.62	0.42
1:E:296:ILE:N	1:E:297:PRO:HD2	2.35	0.42
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.50	0.42
1:A:397:PHE:HD1	1:A:437:MET:HG3	1.84	0.42
1:A:495:VAL:HA	1:A:554:LEU:HD23	2.01	0.42
1:A:565:GLU:HG2	1:A:676:ILE:HD12	2.02	0.42
1:A:644:ASN:ND2	1:A:684:VAL:H	2.17	0.42
1:C:116:THR:C	1:C:481:MET:HE1	2.44	0.42
1:C:419:VAL:O	1:C:420:PRO:C	2.63	0.42
1:C:487:PRO:HB3	1:C:531:ALA:HB1	2.02	0.42
1:C:495:VAL:HG12	1:C:554:LEU:HD23	2.01	0.42
1:C:626:ASP:O	1:C:628:THR:N	2.53	0.42
1:C:659:ILE:HD13	1:C:693:LEU:HD21	2.02	0.42
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.48	0.42
1:E:306:VAL:HG23	1:E:306:VAL:O	2.19	0.42
1:E:500:ASP:CB	1:E:552:VAL:CG1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:479:TYR:CE2	2:F:582:LEU:HD13	2.54	0.42
1:A:106:PRO:CG	1:A:114:GLU:HG3	2.48	0.42
1:A:392:GLY:CA	1:A:513:LYS:HE2	2.43	0.42
1:C:547:HIS:CD2	1:C:548:ASP:OD1	2.72	0.42
1:C:799:ASP:OD1	1:C:800:HIS:HD2	2.03	0.42
2:D:467:ARG:HG3	2:D:558:TRP:CD1	2.54	0.42
1:E:295:GLU:C	1:E:297:PRO:HD2	2.45	0.42
1:E:412:ARG:HH12	1:E:428:ILE:CD1	2.32	0.42
1:E:500:ASP:HB3	1:E:552:VAL:CG1	2.50	0.42
1:E:773:PRO:HB2	1:E:776:GLU:HB2	2.01	0.42
2:F:437:VAL:HG11	2:F:511:PHE:CE2	2.54	0.42
1:A:406:LYS:O	1:A:409:GLN:HB3	2.19	0.42
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.31	0.42
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.84	0.42
1:C:288:ILE:HG21	1:C:319:LEU:HG	2.01	0.42
1:C:576:LEU:HD12	1:C:577:SER:N	2.34	0.42
1:E:485:VAL:HG22	1:E:485:VAL:O	2.20	0.42
1:E:500:ASP:OD1	1:E:503:LYS:CD	2.68	0.42
2:F:472:ALA:HB2	3:F:702:P34:HAE	2.02	0.42
1:A:782:GLY:O	1:A:785:ARG:HB3	2.20	0.42
1:C:211:PHE:O	1:C:219:ALA:HA	2.19	0.42
1:C:258:THR:HG22	1:C:260:LYS:N	2.29	0.42
1:C:529:ILE:HG22	1:C:530:VAL:H	1.83	0.42
1:C:536:LEU:HD12	1:C:537:HIS:H	1.75	0.42
1:C:536:LEU:O	1:C:537:HIS:C	2.62	0.42
1:E:9:MET:HE3	1:E:436:LEU:HD13	2.01	0.42
1:E:25:ILE:HG23	1:E:142:VAL:HG11	2.02	0.42
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.55	0.42
1:E:171:LYS:HZ1	1:E:283:ARG:NH2	2.18	0.42
1:A:153:PRO:HD2	1:A:200:VAL:HG13	2.01	0.41
1:C:251:ASN:HB2	1:C:254:THR:HG1	1.83	0.41
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.55	0.41
1:E:736:PRO:CB	1:E:738:GLN:HG2	2.49	0.41
1:A:161:ASP:CG	1:A:162:ARG:N	2.79	0.41
1:A:550:ALA:C	1:A:552:VAL:H	2.28	0.41
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.55	0.41
2:B:522:GLU:OE1	2:B:522:GLU:N	2.41	0.41
1:C:521:TYR:O	1:C:529:ILE:CD1	2.67	0.41
1:E:25:ILE:HG23	1:E:142:VAL:CG1	2.49	0.41
1:E:123:ASP:O	1:E:151:ILE:HG23	2.20	0.41
2:F:486:GLU:C	2:F:493:ILE:HD11	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG22	1:A:91:GLN:HG2	2.02	0.41
1:C:277:ILE:O	1:C:280:PRO:HD2	2.20	0.41
1:C:406:LYS:O	1:C:409:GLN:HB3	2.20	0.41
1:C:751:ARG:NH2	1:C:776:GLU:HG3	2.35	0.41
1:E:307:LEU:HB2	1:E:312:LYS:CD	2.50	0.41
1:C:276:PHE:C	1:C:277:ILE:HD12	2.45	0.41
1:C:466:THR:HG22	1:C:467:GLY:N	2.35	0.41
2:D:507:SER:C	2:D:509:PRO:CD	2.94	0.41
1:E:143:LEU:O	1:E:144:ARG:C	2.62	0.41
1:E:188:ILE:HG23	1:E:192:TYR:CD2	2.56	0.41
1:E:759:GLN:HB2	1:E:766:PHE:HE2	1.81	0.41
1:A:160:VAL:O	1:A:163:ALA:HB3	2.21	0.41
1:A:521:TYR:CZ	1:A:529:ILE:HD12	2.55	0.41
1:A:737:GLU:CG	1:A:766:PHE:CD2	3.03	0.41
1:C:37:ASP:O	1:C:40:VAL:N	2.53	0.41
1:C:70:ILE:HG12	1:C:440:ARG:C	2.45	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.55	0.41
1:E:46:ILE:HD12	1:E:46:ILE:H	1.85	0.41
1:E:736:PRO:CB	1:E:738:GLN:CG	2.95	0.41
2:F:495:ASN:OD1	2:F:495:ASN:N	2.54	0.41
1:A:112:SER:HB3	1:A:794:PRO:O	2.19	0.41
1:A:137:VAL:O	1:A:140:GLU:HB3	2.20	0.41
1:A:374:PRO:O	1:A:404:THR:HG23	2.21	0.41
2:B:520:ALA:HB1	2:B:522:GLU:OE1	2.21	0.41
1:C:132:ILE:CG2	1:C:133:GLU:H	2.33	0.41
1:C:493:VAL:HG21	1:C:545:LEU:CD2	2.46	0.41
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.79	0.41
1:C:581:ASN:O	1:C:582:LYS:CB	2.68	0.41
1:C:613:LYS:HD3	1:C:631:ARG:NH1	2.35	0.41
1:E:126:LEU:HD11	1:E:156:VAL:HG23	2.02	0.41
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.85	0.41
1:E:374:PRO:O	1:E:404:THR:HG23	2.21	0.41
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.81	0.41
1:A:2:VAL:HG22	1:A:3:ALA:H	1.84	0.41
1:A:111:PHE:O	1:A:112:SER:C	2.63	0.41
1:A:254:THR:O	1:A:255:LYS:HB2	2.20	0.41
1:A:485:VAL:O	1:A:487:PRO:HD3	2.21	0.41
1:A:656:LEU:O	1:A:659:ILE:HG12	2.21	0.41
1:A:735:CYS:HG	1:A:739:ALA:HB3	1.85	0.41
2:B:450:ILE:HG23	2:B:455:VAL:CG2	2.51	0.41
1:C:111:PHE:O	1:C:112:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:HA	1:C:240:MET:HB3	2.03	0.41
1:C:459:ILE:HA	1:C:462:PHE:HD2	1.84	0.41
1:C:563:TYR:O	1:C:564:ARG:CD	2.67	0.41
1:C:619:MET:HE1	1:C:633:ILE:HD12	2.03	0.41
2:F:467:ARG:HG3	2:F:558:TRP:HD1	1.84	0.41
1:A:550:ALA:O	1:A:552:VAL:N	2.54	0.41
1:A:636:PHE:CD1	1:A:645:LEU:HD21	2.56	0.41
1:C:18:ASN:HB3	1:C:97:SER:O	2.21	0.41
1:C:268:PRO:C	1:C:269:LEU:HD23	2.45	0.41
1:C:459:ILE:O	1:C:462:PHE:N	2.46	0.41
1:C:560:VAL:HG12	1:C:561:VAL:N	2.35	0.41
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.03	0.41
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.56	0.41
1:A:258:THR:CG2	1:A:259:ASN:H	2.29	0.41
1:A:391:LYS:O	1:A:513:LYS:HE2	2.20	0.41
1:A:578:LYS:HG2	1:A:840:ASP:OD2	2.20	0.41
1:A:637:GLY:O	1:A:642:GLY:HA3	2.21	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.88	0.41
2:B:482:ALA:O	2:B:483:GLN:HB3	2.20	0.41
2:B:490:ARG:CG	2:B:492:ARG:HD2	2.51	0.41
2:B:499:LEU:HB3	2:B:566:VAL:HG11	2.03	0.41
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.85	0.41
1:C:70:ILE:HG12	1:C:440:ARG:O	2.21	0.41
1:C:279:ASP:O	1:C:280:PRO:C	2.64	0.41
1:C:308:LYS:HB2	1:C:311:GLU:OE1	2.20	0.41
1:C:436:LEU:O	1:C:442:VAL:HA	2.21	0.41
1:C:630:ALA:O	1:C:633:ILE:HG13	2.21	0.41
1:C:698:ILE:CG2	1:C:699:DDE:N	2.83	0.41
1:C:807:ASP:OD2	1:C:808:PRO:N	2.54	0.41
1:C:823:ARG:HH11	1:C:828:MET:HB2	1.86	0.41
2:D:531:ILE:CG1	2:D:532:GLY:N	2.84	0.41
1:E:89:ILE:C	1:E:91:GLN:N	2.68	0.41
1:E:186:ASN:CG	1:E:201:GLN:NE2	2.74	0.41
1:E:488:VAL:HG23	1:E:489:VAL:HG22	2.03	0.41
1:E:710:ARG:HH11	1:E:710:ARG:CG	2.30	0.41
1:E:733:ILE:O	1:E:767:THR:HA	2.21	0.41
1:E:759:GLN:HB2	1:E:766:PHE:CD2	2.56	0.41
2:F:531:ILE:HG22	2:F:533:HIS:H	1.85	0.41
1:A:228:ARG:HG2	1:A:229:TYR:N	2.36	0.41
1:A:589:LYS:HE3	1:A:689:LEU:HD11	2.03	0.41
2:B:471:ILE:HD12	2:B:472:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:MET:O	1:C:96:ASN:HB3	2.21	0.41
1:C:388:THR:HG21	1:C:395:TYR:CG	2.56	0.41
1:C:506:GLU:HG3	1:C:510:ARG:HE	1.86	0.41
1:C:530:VAL:O	1:C:538:LEU:HD13	2.18	0.41
1:E:511:LEU:HA	1:E:549:HIS:CE1	2.56	0.41
1:E:737:GLU:HG3	1:E:766:PHE:CZ	2.56	0.41
1:A:488:VAL:HG23	1:A:489:VAL:CG2	2.51	0.40
2:B:529:ARG:NH1	2:B:604:PRO:HG3	2.36	0.40
1:C:637:GLY:O	1:C:642:GLY:CA	2.69	0.40
1:C:749:LYS:C	1:C:750:LYS:HD2	2.46	0.40
1:C:773:PRO:O	1:C:774:VAL:C	2.65	0.40
1:E:145:GLN:CD	1:E:793:PHE:CE1	2.99	0.40
1:E:744:TYR:O	1:E:748:ASN:ND2	2.53	0.40
2:F:486:GLU:HB2	2:F:487:PRO:HD2	2.03	0.40
1:A:169:VAL:CG2	1:A:173:ASP:HB2	2.51	0.40
1:A:677:PHE:CD2	1:A:677:PHE:N	2.89	0.40
1:C:71:LYS:HB3	1:C:386:VAL:HG23	2.03	0.40
1:C:156:VAL:HG21	1:C:334:LEU:CD2	2.51	0.40
1:C:484:SER:CB	1:C:797:VAL:HG23	2.48	0.40
1:C:730:LEU:CD2	1:C:730:LEU:C	2.94	0.40
1:C:807:ASP:OD2	1:C:808:PRO:CD	2.69	0.40
1:E:419:VAL:O	1:E:420:PRO:C	2.63	0.40
1:E:498:ALA:C	1:E:500:ASP:N	2.78	0.40
1:A:522:MET:HA	1:A:527:GLU:O	2.21	0.40
1:A:590:ALA:HA	1:A:685:ARG:O	2.21	0.40
2:B:486:GLU:HB3	2:B:487:PRO:HD2	2.03	0.40
2:B:542:ILE:O	2:B:542:ILE:HG23	2.22	0.40
1:C:226:ALA:HB2	1:C:241:MET:HB3	2.03	0.40
1:C:291:PHE:CE1	1:C:316:GLY:N	2.89	0.40
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.56	0.40
1:E:156:VAL:CG2	1:E:337:MET:HE1	2.51	0.40
1:E:241:MET:HA	1:E:244:LEU:HD12	2.03	0.40
1:E:360:PRO:C	1:E:362:ASP:N	2.79	0.40
1:E:587:TYR:CD2	1:E:690:ASP:HB3	2.57	0.40
1:E:637:GLY:O	1:E:642:GLY:HA3	2.21	0.40
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.92	0.40
1:A:515:ASP:OD1	1:A:516:PRO:HD2	2.21	0.40
1:C:360:PRO:C	1:C:362:ASP:N	2.79	0.40
1:C:386:VAL:HG11	1:C:437:MET:CE	2.51	0.40
1:C:591:GLU:HG2	1:C:685:ARG:CG	2.49	0.40
2:D:488:ASP:CG	2:D:489:ALA:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:527:VAL:HG22	2:D:542:ILE:HD12	2.03	0.40
1:E:739:ALA:HB1	1:E:788:THR:HB	2.03	0.40
2:F:571:ILE:CD1	2:F:587:ILE:HD12	2.51	0.40
1:A:319:LEU:O	1:A:320:LEU:C	2.62	0.40
1:A:390:ASP:O	1:A:391:LYS:CB	2.67	0.40
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.56	0.40
1:A:490:GLN:HA	1:A:530:VAL:O	2.21	0.40
1:A:576:LEU:HD12	1:A:577:SER:N	2.36	0.40
1:C:581:ASN:ND2	1:C:699:DDE:O	2.55	0.40
1:C:733:ILE:O	1:C:767:THR:HA	2.21	0.40
2:D:555:ILE:O	2:D:555:ILE:HG22	2.21	0.40
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.51	0.40
1:E:92:LYS:HB2	1:E:92:LYS:HE3	1.72	0.40
1:E:158:ASN:HA	1:E:212:GLY:O	2.21	0.40
1:E:188:ILE:HG23	1:E:192:TYR:CE2	2.57	0.40
1:E:325:ARG:HG2	1:E:325:ARG:NH1	2.36	0.40
1:E:337:MET:O	1:E:338:ILE:C	2.63	0.40
1:E:823:ARG:NH2	1:E:833:PRO:HD3	2.35	0.40
2:F:560:LEU:O	2:F:563:ARG:HB2	2.21	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%)	729 (89%)	76 (9%)	13 (2%)	7	27
1	C	818/842 (97%)	726 (89%)	75 (9%)	17 (2%)	5	20
1	E	818/842 (97%)	714 (87%)	87 (11%)	17 (2%)	5	20
2	B	205/207 (99%)	183 (89%)	21 (10%)	1 (0%)	24	55
2	D	205/207 (99%)	177 (86%)	24 (12%)	4 (2%)	6	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	205/207 (99%)	180 (88%)	24 (12%)	1 (0%)	24	55
All	All	3069/3147 (98%)	2709 (88%)	307 (10%)	53 (2%)	7	25

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	498	ALA
1	A	761	PRO
2	B	518	LEU
1	C	235	VAL
1	C	264	ALA
1	C	546	GLU
1	C	761	PRO
1	E	112	SER
1	E	761	PRO
1	A	309	GLY
1	A	677	PHE
1	C	112	SER
1	C	309	GLY
1	E	90	LYS
1	E	233	PHE
1	E	304	GLU
1	E	479	LYS
1	A	390	ASP
1	A	479	LYS
1	C	266	GLY
1	C	479	LYS
1	C	525	SER
1	C	677	PHE
2	D	491	GLY
2	D	506	SER
1	E	390	ASP
1	E	558	PRO
1	E	621	ASP
1	A	111	PHE
1	A	446	ASP
1	A	460	ASP
1	C	265	GLU
1	E	446	ASP
1	E	677	PHE
1	C	446	ASP

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Mol	Chain	Res	Type
1	E	302	LYS
1	E	737	GLU
2	F	404	GLY
1	C	329	PRO
2	D	604	PRO
1	E	460	ASP
1	C	493	VAL
1	C	558	PRO
1	C	743	ILE
1	E	743	ILE
1	A	329	PRO
1	C	491	VAL
1	E	309	GLY
1	E	338	ILE
2	D	404	GLY
1	A	743	ILE
1	A	764	PRO

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%)	649 (93%)	50 (7%)	13	39
1	C	699/714 (98%)	626 (90%)	73 (10%)	7	22
1	E	699/714 (98%)	661 (95%)	38 (5%)	20	51
2	B	161/162 (99%)	147 (91%)	14 (9%)	9	30
2	D	161/162 (99%)	143 (89%)	18 (11%)	6	19
2	F	161/162 (99%)	145 (90%)	16 (10%)	7	24
All	All	2580/2628 (98%)	2371 (92%)	209 (8%)	11	33

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP

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Mol	Chain	Res	Type
1	A	36	THR
1	A	46	ILE
1	A	68	ILE
1	A	81	MET
1	A	83	ASP
1	A	91	GLN
1	A	94	ASP
1	A	113	SER
1	A	151	ILE
1	A	152	LYS
1	A	154	VAL
1	A	183	GLU
1	A	195	GLU
1	A	200	VAL
1	A	222	ILE
1	A	228	ARG
1	A	236	ASP
1	A	262	THR
1	A	275	MET
1	A	295	GLU
1	A	300	LEU
1	A	308	LYS
1	A	347	THR
1	A	362	ASP
1	A	406	LYS
1	A	429	LYS
1	A	432	GLN
1	A	460	ASP
1	A	489	VAL
1	A	536	LEU
1	A	597	VAL
1	A	599	LEU
1	A	625	TRP
1	A	698	ILE
1	A	710	ARG
1	A	718	LEU
1	A	723	LYS
1	A	724	ILE
1	A	730	LEU
1	A	734	GLN
1	A	737	GLU
1	A	738	GLN

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Mol	Chain	Res	Type
1	A	761	PRO
1	A	767	THR
1	A	775	ASN
1	A	785	ARG
1	A	795	GLN
1	A	804	LEU
1	A	836	GLN
2	B	422	LEU
2	B	456	ARG
2	B	467	ARG
2	B	470	TYR
2	B	488	ASP
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	552	LEU
2	B	559	PRO
2	B	560	LEU
1	C	14	ASP
1	C	36	THR
1	C	46	ILE
1	C	68	ILE
1	C	81	MET
1	C	83	ASP
1	C	84	GLU
1	C	91	GLN
1	C	94	ASP
1	C	105	SER
1	C	112	SER
1	C	113	SER
1	C	154	VAL
1	C	159	LYS
1	C	164	LEU
1	C	167	LEU
1	C	170	SER
1	C	172	GLU
1	C	183	GLU
1	C	195	GLU
1	C	200	VAL

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Mol	Chain	Res	Type
1	C	222	ILE
1	C	231	LYS
1	C	235	VAL
1	C	242	ASP
1	C	253	LYS
1	C	256	LYS
1	C	269	LEU
1	C	299	LEU
1	C	300	LEU
1	C	312	LYS
1	C	317	LYS
1	C	320	LEU
1	C	324	MET
1	C	347	THR
1	C	432	GLN
1	C	440	ARG
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	493	VAL
1	C	494	GLU
1	C	495	VAL
1	C	497	ASN
1	C	499	ASN
1	C	500	ASP
1	C	501	LEU
1	C	512	SER
1	C	524	GLU
1	C	528	HIS
1	C	529	ILE
1	C	543	GLN
1	C	546	GLU
1	C	549	HIS
1	C	556	ILE
1	C	582	LYS
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	724	ILE

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Mol	Chain	Res	Type
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	820	LEU
1	C	836	GLN
1	C	837	GLU
2	D	410	SER
2	D	411	THR
2	D	422	LEU
2	D	427	ARG
2	D	465	ILE
2	D	483	GLN
2	D	486	GLU
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	538	ARG
2	D	540	ASP
2	D	542	ILE
2	D	547	GLU
2	D	551	ARG
2	D	552	LEU
2	D	560	LEU
2	D	602	SER
1	E	46	ILE
1	E	94	ASP
1	E	161	ASP
1	E	183	GLU
1	E	186	ASN
1	E	195	GLU
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	352	ARG
1	E	362	ASP

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Mol	Chain	Res	Type
1	E	440	ARG
1	E	460	ASP
1	E	489	VAL
1	E	524	GLU
1	E	527	GLU
1	E	597	VAL
1	E	599	LEU
1	E	625	TRP
1	E	677	PHE
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	723	LYS
1	E	724	ILE
1	E	730	LEU
1	E	734	GLN
1	E	738	GLN
1	E	749	LYS
1	E	761	PRO
1	E	767	THR
1	E	775	ASN
1	E	786	GLN
1	E	836	GLN
1	E	837	GLU
2	F	411	THR
2	F	422	LEU
2	F	437	VAL
2	F	467	ARG
2	F	494	ARG
2	F	498	LEU
2	F	513	ARG
2	F	522	GLU
2	F	538	ARG
2	F	540	ASP
2	F	547	GLU
2	F	548	GLU
2	F	552	LEU
2	F	560	LEU
2	F	599	ASP
2	F	602	SER

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

Mol	Chain	Res	Type
1	A	27	HIS
1	A	91	GLN
1	A	138	GLN
1	A	176	GLN
1	A	201	GLN
1	A	274	ASN
1	A	371	ASN
1	A	414	GLN
1	A	528	HIS
1	A	537	HIS
1	A	549	HIS
1	A	581	ASN
1	A	584	ASN
1	A	644	ASN
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	800	HIS
1	A	836	GLN
2	B	424	GLN
2	B	428	GLN
2	B	460	GLN
2	B	495	ASN
2	B	577	ASN
1	C	27	HIS
1	C	91	GLN
1	C	138	GLN
1	C	201	GLN
1	C	251	ASN
1	C	341	HIS
1	C	414	GLN
1	C	490	GLN
1	C	497	ASN
1	C	537	HIS
1	C	547	HIS
1	C	581	ASN
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	649	GLN

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Mol	Chain	Res	Type
1	C	687	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
2	D	448	GLN
2	D	577	ASN
1	E	27	HIS
1	E	91	GLN
1	E	138	GLN
1	E	201	GLN
1	E	259	ASN
1	E	290	ASN
1	E	371	ASN
1	E	414	GLN
1	E	476	HIS
1	E	528	HIS
1	E	537	HIS
1	E	549	HIS
1	E	581	ASN
1	E	584	ASN
1	E	644	ASN
1	E	649	GLN
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	428	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	A	699	1	9,10,21	0.59	0	8,12,30	0.98	0
1	DDE	C	699	1	9,10,21	0.54	0	8,12,30	1.02	0
1	DDE	E	699	1	9,10,21	0.49	0	8,12,30	1.00	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	A	699	1	-	0/5/6/23	0/1/1/1
1	DDE	C	699	1	-	0/5/6/23	0/1/1/1
1	DDE	E	699	1	-	0/5/6/23	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	3	0
1	E	699	DDE	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands 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$
3	P34	F	702	-	24,24,24	2.48	15 (62%)	33,34,34	2.03	7 (21%)
3	P34	D	701	-	24,24,24	2.23	14 (58%)	33,34,34	1.98	8 (24%)
3	P34	B	700	-	24,24,24	2.44	13 (54%)	33,34,34	2.03	9 (27%)

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	P34	F	702	-	-	3/8/8/8	0/3/3/3
3	P34	D	701	-	-	2/8/8/8	0/3/3/3
3	P34	B	700	-	-	4/8/8/8	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	702	P34	CAS-CAT	4.27	1.47	1.40
3	B	700	P34	CAG-CAP	3.97	1.46	1.39
3	B	700	P34	CAU-CAR	3.96	1.46	1.40
3	F	702	P34	CAU-CAR	3.81	1.45	1.40
3	D	701	P34	CAS-CAT	3.64	1.46	1.40
3	B	700	P34	CAS-CAT	3.48	1.46	1.40
3	F	702	P34	CAG-CAP	3.43	1.45	1.39
3	F	702	P34	CAH-CAS	3.42	1.45	1.39
3	F	702	P34	CAG-CAJ	3.41	1.44	1.38
3	D	701	P34	CAU-CAR	3.29	1.45	1.40
3	B	700	P34	CAQ-NAN	3.23	1.42	1.36
3	B	700	P34	CAK-CAU	3.20	1.45	1.39
3	D	701	P34	CAP-NAM	-3.19	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	P34	CAG-CAJ	3.11	1.43	1.38
3	D	701	P34	CAG-CAP	3.11	1.44	1.39
3	F	702	P34	CAP-NAM	-3.06	1.35	1.41
3	B	700	P34	CAS-CAQ	-3.02	1.42	1.47
3	F	702	P34	CAJ-CAR	2.97	1.44	1.39
3	F	702	P34	CAI-CAT	2.93	1.44	1.40
3	D	701	P34	CAQ-NAN	2.92	1.41	1.36
3	D	701	P34	CAH-CAS	2.91	1.44	1.39
3	B	700	P34	CAJ-CAR	2.78	1.44	1.39
3	F	702	P34	CAK-CAU	2.76	1.44	1.39
3	D	701	P34	CAI-CAT	2.70	1.44	1.40
3	B	700	P34	CAP-NAM	-2.68	1.36	1.41
3	D	701	P34	CAS-CAQ	-2.65	1.42	1.47
3	F	702	P34	CAK-CAP	2.61	1.43	1.39
3	F	702	P34	CAS-CAQ	-2.59	1.42	1.47
3	B	700	P34	CAI-CAT	2.56	1.43	1.40
3	B	700	P34	CA-C	2.56	1.57	1.52
3	D	701	P34	CAT-CAU	-2.54	1.42	1.47
3	F	702	P34	CA-C	2.51	1.57	1.52
3	B	700	P34	CAH-CAS	2.50	1.43	1.39
3	D	701	P34	CAE-CAH	2.40	1.43	1.38
3	F	702	P34	CAQ-NAN	2.39	1.40	1.36
3	B	700	P34	CAE-CAH	2.37	1.43	1.38
3	D	701	P34	CAK-CAU	2.34	1.43	1.39
3	D	701	P34	CAF-CAI	2.27	1.42	1.38
3	F	702	P34	CAF-CAI	2.18	1.42	1.38
3	D	701	P34	CA-C	2.10	1.56	1.52
3	F	702	P34	CAE-CAH	2.06	1.42	1.38
3	D	701	P34	CAJ-CAR	2.03	1.43	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	P34	CAP-NAM-C	6.08	138.28	127.52
3	B	700	P34	CAP-NAM-C	5.89	137.95	127.52
3	D	701	P34	CAP-NAM-C	5.52	137.30	127.52
3	F	702	P34	CA-C-NAM	5.24	123.94	114.23
3	D	701	P34	CA-C-NAM	4.82	123.15	114.23
3	B	700	P34	CA-C-NAM	4.55	122.65	114.23
3	F	702	P34	O-C-NAM	-4.50	115.58	123.64
3	B	700	P34	O-C-NAM	-4.24	116.04	123.64
3	D	701	P34	O-C-NAM	-4.00	116.47	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	P34	CAS-CAQ-NAN	3.81	120.35	115.56
3	D	701	P34	CAS-CAQ-NAN	3.49	119.96	115.56
3	F	702	P34	CAS-CAQ-NAN	3.46	119.91	115.56
3	B	700	P34	CAG-CAP-NAM	2.99	130.45	120.41
3	B	700	P34	CAK-CAP-NAM	-2.91	110.69	120.13
3	F	702	P34	CAK-CAP-NAM	-2.82	110.95	120.13
3	F	702	P34	CAG-CAP-NAM	2.80	129.81	120.41
3	D	701	P34	CAG-CAP-NAM	2.77	129.73	120.41
3	D	701	P34	CAK-CAP-NAM	-2.63	111.59	120.13
3	D	701	P34	CAJ-CAR-CAU	2.59	123.00	119.99
3	D	701	P34	CAR-NAN-CAQ	-2.58	121.17	124.85
3	B	700	P34	CAJ-CAR-CAU	2.27	122.62	119.99
3	B	700	P34	CAR-NAN-CAQ	-2.26	121.62	124.85
3	F	702	P34	CAJ-CAR-CAU	2.21	122.56	119.99
3	B	700	P34	CAB-N-CA	2.02	113.69	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	P34	C-CA-N-CAA
3	B	700	P34	C-CA-N-CAB
3	B	700	P34	CA-C-NAM-CAP
3	D	701	P34	CA-C-NAM-CAP
3	F	702	P34	C-CA-N-CAB
3	F	702	P34	CA-C-NAM-CAP
3	B	700	P34	O-C-NAM-CAP
3	D	701	P34	O-C-NAM-CAP
3	F	702	P34	O-C-NAM-CAP

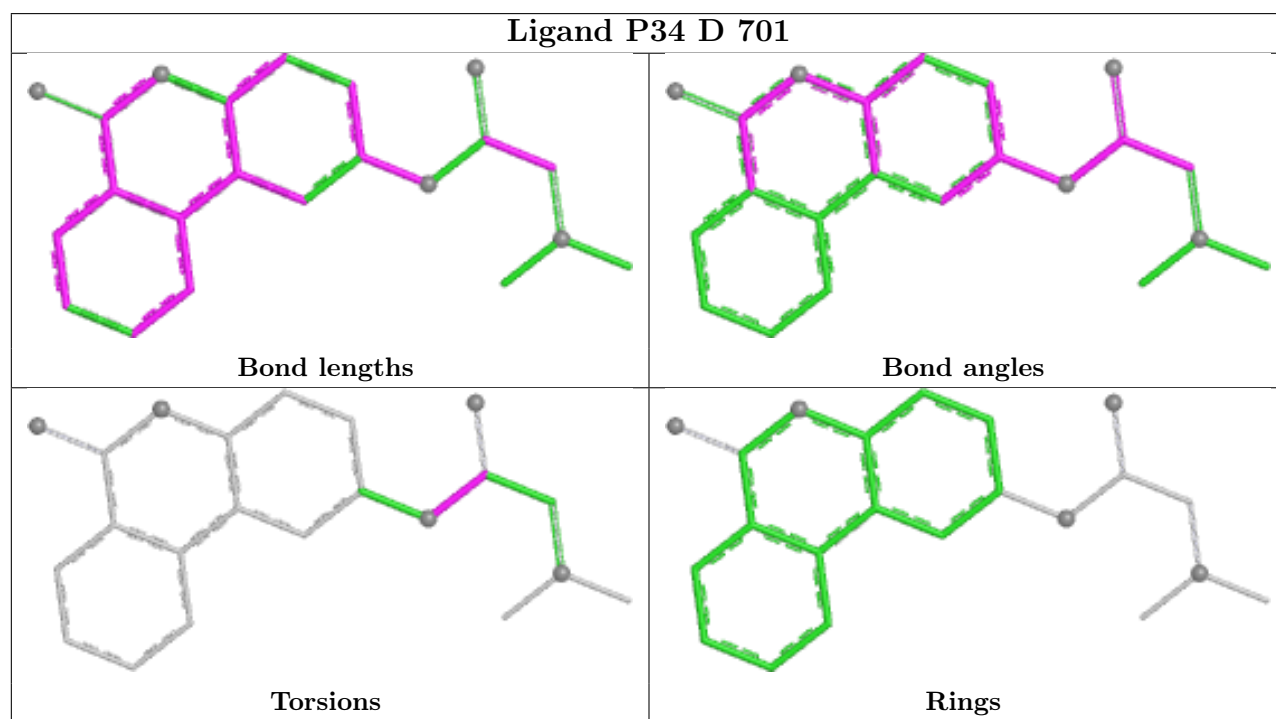
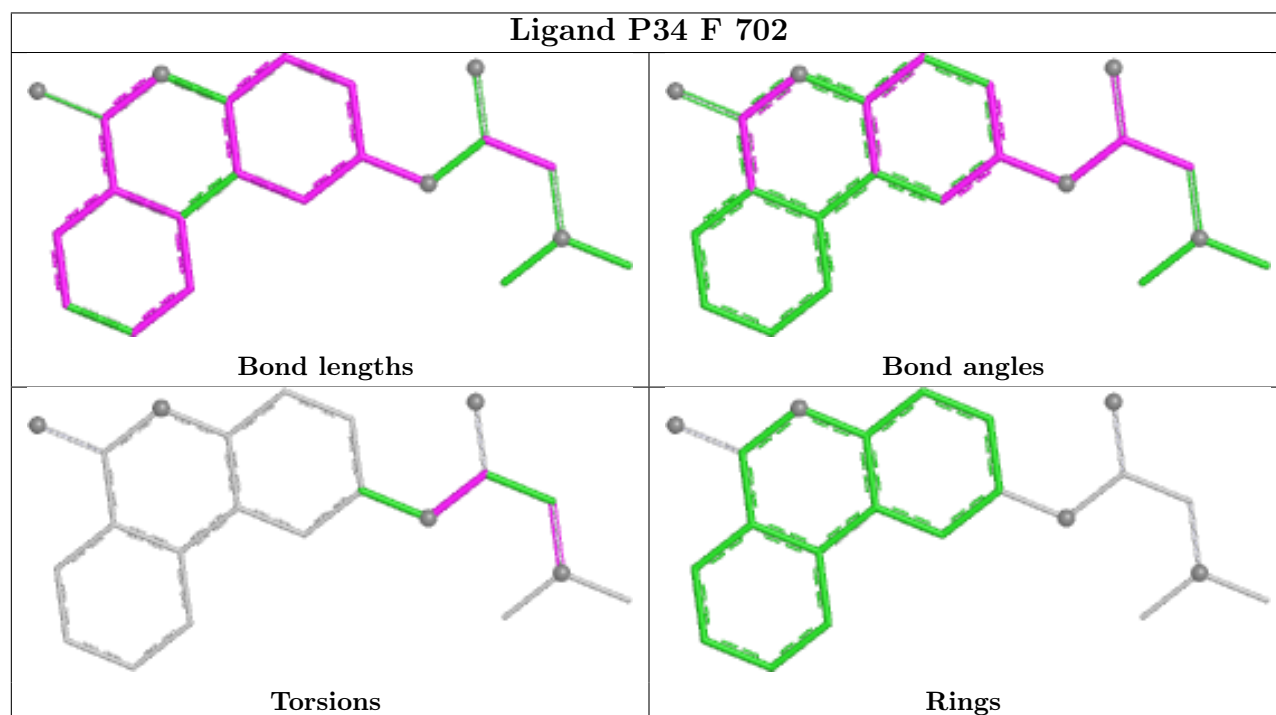
There are no ring outliers.

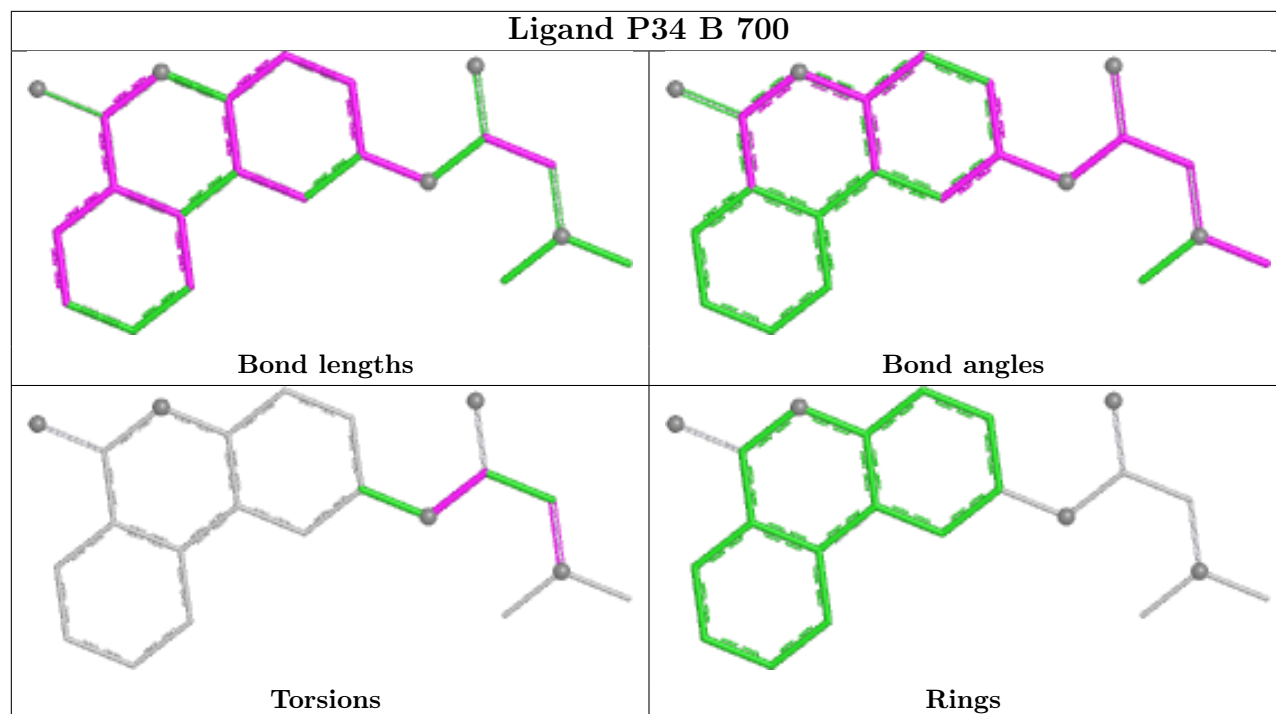
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	702	P34	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	822/842 (97%)	0.56	48 (5%) 29 22	16, 52, 85, 106	0
1	C	822/842 (97%)	1.00	138 (16%) 4 3	19, 66, 124, 136	0
1	E	822/842 (97%)	1.78	343 (41%) 0 0	20, 105, 128, 148	0
2	B	207/207 (100%)	-0.06	7 (3%) 48 39	9, 32, 61, 79	0
2	D	207/207 (100%)	0.11	6 (2%) 53 43	11, 33, 64, 79	0
2	F	207/207 (100%)	0.18	7 (3%) 48 39	18, 38, 70, 84	0
All	All	3087/3147 (98%)	0.91	549 (17%) 4 3	9, 58, 122, 148	0

All (549) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	335	LEU	7.0
1	E	146	ALA	6.8
1	E	731	VAL	6.6
1	E	781	THR	6.6
1	E	126	LEU	6.2
1	E	364	ALA	6.0
1	C	552	VAL	6.0
1	E	790	GLY	5.9
1	E	200	VAL	5.8
1	E	143	LEU	5.7
1	E	765	LEU	5.7
1	E	205	ALA	5.7
1	E	770	ALA	5.6
1	C	507	GLY	5.6
1	E	780	PHE	5.6
1	E	475	ALA	5.6
1	E	127	VAL	5.5
1	C	492	ALA	5.5
1	E	784	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	764	PRO	5.5
1	E	10	ARG	5.4
1	E	338	ILE	5.4
1	E	21	ASN	5.2
1	E	339	VAL	5.2
1	E	761	PRO	5.2
1	E	746	VAL	5.2
1	E	179	ALA	5.2
1	E	93	THR	5.1
1	E	104	ASP	5.1
1	C	505	VAL	5.0
1	E	343	PRO	5.0
1	E	17	THR	5.0
1	E	128	VAL	4.8
1	E	348	ALA	4.8
1	E	492	ALA	4.8
1	C	281	ILE	4.8
1	E	259	ASN	4.7
1	E	188	ILE	4.7
1	E	189	VAL	4.6
1	C	318	ALA	4.6
1	E	347	THR	4.6
1	E	346	VAL	4.5
1	E	86	VAL	4.4
1	E	526	GLY	4.4
1	E	196	VAL	4.4
1	E	222	ILE	4.4
1	E	99	LEU	4.3
1	C	493	VAL	4.3
1	E	277	ILE	4.2
1	E	789	GLY	4.2
1	E	92	LYS	4.2
1	C	554	LEU	4.2
1	C	504	LEU	4.1
1	E	280	PRO	4.1
1	E	331	ALA	4.1
1	E	763	THR	4.0
1	C	163	ALA	4.0
1	C	445	ILE	4.0
1	E	760	ARG	4.0
1	C	549	HIS	4.0
1	E	202	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	334	LEU	4.0
1	E	441	PHE	3.9
1	C	545	LEU	3.9
1	E	554	LEU	3.9
1	E	278	LEU	3.9
1	C	235	VAL	3.9
1	E	369	ILE	3.9
1	E	736	PRO	3.9
1	E	546	GLU	3.8
1	C	226	ALA	3.8
1	C	258	THR	3.8
1	E	131	THR	3.8
1	C	261	ASP	3.8
1	C	233	PHE	3.8
1	E	342	LEU	3.8
1	C	550	ALA	3.8
1	E	752	GLY	3.8
1	E	154	VAL	3.7
1	E	523	SER	3.7
1	E	122	THR	3.7
1	C	282	PHE	3.7
1	A	758	GLU	3.7
1	E	235	VAL	3.7
1	E	281	ILE	3.7
1	E	340	LEU	3.7
1	E	257	TRP	3.7
1	E	254	THR	3.7
1	E	788	THR	3.7
1	C	553	PRO	3.6
1	E	204	PRO	3.6
1	C	299	LEU	3.6
1	E	142	VAL	3.6
1	E	552	VAL	3.6
1	E	796	MET	3.6
1	E	248	SER	3.6
1	E	67	GLY	3.6
1	E	321	LYS	3.6
1	E	556	ILE	3.6
1	E	442	VAL	3.6
1	E	197	LEU	3.6
1	A	309	GLY	3.6
1	E	116	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	229	TYR	3.5
1	E	175	TYR	3.5
1	E	98	PHE	3.5
1	E	276	PHE	3.5
1	C	551	GLY	3.5
1	C	501	LEU	3.5
1	E	437	MET	3.5
1	E	474	THR	3.5
1	E	216	HIS	3.5
1	E	157	ILE	3.5
1	E	296	ILE	3.4
1	E	345	PRO	3.4
1	E	77	LEU	3.4
1	E	182	VAL	3.4
1	E	794	PRO	3.4
1	C	498	ALA	3.4
1	E	110	ASP	3.4
1	C	165	LEU	3.4
1	C	234	GLY	3.4
1	E	136	CYS	3.4
1	E	328	LEU	3.3
1	E	139	THR	3.3
1	E	747	LEU	3.3
1	A	235	VAL	3.3
1	C	277	ILE	3.3
1	E	163	ALA	3.3
1	E	787	ALA	3.3
1	A	310	ASP	3.3
1	E	308	LYS	3.3
1	C	319	LEU	3.3
1	C	306	VAL	3.3
1	E	187	VAL	3.3
1	E	176	GLN	3.3
1	E	745	SER	3.3
1	E	553	PRO	3.2
1	E	125	ALA	3.2
1	E	256	LYS	3.2
1	E	366	CYS	3.2
2	F	459	SER	3.2
1	E	194	ASP	3.2
1	C	251	ASN	3.2
1	E	431	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	312	LYS	3.2
1	E	84	GLU	3.2
1	E	27	HIS	3.2
1	E	476	HIS	3.2
1	E	759	GLN	3.2
1	E	95	GLY	3.2
1	E	148	GLY	3.2
1	E	81	MET	3.2
1	E	245	TRP	3.2
1	C	278	LEU	3.2
1	C	291	PHE	3.2
1	E	255	LYS	3.2
1	E	234	GLY	3.2
1	E	536	LEU	3.1
1	E	6	VAL	3.1
1	E	298	VAL	3.1
1	E	25	ILE	3.1
1	E	273	PHE	3.1
1	E	742	GLY	3.1
1	E	387	PRO	3.1
1	E	109	VAL	3.1
1	E	495	VAL	3.1
1	E	548	ASP	3.1
1	E	372	CYS	3.0
1	C	829	LYS	3.0
1	E	167	LEU	3.0
1	E	333	ALA	3.0
1	A	236	ASP	3.0
1	E	70	ILE	3.0
1	E	75	ILE	3.0
1	E	87	LYS	3.0
1	E	730	LEU	3.0
1	E	238	ALA	3.0
1	E	322	VAL	3.0
1	C	158	ASN	3.0
1	E	279	ASP	3.0
1	E	753	GLN	3.0
1	E	48	ALA	3.0
1	E	282	PHE	3.0
1	E	314	LEU	3.0
1	E	534	GLY	3.0
1	E	782	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	129	VAL	3.0
1	E	306	VAL	3.0
1	A	232	LYS	2.9
1	E	165	LEU	2.9
1	E	779	GLY	2.9
1	E	82	SER	2.9
1	C	495	VAL	2.9
1	C	503	LYS	2.9
1	C	320	LEU	2.9
1	C	500	ASP	2.9
1	E	241	MET	2.9
1	E	472	SER	2.9
1	E	185	VAL	2.9
1	E	119	LEU	2.9
1	E	360	PRO	2.9
1	E	13	MET	2.9
1	C	807	ASP	2.9
1	E	123	ASP	2.9
1	E	74	ALA	2.9
1	E	768	VAL	2.9
1	C	222	ILE	2.9
1	C	284	LEU	2.9
1	E	332	ASP	2.9
1	E	777	SER	2.9
1	E	177	THR	2.9
1	E	45	ILE	2.9
1	E	252	PRO	2.8
1	A	766	PHE	2.8
1	E	184	SER	2.8
2	B	518	LEU	2.8
2	F	518	LEU	2.8
1	E	120	ARG	2.8
1	E	498	ALA	2.8
1	C	515	ASP	2.8
1	C	170	SER	2.8
1	E	47	SER	2.8
1	E	72	SER	2.8
1	E	239	LYS	2.8
1	E	155	VAL	2.8
1	E	226	ALA	2.8
1	C	307	LEU	2.8
1	E	269	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	73	THR	2.8
1	C	785	ARG	2.8
1	E	180	ARG	2.8
1	E	361	ALA	2.8
1	E	792	ALA	2.8
1	C	164	LEU	2.8
1	C	508	LEU	2.8
1	E	542	LEU	2.8
1	E	743	ILE	2.8
1	C	108	HIS	2.8
1	E	14	ASP	2.8
1	C	2	VAL	2.7
1	C	257	TRP	2.7
1	E	26	ALA	2.7
1	E	233	PHE	2.7
1	E	739	ALA	2.7
2	F	489	ALA	2.7
1	E	147	LEU	2.7
1	C	446	ASP	2.7
1	E	424	ASP	2.7
1	C	268	PRO	2.7
1	A	759	GLN	2.7
1	E	386	VAL	2.7
1	C	45	ILE	2.7
1	E	291	PHE	2.7
1	E	207	GLY	2.7
1	E	791	GLN	2.7
1	E	39	LEU	2.7
1	E	210	ALA	2.7
1	E	80	GLU	2.7
1	E	145	GLN	2.7
1	E	2	VAL	2.7
1	E	493	VAL	2.7
1	E	193	ALA	2.7
1	E	368	ALA	2.7
1	E	735	CYS	2.7
1	E	134	GLY	2.7
1	C	300	LEU	2.7
1	E	174	LEU	2.7
1	E	350	ALA	2.6
1	E	547	HIS	2.6
2	B	549	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	495	VAL	2.6
1	C	237	LYS	2.6
1	C	491	VAL	2.6
1	C	546	GLU	2.6
1	E	247	ASP	2.6
1	E	303	LEU	2.6
1	E	370	LYS	2.6
1	A	549	HIS	2.6
2	F	490	ARG	2.6
1	A	451	GLY	2.6
1	E	172	GLU	2.6
1	E	795	GLN	2.6
1	E	130	ASP	2.6
1	E	236	ASP	2.6
1	E	362	ASP	2.6
1	E	20	ARG	2.6
1	E	293	LYS	2.6
1	E	436	LEU	2.6
1	A	431	ILE	2.6
1	E	89	ILE	2.6
1	E	401	PHE	2.6
1	E	190	SER	2.6
1	E	78	TYR	2.6
1	E	153	PRO	2.6
1	E	351	TYR	2.6
1	E	771	TYR	2.6
1	E	519	LEU	2.6
1	E	137	VAL	2.6
1	E	305	ILE	2.6
1	C	285	PHE	2.6
1	E	225	PHE	2.6
1	A	513	LYS	2.5
1	E	260	LYS	2.5
1	E	501	LEU	2.5
1	E	762	GLY	2.5
1	E	740	VAL	2.5
1	C	427	PHE	2.5
1	E	376	ALA	2.5
1	A	748	ASN	2.5
1	A	515	ASP	2.5
1	E	144	ARG	2.5
1	C	806	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	90	LYS	2.5
1	C	269	LEU	2.5
1	C	761	PRO	2.5
1	E	300	LEU	2.5
1	A	305	ILE	2.5
1	A	480	VAL	2.5
1	C	325	ARG	2.5
1	C	557	SER	2.5
1	E	557	SER	2.5
1	E	268	PRO	2.5
1	E	385	MET	2.5
1	E	438	MET	2.5
1	E	444	PRO	2.5
1	C	789	GLY	2.5
1	E	124	GLY	2.5
1	E	458	GLY	2.5
2	B	490	ARG	2.5
1	C	541	CYS	2.5
1	E	100	ILE	2.5
1	E	344	SER	2.5
1	E	491	VAL	2.5
1	C	418	TYR	2.5
1	E	203	TYR	2.5
1	E	250	PHE	2.5
1	E	227	THR	2.5
1	E	272	ALA	2.5
1	C	256	LYS	2.5
1	E	32	LYS	2.5
1	E	341	HIS	2.5
1	C	174	LEU	2.4
1	C	481	MET	2.4
1	E	46	ILE	2.4
1	C	731	VAL	2.4
1	E	754	VAL	2.4
1	E	336	GLU	2.4
1	E	737	GLU	2.4
1	C	321	LYS	2.4
1	E	215	LEU	2.4
1	E	288	ILE	2.4
1	A	67	GLY	2.4
1	A	84	GLU	2.4
1	A	473	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	766	PHE	2.4
2	D	523	ALA	2.4
1	E	744	TYR	2.4
1	E	497	ASN	2.4
1	C	502	PRO	2.4
1	E	478	MET	2.4
1	E	232	LYS	2.4
1	E	551	GLY	2.4
1	E	220	PHE	2.4
1	A	830	GLU	2.4
1	C	286	THR	2.4
1	C	167	LEU	2.4
1	E	158	ASN	2.3
1	E	451	GLY	2.3
1	E	734	GLN	2.3
1	C	536	LEU	2.3
1	C	817	GLU	2.3
1	E	195	GLU	2.3
1	E	494	GLU	2.3
1	C	759	GLN	2.3
1	E	192	TYR	2.3
1	E	221	THR	2.3
1	C	509	LYS	2.3
1	C	10	ARG	2.3
1	C	86	VAL	2.3
1	E	16	VAL	2.3
1	E	287	ALA	2.3
1	C	542	LEU	2.3
1	C	556	ILE	2.3
1	A	812	THR	2.3
1	C	162	ARG	2.3
1	E	418	TYR	2.3
2	D	549	GLY	2.3
1	E	427	PHE	2.3
1	C	241	MET	2.3
1	E	240	MET	2.3
1	E	201	GLN	2.3
1	E	432	GLN	2.3
1	C	171	LYS	2.3
1	C	812	THR	2.3
1	E	170	SER	2.3
1	C	345	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	434	VAL	2.3
1	E	741	GLY	2.3
2	B	405	GLY	2.3
1	A	607	ASN	2.2
1	E	186	ASN	2.2
1	E	697	ALA	2.2
1	C	314	LEU	2.2
1	E	284	LEU	2.2
1	E	479	LYS	2.2
1	C	14	ASP	2.2
1	C	46	ILE	2.2
1	E	367	ILE	2.2
1	E	113	SER	2.2
1	E	359	GLY	2.2
1	E	379	MET	2.2
1	A	195	GLU	2.2
1	A	475	ALA	2.2
1	C	443	GLU	2.2
1	E	114	GLU	2.2
1	E	783	GLU	2.2
1	E	18	ASN	2.2
1	C	296	ILE	2.2
1	C	540	ILE	2.2
1	A	446	ASP	2.2
1	C	280	PRO	2.2
1	E	135	VAL	2.2
1	E	449	PRO	2.2
1	C	394	PHE	2.2
1	E	211	PHE	2.2
1	A	237	LYS	2.2
1	A	596	GLU	2.2
1	C	238	ALA	2.2
1	C	303	LEU	2.2
1	E	320	LEU	2.2
1	E	550	ALA	2.2
1	E	749	LYS	2.2
1	C	315	GLU	2.2
1	E	149	GLU	2.2
2	D	548	GLU	2.2
1	E	352	ARG	2.2
1	E	261	ASP	2.2
1	C	322	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	471	THR	2.2
1	C	324	MET	2.2
1	C	762	GLY	2.2
1	E	525	SER	2.2
1	C	255	LYS	2.2
1	C	519	LEU	2.2
1	E	102	LEU	2.2
2	F	523	ALA	2.2
1	E	151	ILE	2.2
2	F	492	ARG	2.2
1	C	93	THR	2.2
1	C	289	MET	2.2
1	C	232	LYS	2.2
1	E	15	LYS	2.2
1	E	246	GLY	2.2
1	C	521	TYR	2.2
1	A	300	LEU	2.2
1	C	523	SER	2.2
1	A	737	GLU	2.2
1	E	402	ALA	2.2
2	B	519	ALA	2.2
2	B	548	GLU	2.2
1	C	606	ILE	2.1
1	C	734	GLN	2.1
1	C	442	VAL	2.1
1	E	505	VAL	2.1
1	A	110	ASP	2.1
1	A	437	MET	2.1
1	C	83	ASP	2.1
1	E	218	TRP	2.1
1	E	538	LEU	2.1
1	E	512	SER	2.1
1	E	541	CYS	2.1
1	E	271	ARG	2.1
1	E	132	ILE	2.1
1	A	795	GLN	2.1
1	C	101	ASN	2.1
1	C	259	ASN	2.1
1	E	516	PRO	2.1
1	E	532	GLY	2.1
1	A	111	PHE	2.1
1	E	285	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	545	LEU	2.1
2	D	518	LEU	2.1
1	E	358	GLU	2.1
1	A	92	LYS	2.1
1	E	522	MET	2.1
1	C	244	LEU	2.1
1	A	233	PHE	2.1
1	A	548	ASP	2.1
1	C	227	THR	2.1
1	E	5	THR	2.1
1	E	778	PHE	2.1
1	E	229	TYR	2.1
1	C	190	SER	2.1
1	E	349	GLN	2.1
1	E	400	VAL	2.1
1	E	356	LEU	2.1
1	A	439	GLY	2.1
1	C	250	PHE	2.1
1	E	793	PHE	2.1
1	A	104	ASP	2.1
1	E	181	THR	2.1
1	C	48	ALA	2.1
1	E	118	ALA	2.1
1	E	318	ALA	2.1
1	C	732	GLU	2.1
1	C	38	SER	2.0
1	C	113	SER	2.0
1	C	749	LYS	2.0
1	C	802	SER	2.0
1	E	79	SER	2.0
1	A	411	VAL	2.0
1	E	28	VAL	2.0
1	E	411	VAL	2.0
1	A	761	PRO	2.0
1	C	811	PRO	2.0
1	E	773	PRO	2.0
1	A	314	LEU	2.0
1	E	35	LEU	2.0
1	C	42	ARG	2.0
1	E	327	PHE	2.0
2	D	605	GLY	2.0
1	A	763	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	767	THR	2.0
1	C	94	ASP	2.0
1	A	231	LYS	2.0
1	A	484	SER	2.0
1	A	518	VAL	2.0
1	C	583	HIS	2.0
1	C	657	HIS	2.0
1	E	435	VAL	2.0
1	C	764	PRO	2.0
1	E	420	PRO	2.0
1	C	765	LEU	2.0
1	C	316	GLY	2.0
1	C	439	GLY	2.0
1	E	178	PHE	2.0
1	E	397	PHE	2.0
1	E	103	ILE	2.0
1	E	698	ILE	2.0
1	E	353	ALA	2.0
2	D	517	THR	2.0
2	F	519	ALA	2.0
1	A	311	GLU	2.0
1	C	527	GLU	2.0
1	E	294	ASP	2.0
2	B	581	ASP	2.0
1	E	171	LYS	2.0
1	E	337	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	DDE	E	699	10/21	0.87	0.10	42,46,47,48	0
1	DDE	C	699	10/21	0.89	0.11	49,55,57,58	0
1	DDE	A	699	10/21	0.91	0.09	42,44,47,48	0

6.3 Carbohydrates [i](#)

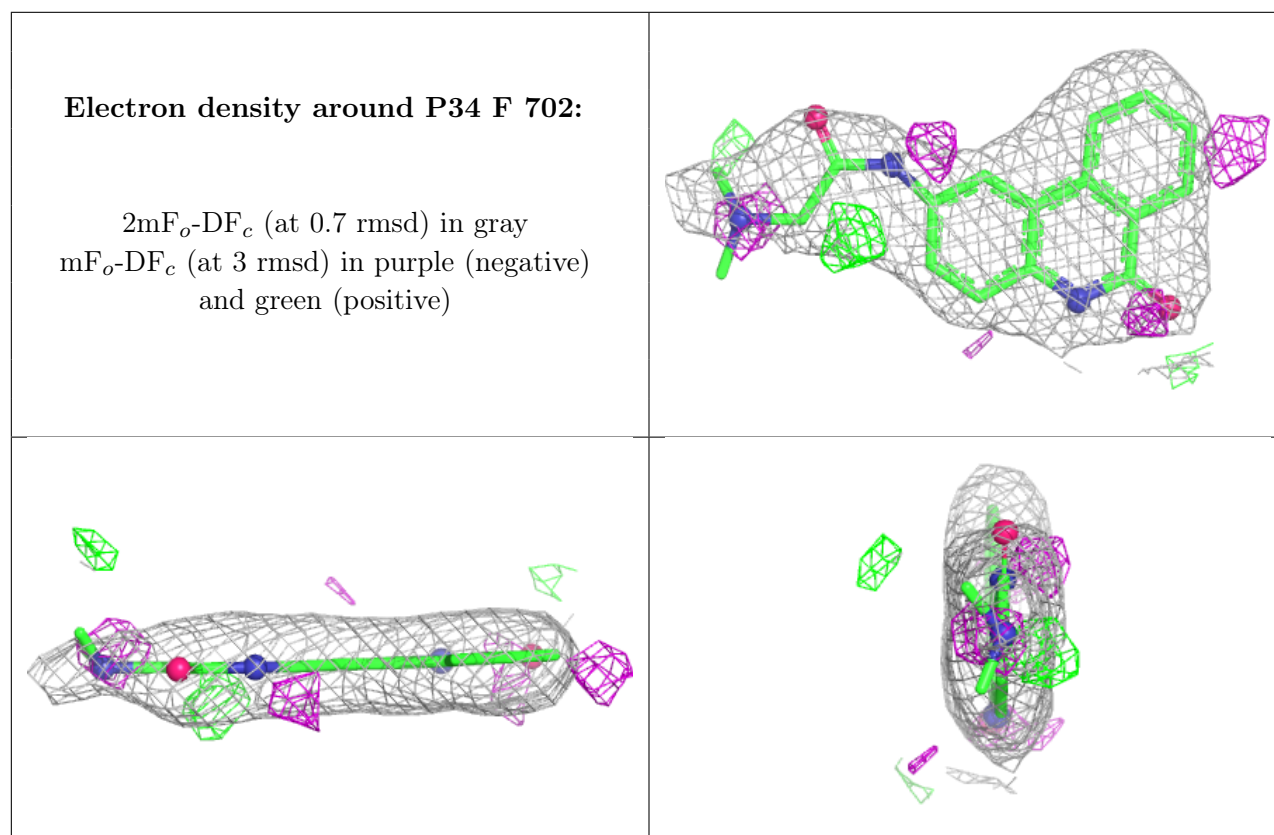
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

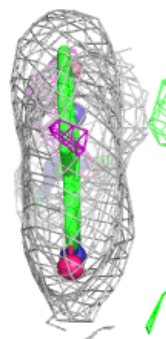
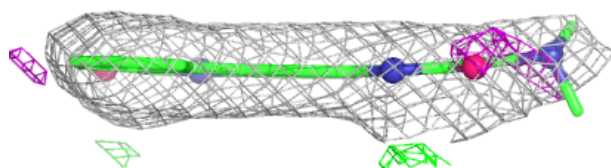
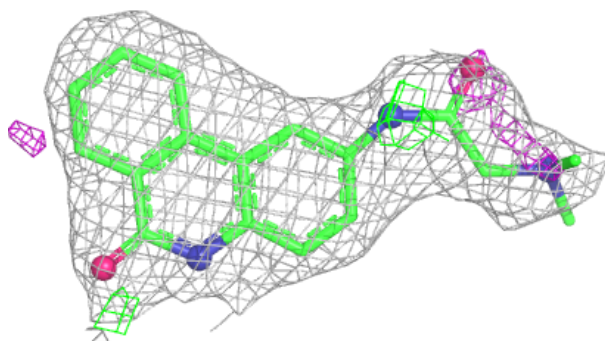
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P34	F	702	22/22	0.88	0.14	12,17,57,58	0
3	P34	D	701	22/22	0.91	0.12	18,24,54,55	0
3	P34	B	700	22/22	0.91	0.10	8,13,34,35	0

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

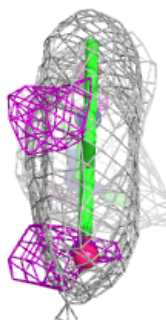
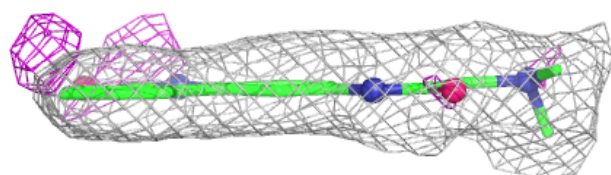
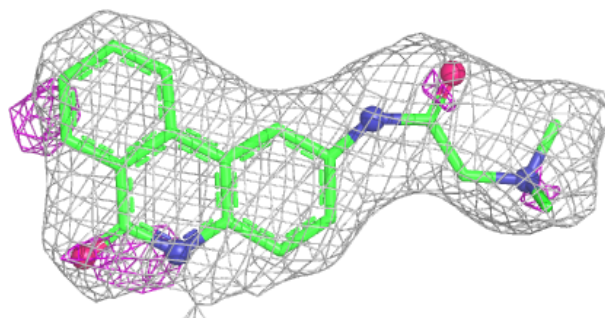


Electron density around P34 D 701:

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

**Electron density around P34 B 700:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.