



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 AM UTC

PDB ID : 1K90 / pdb_00001k90
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 3' deoxy-ATP
Authors : Drum, C.L.; Yan, S.-Z.; Bard, J.; Shen, Y.-Q.; Lu, D.; Soelaiman, S.; Grabarek, Z.; Bohm, A.; Tang, W.-J.
Deposited on : 2001-10-26
Resolution : 2.75 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

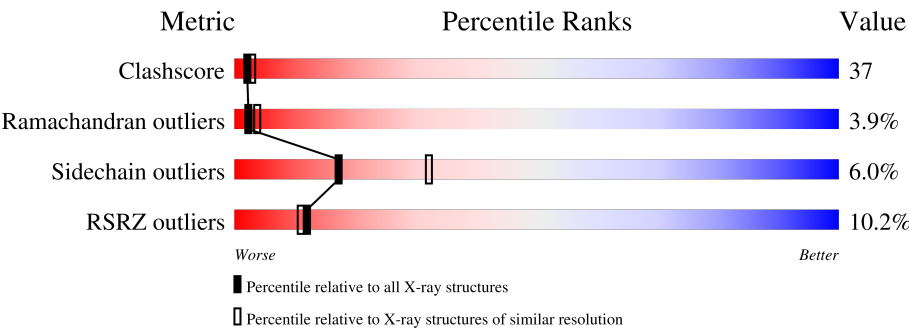
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	510	5% 45% 43% 6% 5%
1	B	510	11% 33% 49% 9% 9%
1	C	510	5% 47% 45% 6%
2	D	148	15% 42% 49%
2	E	148	26% 40% 53%
2	F	148	17% 36% 55% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15357 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CALMODULIN-SENSITIVE ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	465	Total	C	N	O	S	113	0	0
			3794	2431	642	718	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

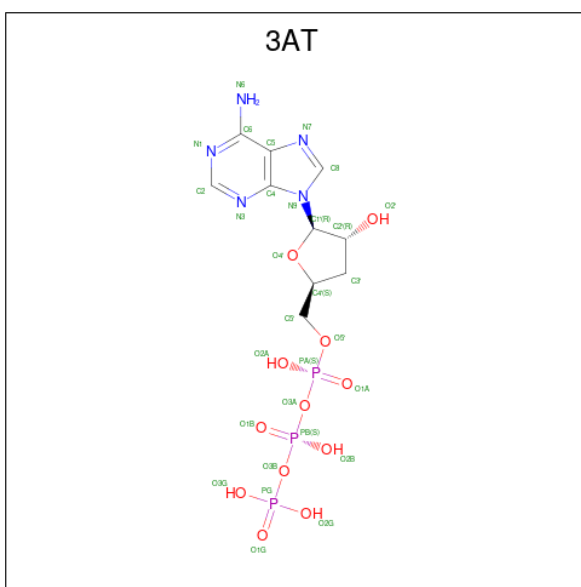
- Molecule 2 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

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

- Molecule 4 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	C	1	Total 30	C 10	N 5	O 12	P 3	0	0

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	D	1	Total O 1 1	0	0
6	B	8	Total O 8 8	0	0

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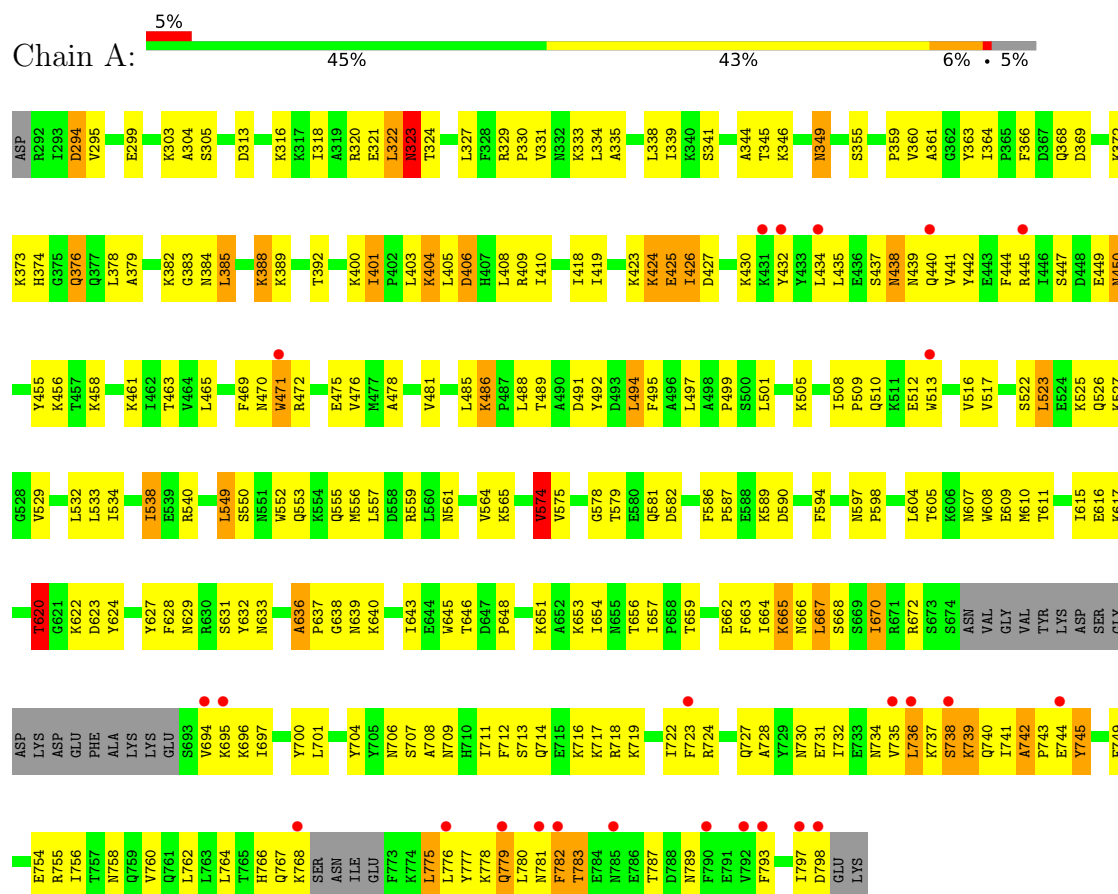
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	22	Total	O	0	0
			22	22		
6	F	2	Total	O	0	0
			2	2		

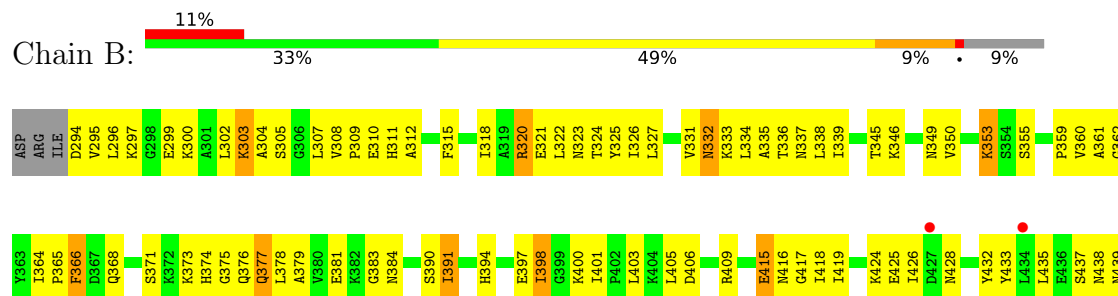
3 Residue-property plots

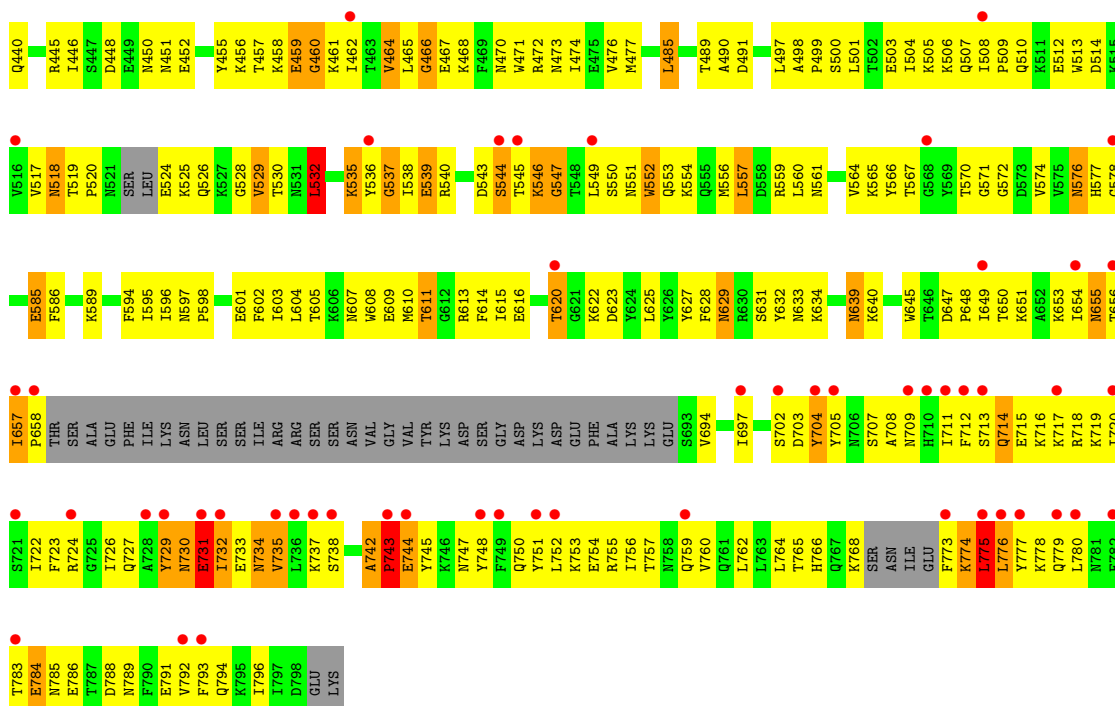
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

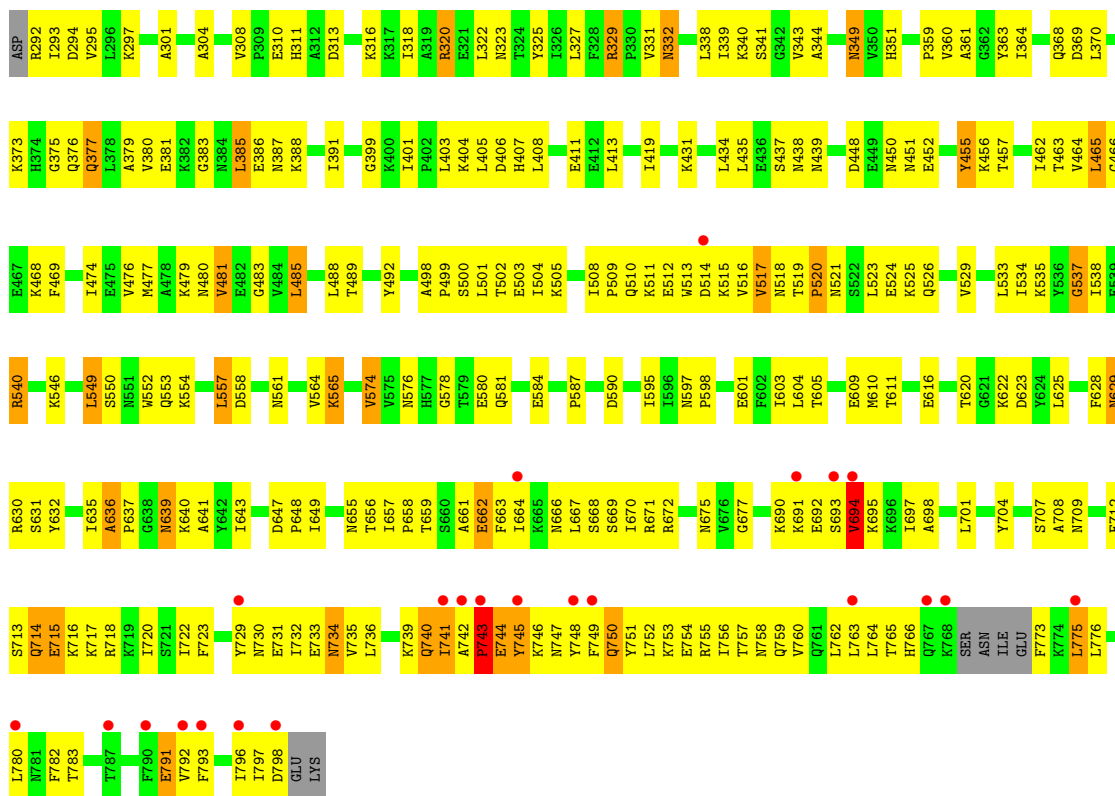


• Molecule 1: CALMODULIN-SENSITIVE ADENYLATE CYCLASE

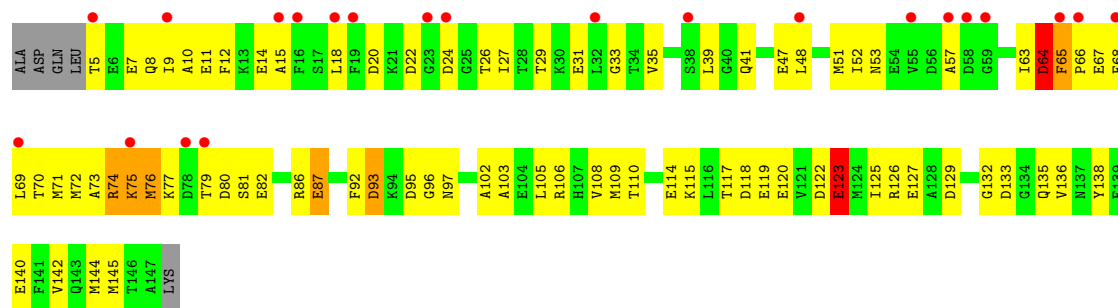
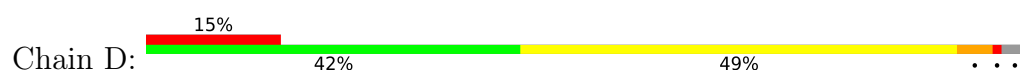




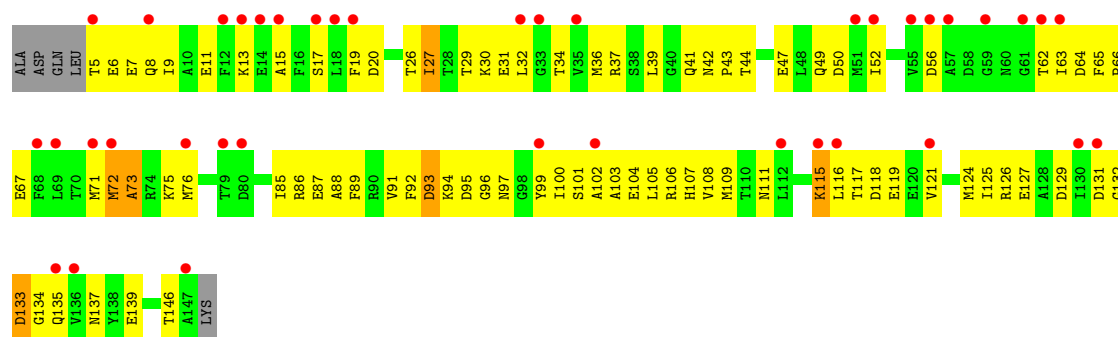
• Molecule 1: CALMODULIN-SENSITIVE ADENYLATE CYCLASE



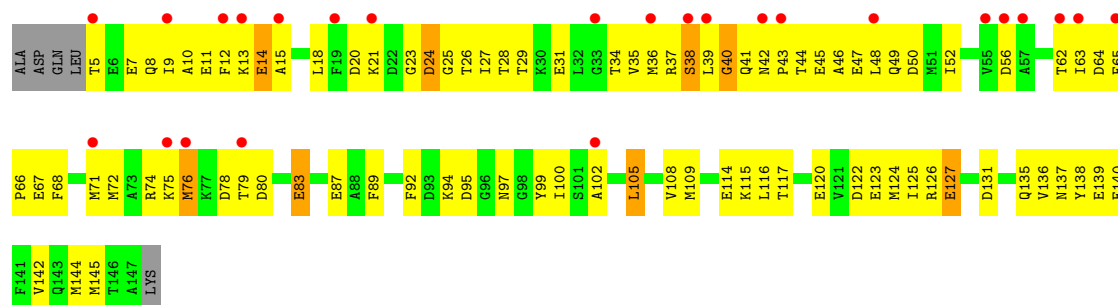
• Molecule 2: CALMODULIN



• Molecule 2: CALMODULIN



• Molecule 2: CALMODULIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.10Å 166.10Å 343.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.75 19.97 – 2.75	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.97-2.75) 99.4 (19.97-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.64Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.286 0.243 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15357	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 3AT, YB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/4027	0.95	18/5419 (0.3%)
1	B	0.34	0/3867	0.94	16/5204 (0.3%)
1	C	0.37	0/4172	0.88	11/5613 (0.2%)
2	D	0.31	0/1137	0.78	1/1527 (0.1%)
2	E	0.29	0/1137	0.74	1/1527 (0.1%)
2	F	0.33	0/1137	0.83	3/1527 (0.2%)
All	All	0.35	0/15477	0.89	50/20817 (0.2%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	SER	N-CA-C	-16.51	83.07	108.67
1	C	745	TYR	N-CA-C	-13.31	96.14	112.38
1	B	735	VAL	N-CA-C	-12.46	100.97	112.43
1	B	742	ALA	CA-C-N	11.69	134.45	119.84
1	B	742	ALA	C-N-CA	11.69	134.45	119.84
1	B	775	LEU	N-CA-C	-11.02	98.46	112.90
1	A	779	GLN	N-CA-C	-7.68	102.76	113.20
1	B	783	THR	N-CA-C	-7.52	106.05	114.62
1	B	731	GLU	N-CA-C	-7.37	102.93	110.97
1	A	620	THR	N-CA-C	7.26	119.19	111.28
1	A	667	LEU	N-CA-C	-6.97	104.44	114.12
1	B	743	PRO	N-CA-C	6.96	126.80	112.47
1	B	366	PHE	N-CA-C	-6.90	103.69	111.14
1	C	750	GLN	N-CA-C	-6.81	104.84	113.01
1	C	636	ALA	CA-C-N	6.66	126.44	119.05
1	C	636	ALA	C-N-CA	6.66	126.44	119.05
1	B	546	LYS	N-CA-C	-6.62	98.91	109.76
1	A	636	ALA	CA-C-N	6.42	125.92	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	ALA	C-N-CA	6.42	125.92	119.24
1	A	574	VAL	N-CA-C	-6.21	107.44	113.53
1	B	647	ASP	CA-C-N	5.98	127.31	119.84
1	B	647	ASP	C-N-CA	5.98	127.31	119.84
1	A	486	LYS	CA-C-N	5.94	125.95	119.89
1	A	486	LYS	C-N-CA	5.94	125.95	119.89
1	A	738	SER	CA-C-O	-5.87	113.97	120.60
1	B	729	TYR	N-CA-C	-5.85	104.25	111.33
1	C	783	THR	N-CA-C	-5.77	106.03	114.39
1	B	532	LEU	N-CA-C	-5.76	105.92	113.12
2	F	38	SER	N-CA-C	-5.67	106.07	112.87
2	D	123	GLU	N-CA-C	-5.65	104.74	111.69
2	F	76	MET	N-CA-C	-5.52	104.32	111.71
1	A	672	ARG	N-CA-C	-5.50	105.62	112.93
1	B	576	ASN	N-CA-C	5.49	120.25	113.50
1	A	408	LEU	N-CA-C	5.35	116.80	111.07
2	F	40	GLY	N-CA-C	5.33	125.81	113.18
1	B	577	HIS	N-CA-C	5.32	116.74	109.18
1	C	574	VAL	N-CA-C	-5.31	107.20	113.42
1	C	369	ASP	N-CA-C	-5.24	106.73	113.01
1	A	495	PHE	N-CA-C	-5.18	106.11	112.90
1	B	448	ASP	N-CA-C	-5.11	107.17	113.41
1	A	401	ILE	CA-C-N	5.11	125.02	119.76
1	A	401	ILE	C-N-CA	5.11	125.02	119.76
1	A	538	ILE	N-CA-C	5.10	115.77	110.82
1	C	576	ASN	N-CA-C	5.09	119.59	113.17
2	E	146	THR	N-CA-C	-5.08	106.92	113.01
1	C	329	ARG	N-CA-C	-5.04	103.61	110.36
1	C	565	LYS	N-CA-C	-5.04	105.79	111.28
1	C	744	GLU	N-CA-C	5.04	117.33	110.88
1	A	366	PHE	N-CA-C	-5.01	105.71	111.07
1	A	745	TYR	N-CA-C	-5.01	107.72	113.88

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	3952	0	3999	274	0
1	B	3794	0	3828	351	0
1	C	4094	0	4134	270	0
2	D	1125	0	1049	74	0
2	E	1125	0	1049	96	0
2	F	1125	0	1049	98	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	30	0	12	2	0
4	B	30	0	12	1	0
4	C	30	0	12	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
6	A	10	0	0	0	0
6	B	8	0	0	1	0
6	C	22	0	0	1	0
6	D	1	0	0	0	0
6	F	2	0	0	0	0
All	All	15357	0	15144	1113	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 37.

All (1113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:GLU:HA	1:B:620:THR:HG22	1.37	1.06
1:B:489:THR:HG22	1:B:490:ALA:H	1.21	1.03
1:B:325:TYR:HB2	1:B:498:ALA:HB3	1.37	1.03
1:C:659:THR:HG22	1:C:661:ALA:H	1.21	1.03
1:A:783:THR:HB	1:A:789:ASN:HD21	1.30	0.96
1:B:324:THR:HG22	1:B:499:PRO:HA	1.48	0.96
1:B:730:ASN:HD21	1:B:734:ASN:HB2	1.29	0.96
1:C:691:LYS:HB2	1:C:694:VAL:HG13	1.48	0.94
1:C:744:GLU:HB3	1:C:747:ASN:HB2	1.49	0.94
1:B:597:ASN:HD21	1:B:601:GLU:HB2	1.33	0.93
2:F:37:ARG:HD2	2:F:42:ASN:HA	1.48	0.93
1:A:434:LEU:HA	1:A:445:ARG:HD3	1.52	0.92
1:B:729:TYR:HE2	1:B:773:PHE:HE1	1.18	0.91
1:B:353:LYS:H	1:B:368:GLN:NE2	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:HG	1:B:595:ILE:HG12	1.52	0.91
1:B:464:VAL:HG23	1:B:465:LEU:H	1.36	0.91
1:B:629:ASN:HD22	1:B:631:SER:H	1.19	0.90
1:A:776:LEU:HD12	1:A:776:LEU:H	1.37	0.90
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.53	0.89
1:B:514:ASP:HA	1:B:517:VAL:HG12	1.55	0.89
1:B:353:LYS:N	1:B:368:GLN:HE22	1.70	0.88
1:C:775:LEU:HD23	1:C:775:LEU:H	1.37	0.88
1:B:561:ASN:O	1:B:564:VAL:HG22	1.72	0.88
2:E:26:THR:HG22	2:E:64:ASP:HB3	1.54	0.88
1:B:529:VAL:HG11	2:E:109:MET:HE1	1.54	0.87
1:C:464:VAL:HG23	1:C:465:LEU:HD23	1.56	0.87
1:B:508:ILE:HG12	1:B:536:TYR:HD1	1.40	0.87
1:C:605:THR:HG21	1:C:611:THR:HA	1.57	0.86
1:C:351:HIS:HB2	1:C:386:GLU:HG2	1.58	0.85
1:B:729:TYR:HE2	1:B:773:PHE:CE1	1.94	0.85
1:B:543:ASP:OD1	1:B:544:SER:N	2.08	0.85
1:C:714:GLN:HE21	1:C:714:GLN:HA	1.37	0.85
1:A:775:LEU:HD12	1:A:775:LEU:H	1.42	0.84
1:A:697:ILE:HD13	1:A:732:ILE:HG12	1.59	0.84
1:B:526:GLN:HE21	2:E:124:MET:HE2	1.41	0.84
1:B:535:LYS:HE2	1:B:535:LYS:HA	1.60	0.83
2:F:138:TYR:O	2:F:142:VAL:HG23	1.77	0.83
1:B:381:GLU:HG2	1:B:465:LEU:HD11	1.59	0.83
1:B:366:PHE:HD1	1:B:477:MET:HE1	1.44	0.82
1:B:489:THR:HG22	1:B:490:ALA:N	1.95	0.82
1:C:715:GLU:H	1:C:715:GLU:CD	1.86	0.82
1:B:509:PRO:HG2	1:B:512:GLU:HB3	1.60	0.81
2:E:49:GLN:HA	2:E:52:ILE:HG22	1.61	0.81
1:A:797:ILE:HG23	1:A:798:ASP:H	1.45	0.81
1:C:736:LEU:HD22	1:C:746:LYS:HG2	1.62	0.81
1:A:611:THR:O	1:A:615:ILE:HG12	1.81	0.81
1:A:425:GLU:CD	1:A:445:ARG:HH12	1.89	0.81
1:C:526:GLN:HB2	2:F:124:MET:HE2	1.63	0.81
2:F:97:ASN:HD21	2:F:99:TYR:HB2	1.43	0.81
2:F:76:MET:SD	2:F:79:THR:HG21	2.20	0.81
1:A:456:LYS:HD3	1:A:471:TRP:HD1	1.45	0.81
1:B:518:ASN:C	1:B:520:PRO:HD3	2.06	0.80
1:B:597:ASN:ND2	1:B:601:GLU:HB2	1.97	0.80
1:B:543:ASP:HB3	1:B:546:LYS:O	1.81	0.80
1:C:526:GLN:HE22	2:F:144:MET:HE1	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:101:SER:HB2	2:E:104:GLU:HG3	1.64	0.79
1:C:629:ASN:HD22	1:C:631:SER:H	1.30	0.79
1:A:694:VAL:HG11	1:A:731:GLU:CD	2.08	0.79
1:C:639:ASN:ND2	1:C:641:ALA:H	1.82	0.78
1:A:616:GLU:HA	1:A:620:THR:HG22	1.65	0.78
1:B:320:ARG:HB3	1:B:320:ARG:HH21	1.48	0.78
1:B:526:GLN:HG3	2:E:124:MET:HE2	1.65	0.78
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.65	0.77
1:B:508:ILE:HD13	1:B:532:LEU:HD22	1.66	0.77
1:B:360:VAL:HG21	1:B:365:PRO:HG3	1.66	0.77
1:A:780:LEU:HD13	1:A:782:PHE:CZ	2.19	0.77
2:F:5:THR:N	2:F:9:ILE:HG12	2.00	0.77
1:B:353:LYS:H	1:B:368:GLN:HE22	0.86	0.77
1:B:730:ASN:ND2	1:B:734:ASN:HB2	1.99	0.77
1:A:629:ASN:HD22	1:A:631:SER:H	1.33	0.77
1:C:629:ASN:ND2	1:C:631:SER:H	1.82	0.76
2:E:103:ALA:O	2:E:107:HIS:HB2	1.85	0.76
1:A:731:GLU:HA	1:A:734:ASN:HD21	1.48	0.76
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.67	0.76
1:B:335:ALA:HB1	1:B:489:THR:CG2	2.16	0.75
1:B:549:LEU:HD12	1:B:553:GLN:HE21	1.51	0.75
1:B:311:HIS:HD2	1:B:564:VAL:HB	1.49	0.75
1:C:351:HIS:HB2	1:C:386:GLU:CG	2.16	0.75
1:B:322:LEU:O	1:B:324:THR:HG23	1.86	0.74
1:C:587:PRO:HB2	1:C:643:ILE:HD12	1.69	0.74
1:B:324:THR:CG2	1:B:499:PRO:HA	2.16	0.74
1:A:440:GLN:HE21	1:A:441:VAL:HG23	1.51	0.74
1:A:694:VAL:HG11	1:A:731:GLU:OE2	1.88	0.74
1:B:629:ASN:ND2	1:B:631:SER:H	1.85	0.74
1:B:720:ILE:O	1:B:724:ARG:HG2	1.87	0.74
1:B:730:ASN:HD21	1:B:734:ASN:CB	2.00	0.74
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.70	0.73
1:B:525:LYS:HZ3	2:E:116:LEU:HD21	1.54	0.73
2:E:92:PHE:HD2	2:E:108:VAL:HG21	1.51	0.73
1:C:419:ILE:HD12	1:C:435:LEU:HD22	1.70	0.73
1:A:559:ARG:NH1	1:A:559:ARG:HB3	2.03	0.73
1:B:320:ARG:HG3	1:B:321:GLU:N	2.04	0.73
1:A:629:ASN:ND2	1:A:631:SER:H	1.86	0.72
1:C:313:ASP:HA	1:C:316:LYS:HE2	1.70	0.72
1:C:581:GLN:HE21	1:C:628:PHE:HA	1.54	0.72
1:C:550:SER:H	1:C:553:GLN:NE2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HG22	1:C:465:LEU:H	1.54	0.72
1:C:755:ARG:HA	1:C:758:ASN:ND2	2.04	0.72
1:C:690:LYS:HG2	1:C:691:LYS:N	2.05	0.71
1:A:633:ASN:HD21	1:A:645:TRP:H	1.38	0.71
1:C:549:LEU:HD12	1:C:549:LEU:H	1.55	0.71
1:C:310:GLU:OE1	1:C:340:LYS:HD2	1.90	0.71
2:F:39:LEU:O	2:F:41:GLN:N	2.24	0.71
1:B:653:LYS:HE2	1:B:755:ARG:HH12	1.54	0.71
1:C:295:VAL:HG12	1:C:610:MET:SD	2.30	0.71
1:A:581:GLN:HE21	1:A:628:PHE:HA	1.56	0.71
1:B:549:LEU:HD12	1:B:553:GLN:NE2	2.04	0.71
1:B:788:ASP:O	1:B:791:GLU:HG2	1.89	0.70
1:C:519:THR:OG1	1:C:520:PRO:HD2	1.90	0.70
1:A:697:ILE:HD11	1:A:731:GLU:O	1.92	0.70
1:C:525:LYS:O	1:C:529:VAL:HG23	1.92	0.70
2:F:102:ALA:HA	2:F:125:ILE:HG13	1.71	0.70
2:E:99:TYR:CE2	2:E:137:ASN:HB3	2.27	0.69
2:E:63:ILE:HG23	2:E:67:GLU:HB2	1.72	0.69
1:A:555:GLN:O	1:A:559:ARG:HG2	1.92	0.69
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.74	0.69
1:A:525:LYS:O	1:A:529:VAL:HG23	1.93	0.69
1:B:320:ARG:HG3	1:B:321:GLU:H	1.56	0.69
1:C:479:LYS:HB3	1:C:488:LEU:HD21	1.74	0.69
1:C:797:ILE:HG13	1:C:798:ASP:H	1.57	0.69
2:F:26:THR:HB	2:F:62:THR:HB	1.73	0.69
1:B:320:ARG:HB3	1:B:320:ARG:NH2	2.07	0.69
1:B:549:LEU:HD13	1:B:578:GLY:HA2	1.73	0.69
1:B:730:ASN:ND2	1:B:734:ASN:H	1.91	0.69
1:A:706:ASN:HD21	1:A:708:ALA:HB3	1.57	0.68
1:B:311:HIS:CD2	1:B:564:VAL:HB	2.28	0.68
1:B:792:VAL:O	1:B:796:ILE:HG12	1.92	0.68
1:A:738:SER:O	1:A:739:LYS:C	2.36	0.68
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.28	0.68
1:A:434:LEU:HG	1:A:445:ARG:HE	1.59	0.67
2:E:30:LYS:HB2	2:E:31:GLU:OE1	1.93	0.67
1:C:534:ILE:HA	1:C:538:ILE:HB	1.76	0.67
2:D:133:ASP:OD2	2:D:135:GLN:HG3	1.95	0.67
1:A:731:GLU:HA	1:A:734:ASN:ND2	2.09	0.67
1:B:318:ILE:HG23	1:B:322:LEU:HD12	1.77	0.67
1:C:639:ASN:C	1:C:639:ASN:HD22	2.01	0.67
1:C:718:ARG:HH11	1:C:766:HIS:HB3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASN:ND2	1:A:645:TRP:H	1.93	0.67
1:A:605:THR:HG21	1:A:611:THR:HA	1.77	0.67
1:A:741:ILE:O	1:A:742:ALA:C	2.38	0.67
1:B:335:ALA:HB1	1:B:489:THR:HG22	1.76	0.67
2:E:63:ILE:HG21	2:E:71:MET:HE1	1.75	0.67
1:B:333:LYS:O	1:B:336:THR:HG22	1.95	0.67
1:A:696:LYS:HB2	1:A:731:GLU:HG2	1.77	0.67
1:B:294:ASP:HB3	1:B:610:MET:HE1	1.77	0.66
2:F:68:PHE:HA	2:F:71:MET:HE3	1.77	0.66
1:A:376:GLN:NE2	1:B:466:GLY:HA3	2.11	0.66
1:B:362:GLY:O	1:B:489:THR:HG23	1.95	0.66
1:B:709:ASN:HD21	1:B:720:ILE:HD11	1.60	0.66
2:E:102:ALA:HA	2:E:125:ILE:HD11	1.76	0.66
1:B:460:GLY:HA2	1:B:468:LYS:HZ3	1.59	0.66
1:C:714:GLN:HE21	1:C:714:GLN:CA	2.09	0.66
2:F:97:ASN:HD22	2:F:99:TYR:HD1	1.43	0.66
1:B:320:ARG:HH21	1:B:320:ARG:CB	2.09	0.66
1:B:335:ALA:O	1:B:339:ILE:HG13	1.95	0.66
1:C:292:ARG:HH22	1:C:297:LYS:NZ	1.93	0.66
1:C:752:LEU:O	1:C:756:ILE:HG12	1.96	0.66
1:B:297:LYS:HA	1:B:602:PHE:O	1.95	0.66
2:F:27:ILE:HG13	2:F:63:ILE:HB	1.77	0.66
2:F:89:PHE:CE1	2:F:100:ILE:HG12	2.31	0.66
1:A:322:LEU:O	1:A:323:ASN:C	2.38	0.65
1:B:332:ASN:C	1:B:332:ASN:HD22	2.04	0.65
1:B:722:ILE:HG23	1:B:760:VAL:CG1	2.26	0.65
1:C:661:ALA:C	1:C:663:PHE:H	2.03	0.65
2:F:68:PHE:O	2:F:72:MET:HG2	1.95	0.65
1:A:385:LEU:HD11	1:A:389:LYS:HE3	1.78	0.65
2:D:41:GLN:HE21	2:D:76:MET:HE1	1.61	0.65
1:B:465:LEU:O	1:B:467:GLU:N	2.29	0.65
2:D:9:ILE:HD12	2:D:9:ILE:H	1.60	0.65
1:B:360:VAL:CG2	1:B:365:PRO:HG3	2.25	0.65
1:B:722:ILE:HG12	1:B:760:VAL:HG13	1.77	0.65
1:A:714:GLN:NE2	2:D:126:ARG:HG3	2.12	0.65
2:E:26:THR:HA	2:E:64:ASP:HA	1.77	0.65
1:C:513:TRP:O	1:C:517:VAL:HG12	1.96	0.65
1:A:659:THR:HG22	1:A:662:GLU:HB3	1.78	0.65
1:A:664:ILE:C	1:A:666:ASN:H	2.05	0.65
1:A:445:ARG:HG3	1:A:471:TRP:CZ2	2.32	0.65
1:A:492:TYR:CD2	1:A:574:VAL:HG13	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.79	0.65
1:B:709:ASN:ND2	1:B:720:ILE:HD11	2.12	0.65
1:B:450:ASN:OD1	1:B:452:GLU:HG3	1.97	0.65
1:B:657:ILE:HG12	1:B:658:PRO:HD2	1.78	0.64
1:C:320:ARG:HA	1:C:598:PRO:O	1.96	0.64
1:A:670:ILE:HD12	1:A:745:TYR:CE1	2.33	0.64
1:B:729:TYR:CE2	1:B:773:PHE:HE1	2.07	0.64
1:C:739:LYS:C	1:C:741:ILE:H	2.05	0.64
1:C:318:ILE:HD12	1:C:318:ILE:H	1.62	0.64
1:B:556:MET:O	1:B:560:LEU:HG	1.98	0.64
1:B:735:VAL:HG22	1:B:738:SER:HB2	1.79	0.63
2:E:5:THR:OG1	2:E:8:GLN:HB2	1.97	0.63
1:A:426:ILE:HD12	1:A:426:ILE:N	2.14	0.63
1:B:499:PRO:CG	1:B:504:ILE:HD11	2.28	0.63
1:B:629:ASN:ND2	1:B:631:SER:HB2	2.13	0.63
2:E:131:ASP:HB2	2:E:133:ASP:OD2	1.98	0.63
1:C:595:ILE:HB	1:C:603:ILE:HB	1.80	0.63
1:C:655:ASN:HA	1:C:758:ASN:HB2	1.80	0.63
2:D:26:THR:HG22	2:D:64:ASP:OD1	1.99	0.63
1:B:391:ILE:HD11	1:B:400:LYS:HG2	1.80	0.63
1:B:716:LYS:O	1:B:720:ILE:HG12	1.99	0.63
1:B:514:ASP:HA	1:B:517:VAL:CG1	2.26	0.63
1:C:659:THR:H	1:C:662:GLU:HB2	1.64	0.63
1:C:797:ILE:HG13	1:C:798:ASP:N	2.11	0.63
1:A:440:GLN:O	1:A:458:LYS:HD3	1.99	0.62
1:C:339:ILE:HD13	1:C:492:TYR:HE1	1.64	0.62
1:C:690:LYS:HG2	1:C:691:LYS:H	1.62	0.62
1:B:714:GLN:OE1	1:B:715:GLU:HG3	2.00	0.62
1:A:434:LEU:CA	1:A:445:ARG:HD3	2.26	0.62
2:E:52:ILE:O	2:E:56:ASP:HB3	1.98	0.62
1:A:299:GLU:HG3	1:A:303:LYS:NZ	2.15	0.62
1:B:777:TYR:HD1	1:B:780:LEU:HD12	1.64	0.62
2:E:115:LYS:HZ2	2:E:115:LYS:HB3	1.65	0.62
2:E:115:LYS:HB3	2:E:115:LYS:NZ	2.15	0.62
2:E:7:GLU:O	2:E:11:GLU:HG3	1.98	0.62
1:B:714:GLN:HA	1:B:717:LYS:HD2	1.82	0.62
2:E:124:MET:O	2:E:127:GLU:HB2	1.99	0.62
1:A:559:ARG:HB3	1:A:559:ARG:HH11	1.64	0.62
1:B:349:ASN:OD1	1:B:350:VAL:HG23	2.00	0.62
1:B:750:GLN:O	1:B:754:GLU:HG3	2.00	0.61
1:A:550:SER:H	1:A:553:GLN:NE2	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:39:LEU:HD23	2:E:39:LEU:O	1.99	0.61
1:A:426:ILE:HD12	1:A:426:ILE:H	1.65	0.61
1:A:492:TYR:HD2	1:A:574:VAL:HG13	1.65	0.61
1:A:778:LYS:C	1:A:780:LEU:H	2.07	0.61
1:C:351:HIS:CB	1:C:386:GLU:HG2	2.29	0.61
1:C:731:GLU:O	1:C:735:VAL:HG23	2.00	0.61
2:F:37:ARG:HG2	2:F:43:PRO:HD2	1.82	0.61
1:B:299:GLU:C	1:B:303:LYS:HZ3	2.09	0.61
1:B:615:ILE:HD12	1:B:645:TRP:HH2	1.64	0.61
2:F:114:GLU:HG3	2:F:116:LEU:CD1	2.30	0.61
1:A:323:ASN:C	1:A:323:ASN:HD22	2.08	0.61
1:A:517:VAL:HG13	2:D:114:GLU:OE2	2.00	0.61
1:A:589:LYS:HE3	1:A:608:TRP:CG	2.36	0.61
2:D:79:THR:C	2:D:81:SER:H	2.07	0.61
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.81	0.61
1:B:327:LEU:HG	1:B:595:ILE:CG1	2.29	0.61
1:B:744:GLU:O	1:B:745:TYR:C	2.44	0.61
1:B:538:ILE:CD1	1:B:625:LEU:HD11	2.31	0.61
1:C:722:ILE:HD13	1:C:764:LEU:HD23	1.83	0.61
1:A:561:ASN:O	1:A:565:LYS:HG3	2.01	0.61
1:A:735:VAL:C	1:A:737:LYS:H	2.08	0.61
1:B:639:ASN:C	1:B:639:ASN:HD22	2.09	0.61
1:A:327:LEU:N	1:A:327:LEU:HD12	2.16	0.60
1:A:439:ASN:ND2	1:A:442:TYR:H	1.98	0.60
1:B:305:SER:HB3	1:B:594:PHE:CD1	2.36	0.60
1:C:325:TYR:HB2	1:C:498:ALA:HB3	1.82	0.60
1:B:717:LYS:HZ1	2:E:126:ARG:HG3	1.66	0.60
2:E:71:MET:C	2:E:73:ALA:H	2.09	0.60
1:A:400:LYS:HE2	1:A:475:GLU:OE2	2.02	0.60
1:B:777:TYR:CD1	1:B:780:LEU:HD12	2.36	0.60
1:C:716:LYS:O	1:C:720:ILE:HG12	2.01	0.60
1:C:733:GLU:HG2	1:C:753:LYS:HE2	1.83	0.60
1:C:736:LEU:HD21	1:C:749:PHE:HB2	1.83	0.60
1:A:295:VAL:HG23	1:A:605:THR:HA	1.82	0.60
1:A:334:LEU:HD13	1:A:361:ALA:HB1	1.82	0.60
1:B:616:GLU:HA	1:B:620:THR:CG2	2.25	0.60
2:F:28:THR:OG1	2:F:31:GLU:HG2	2.01	0.60
1:B:366:PHE:HA	1:B:477:MET:HE3	1.84	0.60
1:C:744:GLU:HB3	1:C:747:ASN:CB	2.30	0.60
1:A:368:GLN:HG3	1:A:383:GLY:C	2.26	0.60
1:A:706:ASN:ND2	1:A:708:ALA:HB3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ILE:HB	1:B:477:MET:HB2	1.84	0.60
1:B:697:ILE:HD13	1:B:732:ILE:HD12	1.84	0.60
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.32	0.60
1:A:438:ASN:HD22	1:A:438:ASN:N	2.00	0.59
1:A:497:LEU:HD12	1:A:553:GLN:HG2	1.83	0.59
1:A:664:ILE:HA	1:A:667:LEU:HD12	1.84	0.59
1:A:738:SER:O	1:A:740:GLN:N	2.34	0.59
1:A:463:THR:HG22	1:A:465:LEU:H	1.66	0.59
2:D:9:ILE:HD12	2:D:9:ILE:N	2.17	0.59
1:B:726:ILE:HD13	1:B:780:LEU:HD13	1.82	0.59
1:C:373:LYS:HD2	1:C:379:ALA:HB1	1.84	0.59
1:C:664:ILE:HG21	2:F:15:ALA:HB2	1.83	0.59
1:A:418:ILE:HG22	1:A:419:ILE:HG23	1.84	0.59
1:A:653:LYS:O	1:A:755:ARG:HD3	2.01	0.59
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.36	0.59
1:B:376:GLN:HB2	1:B:379:ALA:HB3	1.84	0.59
1:B:499:PRO:HG2	1:B:625:LEU:HB3	1.84	0.59
1:B:526:GLN:NE2	2:E:124:MET:HE2	2.15	0.59
1:B:744:GLU:OE1	1:B:744:GLU:HA	2.01	0.59
1:B:366:PHE:HD1	1:B:477:MET:CE	2.14	0.59
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.85	0.59
1:C:540:ARG:HH22	2:F:87:GLU:CD	2.11	0.59
1:B:375:GLY:HA2	1:B:464:VAL:HG11	1.84	0.59
1:C:457:THR:HG21	1:C:468:LYS:HA	1.84	0.59
2:F:62:THR:C	2:F:63:ILE:HD12	2.27	0.59
1:A:587:PRO:HB2	1:A:643:ILE:HD12	1.85	0.59
1:B:744:GLU:O	1:B:748:TYR:N	2.36	0.59
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.32	0.59
1:B:464:VAL:HG23	1:B:465:LEU:N	2.14	0.59
1:A:663:PHE:O	1:A:667:LEU:HG	2.03	0.59
1:A:666:ASN:O	1:A:670:ILE:HB	2.02	0.59
1:A:783:THR:CB	1:A:789:ASN:HD21	2.11	0.59
1:A:540:ARG:HH22	2:D:87:GLU:CD	2.11	0.58
1:C:546:LYS:HB3	1:C:549:LEU:HD21	1.84	0.58
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.85	0.58
1:A:736:LEU:HD21	1:A:749:PHE:HB2	1.85	0.58
1:B:546:LYS:HG3	1:B:576:ASN:O	2.02	0.58
2:D:92:PHE:CD2	2:D:108:VAL:HG21	2.39	0.58
1:B:733:GLU:C	1:B:735:VAL:H	2.10	0.58
2:F:44:THR:HG23	2:F:46:ALA:HB3	1.84	0.58
1:A:534:ILE:HA	1:A:538:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:THR:O	1:B:657:ILE:HB	2.02	0.58
1:C:526:GLN:HB2	2:F:124:MET:CE	2.34	0.58
2:F:97:ASN:ND2	2:F:99:TYR:HD1	2.00	0.58
1:C:669:SER:HA	1:C:672:ARG:HG2	1.85	0.58
1:A:349:ASN:N	1:A:349:ASN:HD22	2.02	0.58
2:D:5:THR:OG1	2:D:8:GLN:HG3	2.03	0.58
2:F:10:ALA:O	2:F:14:GLU:HB2	2.03	0.58
1:B:508:ILE:HG12	1:B:536:TYR:CD1	2.30	0.58
1:A:425:GLU:CD	1:A:445:ARG:NH1	2.59	0.58
1:A:629:ASN:HD22	1:A:631:SER:N	1.99	0.58
1:A:734:ASN:O	1:A:737:LYS:HB2	2.04	0.58
1:B:450:ASN:O	1:B:451:ASN:HB2	2.03	0.58
1:C:368:GLN:HG2	1:C:387:ASN:ND2	2.19	0.58
2:F:52:ILE:HD11	2:F:63:ILE:HD11	1.84	0.58
1:A:481:VAL:HG21	1:A:486:LYS:HD2	1.86	0.57
1:A:586:PHE:CE2	1:A:638:GLY:HA3	2.39	0.57
1:B:538:ILE:HD13	1:B:625:LEU:HD11	1.86	0.57
2:D:29:THR:OG1	2:D:52:ILE:HG12	2.04	0.57
1:B:722:ILE:HG23	1:B:760:VAL:HG11	1.85	0.57
2:E:95:ASP:OD2	2:E:97:ASN:HB3	2.04	0.57
1:C:338:LEU:O	1:C:343:VAL:HG23	2.04	0.57
2:F:97:ASN:ND2	2:F:99:TYR:HB2	2.18	0.57
1:A:372:LYS:NZ	4:A:902:3AT:O2G	2.33	0.57
1:A:440:GLN:H	1:A:440:GLN:CD	2.12	0.57
1:A:636:ALA:O	1:A:640:LYS:HA	2.04	0.57
1:B:726:ILE:HA	1:B:729:TYR:HB2	1.85	0.57
2:F:37:ARG:C	2:F:39:LEU:H	2.12	0.57
2:F:45:GLU:HA	2:F:48:LEU:HD12	1.86	0.57
1:A:758:ASN:O	1:A:762:LEU:HB2	2.05	0.57
1:B:514:ASP:CA	1:B:517:VAL:HG12	2.32	0.57
1:A:440:GLN:NE2	1:A:441:VAL:HG23	2.18	0.57
1:B:308:VAL:HB	1:B:311:HIS:HD1	1.69	0.57
1:B:754:GLU:O	1:B:757:THR:HB	2.05	0.57
1:C:293:ILE:HG22	1:C:295:VAL:HG13	1.87	0.57
2:F:115:LYS:O	2:F:116:LEU:HD12	2.05	0.57
1:B:497:LEU:HD13	1:B:556:MET:HG2	1.86	0.57
2:E:44:THR:HG23	2:E:47:GLU:H	1.70	0.57
1:C:636:ALA:HB3	1:C:639:ASN:HD21	1.70	0.57
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.40	0.57
2:F:26:THR:HA	2:F:63:ILE:O	2.05	0.57
1:B:629:ASN:HD21	1:B:631:SER:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:TYR:CD2	2:E:137:ASN:HB3	2.39	0.56
1:C:629:ASN:HD22	1:C:631:SER:N	2.00	0.56
1:A:440:GLN:HG2	1:A:461:LYS:HE2	1.87	0.56
2:D:53:ASN:O	2:D:57:ALA:HB2	2.05	0.56
1:B:296:LEU:HB2	1:B:604:LEU:HB3	1.87	0.56
1:B:368:GLN:HG3	1:B:383:GLY:C	2.31	0.56
1:B:716:LYS:HA	1:B:719:LYS:HE2	1.87	0.56
2:E:64:ASP:OD1	2:E:66:PRO:HD2	2.05	0.56
2:E:89:PHE:HE1	2:E:100:ILE:HG13	1.70	0.56
1:C:546:LYS:HG2	1:C:549:LEU:HD21	1.87	0.56
1:C:670:ILE:HD11	1:C:745:TYR:HA	1.87	0.56
2:F:49:GLN:HA	2:F:52:ILE:HG22	1.88	0.56
1:A:540:ARG:NH2	2:D:87:GLU:OE1	2.39	0.56
2:D:80:ASP:C	2:D:82:GLU:H	2.13	0.56
1:B:732:ILE:HG22	1:B:732:ILE:O	2.06	0.56
2:F:63:ILE:HD12	2:F:63:ILE:N	2.20	0.56
1:A:305:SER:HB3	1:A:594:PHE:CD1	2.41	0.56
1:A:718:ARG:O	1:A:722:ILE:HG13	2.06	0.56
1:B:462:ILE:HG12	1:B:468:LYS:HE3	1.87	0.56
1:B:657:ILE:CG1	1:B:658:PRO:HD2	2.35	0.56
1:B:509:PRO:HD2	1:B:536:TYR:CE1	2.40	0.56
1:C:747:ASN:HA	1:C:750:GLN:CD	2.31	0.56
1:C:775:LEU:H	1:C:775:LEU:CD2	2.15	0.56
2:F:37:ARG:HD2	2:F:42:ASN:CA	2.31	0.56
2:F:49:GLN:HA	2:F:52:ILE:CG2	2.36	0.56
2:F:105:LEU:HD12	2:F:125:ILE:CD1	2.36	0.56
1:B:528:GLY:O	1:B:532:LEU:HB2	2.05	0.56
1:C:329:ARG:HD2	1:C:590:ASP:OD2	2.06	0.56
1:C:639:ASN:ND2	1:C:639:ASN:C	2.63	0.56
2:F:122:ASP:HB3	2:F:126:ARG:HH22	1.71	0.56
1:B:729:TYR:CE2	1:B:773:PHE:CE1	2.85	0.56
1:C:697:ILE:HD13	1:C:732:ILE:HG12	1.88	0.56
1:C:744:GLU:C	1:C:746:LYS:N	2.59	0.56
1:A:668:SER:HB2	2:D:11:GLU:HA	1.88	0.55
1:B:538:ILE:O	1:B:540:ARG:HD3	2.06	0.55
2:F:37:ARG:C	2:F:39:LEU:N	2.62	0.55
2:F:92:PHE:CB	2:F:100:ILE:HD12	2.36	0.55
1:A:529:VAL:HG11	2:D:109:MET:SD	2.47	0.55
1:B:742:ALA:HB1	1:B:743:PRO:HD2	1.87	0.55
1:C:780:LEU:HB3	1:C:782:PHE:HE1	1.71	0.55
1:B:416:ASN:HB2	1:B:418:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:TYR:HB3	2:E:135:GLN:HB3	1.89	0.55
1:A:617:LYS:HD2	1:A:617:LYS:O	2.05	0.55
1:B:733:GLU:O	1:B:735:VAL:N	2.31	0.55
1:C:691:LYS:HB2	1:C:694:VAL:CG1	2.29	0.55
1:B:359:PRO:HB3	1:B:405:LEU:HD11	1.88	0.55
1:B:489:THR:CG2	1:B:490:ALA:H	2.04	0.55
2:E:41:GLN:HB3	2:E:43:PRO:HD3	1.89	0.55
1:A:434:LEU:HG	1:A:445:ARG:NE	2.20	0.55
1:A:659:THR:HG23	1:A:662:GLU:H	1.72	0.55
1:B:401:ILE:HG21	1:B:485:LEU:HB3	1.88	0.55
1:C:663:PHE:CZ	1:C:667:LEU:HD11	2.42	0.55
2:F:35:VAL:O	2:F:39:LEU:HG	2.06	0.55
1:A:709:ASN:HD21	1:A:724:ARG:NH1	2.05	0.55
1:C:308:VAL:HG23	1:C:492:TYR:OH	2.06	0.55
2:D:68:PHE:O	2:D:72:MET:HG2	2.07	0.55
1:B:331:VAL:O	1:B:332:ASN:C	2.50	0.55
1:B:639:ASN:HD22	1:B:640:LYS:N	2.05	0.55
1:B:778:LYS:C	1:B:780:LEU:H	2.14	0.55
2:D:102:ALA:HA	2:D:125:ILE:HG13	1.88	0.55
1:C:437:SER:C	1:C:439:ASN:H	2.15	0.55
1:C:502:THR:O	1:C:505:LYS:HB3	2.07	0.55
2:F:136:VAL:HA	2:F:140:GLU:OE1	2.07	0.54
1:A:607:ASN:ND2	1:A:610:MET:H	2.03	0.54
1:B:585:GLU:HB3	1:B:586:PHE:CD1	2.42	0.54
1:B:629:ASN:HD22	1:B:631:SER:N	1.98	0.54
1:B:697:ILE:HD13	1:B:732:ILE:CD1	2.38	0.54
1:B:403:LEU:HD13	1:B:476:VAL:HG21	1.90	0.54
1:B:756:ILE:O	1:B:760:VAL:HG23	2.06	0.54
2:E:13:LYS:HG2	2:E:65:PHE:CE1	2.43	0.54
2:E:37:ARG:HA	2:E:41:GLN:O	2.08	0.54
1:C:623:ASP:OD1	2:F:94:LYS:HD3	2.07	0.54
2:D:9:ILE:HG23	2:D:69:LEU:HD22	1.90	0.54
1:B:752:LEU:O	1:B:756:ILE:HG13	2.08	0.54
1:C:360:VAL:HG22	1:C:363:TYR:HB2	1.88	0.54
1:C:759:GLN:O	1:C:762:LEU:HB3	2.08	0.54
1:C:775:LEU:HG	1:C:776:LEU:CD1	2.37	0.54
2:F:72:MET:O	2:F:76:MET:HB3	2.08	0.54
1:A:657:ILE:HD11	1:A:704:TYR:CD1	2.42	0.54
1:C:667:LEU:HA	1:C:670:ILE:HG22	1.89	0.54
1:A:318:ILE:O	1:A:322:LEU:HG	2.08	0.54
1:A:329:ARG:HD2	1:A:590:ASP:OD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.43	0.54
1:A:629:ASN:ND2	1:A:631:SER:HB2	2.22	0.54
2:D:12:PHE:HB3	2:D:68:PHE:HE2	1.73	0.54
1:C:639:ASN:HD22	1:C:640:LYS:N	2.04	0.54
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.88	0.54
1:C:746:LYS:HD2	1:C:746:LYS:O	2.08	0.54
1:A:797:ILE:HG23	1:A:798:ASP:N	2.16	0.54
1:C:318:ILE:HD12	1:C:318:ILE:N	2.22	0.54
1:C:791:GLU:OE1	1:C:791:GLU:N	2.36	0.54
2:F:27:ILE:CG1	2:F:63:ILE:HB	2.37	0.54
1:B:535:LYS:HE2	1:B:535:LYS:CA	2.35	0.54
2:E:100:ILE:HA	2:E:104:GLU:OE1	2.08	0.54
1:C:657:ILE:HG13	1:C:759:GLN:CB	2.38	0.54
1:C:659:THR:HG22	1:C:661:ALA:N	2.06	0.54
1:C:722:ILE:HG12	1:C:763:LEU:HB2	1.90	0.54
1:C:730:ASN:ND2	1:C:782:PHE:HB2	2.23	0.54
1:A:368:GLN:HG3	1:A:383:GLY:HA3	1.90	0.54
1:B:368:GLN:HG3	1:B:383:GLY:HA3	1.89	0.54
1:B:530:THR:C	1:B:532:LEU:H	2.16	0.54
1:C:480:ASN:HD21	1:C:483:GLY:CA	2.20	0.54
1:B:322:LEU:HD13	1:B:556:MET:CE	2.38	0.53
1:B:560:LEU:O	1:B:564:VAL:HG13	2.07	0.53
2:D:41:GLN:NE2	2:D:76:MET:HE1	2.22	0.53
1:C:456:LYS:HA	1:C:469:PHE:CE1	2.43	0.53
2:D:63:ILE:HA	2:D:67:GLU:OE2	2.08	0.53
1:B:419:ILE:C	1:B:419:ILE:HD12	2.34	0.53
1:A:616:GLU:HA	1:A:620:THR:CG2	2.37	0.53
1:A:670:ILE:HD13	1:A:670:ILE:O	2.08	0.53
1:B:424:LYS:HE2	1:B:433:TYR:OH	2.08	0.53
1:A:322:LEU:HD12	1:A:556:MET:HE1	1.91	0.53
1:A:360:VAL:HG23	1:A:403:LEU:HD22	1.91	0.53
2:E:63:ILE:HG13	2:E:67:GLU:OE2	2.08	0.53
1:C:698:ALA:O	1:C:701:LEU:HB2	2.08	0.53
1:C:657:ILE:HG13	1:C:759:GLN:CG	2.39	0.53
1:C:747:ASN:HD22	1:C:750:GLN:CD	2.16	0.53
1:A:335:ALA:O	1:A:339:ILE:HG13	2.09	0.53
1:B:445:ARG:HB3	1:B:471:TRP:CH2	2.43	0.53
1:C:301:ALA:HB1	1:C:604:LEU:HB2	1.91	0.53
1:C:751:TYR:O	1:C:754:GLU:HB3	2.09	0.53
1:A:372:LYS:C	1:A:374:HIS:H	2.17	0.53
1:B:519:THR:N	1:B:520:PRO:HD3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:LEU:O	1:B:766:HIS:HB2	2.09	0.53
1:C:450:ASN:O	1:C:451:ASN:HB2	2.09	0.53
1:C:501:LEU:O	1:C:504:ILE:HG12	2.08	0.53
2:F:75:LYS:O	2:F:75:LYS:HG2	2.09	0.53
1:A:526:GLN:NE2	2:D:144:MET:HE2	2.24	0.53
1:A:656:THR:O	1:A:755:ARG:HD2	2.08	0.53
1:B:564:VAL:HG11	1:B:574:VAL:HG11	1.90	0.53
1:C:349:ASN:N	1:C:349:ASN:HD22	2.05	0.53
1:A:385:LEU:CD1	1:A:389:LYS:HE3	2.39	0.52
1:B:705:TYR:CE1	2:E:139:GLU:HB3	2.44	0.52
1:A:540:ARG:HD3	1:A:627:TYR:OH	2.09	0.52
1:A:657:ILE:CG2	1:A:756:ILE:HA	2.39	0.52
2:E:44:THR:HG22	2:E:47:GLU:OE1	2.09	0.52
1:C:509:PRO:O	1:C:511:LYS:N	2.39	0.52
1:C:512:GLU:O	1:C:516:VAL:HG23	2.09	0.52
2:F:52:ILE:O	2:F:56:ASP:HB3	2.09	0.52
2:D:15:ALA:HB1	2:D:35:VAL:HG13	1.90	0.52
1:B:327:LEU:HD12	1:B:327:LEU:N	2.25	0.52
1:B:724:ARG:O	1:B:727:GLN:HB3	2.10	0.52
1:B:773:PHE:C	1:B:775:LEU:H	2.17	0.52
1:C:695:LYS:HD2	2:F:18:LEU:HB3	1.92	0.52
2:F:25:GLY:O	2:F:64:ASP:HA	2.09	0.52
1:A:722:ILE:HG23	1:A:760:VAL:CG1	2.32	0.52
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.91	0.52
1:A:513:TRP:O	1:A:517:VAL:HG23	2.09	0.52
1:B:450:ASN:CG	1:B:452:GLU:HG3	2.34	0.52
1:C:515:LYS:O	1:C:515:LYS:HG2	2.09	0.52
1:C:616:GLU:HA	1:C:620:THR:HG1	1.75	0.52
1:B:419:ILE:HD12	1:B:419:ILE:O	2.09	0.52
1:C:616:GLU:HA	1:C:620:THR:OG1	2.09	0.52
2:F:41:GLN:HB3	2:F:43:PRO:HD3	1.92	0.52
1:A:304:ALA:HB3	1:A:604:LEU:HD13	1.92	0.52
1:A:533:LEU:HG	1:A:538:ILE:HD11	1.92	0.52
1:C:669:SER:C	1:C:671:ARG:H	2.16	0.52
1:B:546:LYS:O	1:B:547:GLY:O	2.28	0.52
1:A:501:LEU:HD23	1:A:623:ASP:C	2.35	0.52
1:B:326:ILE:C	1:B:327:LEU:HD12	2.34	0.52
1:B:334:LEU:N	1:B:334:LEU:HD22	2.25	0.52
1:B:752:LEU:CD2	1:B:756:ILE:HD11	2.40	0.52
2:E:29:THR:HG23	2:E:32:LEU:HD22	1.91	0.52
1:A:456:LYS:HD3	1:A:471:TRP:CD1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:ASN:OD1	1:B:792:VAL:HB	2.10	0.51
1:C:755:ARG:HA	1:C:758:ASN:HD22	1.74	0.51
1:C:775:LEU:HG	1:C:776:LEU:HD12	1.92	0.51
2:F:95:ASP:OD1	2:F:97:ASN:OD1	2.29	0.51
2:D:52:ILE:HD11	2:D:63:ILE:HG12	1.92	0.51
1:B:310:GLU:CD	1:B:310:GLU:H	2.18	0.51
2:D:12:PHE:HD1	2:D:39:LEU:HD21	1.75	0.51
1:B:607:ASN:ND2	1:B:609:GLU:HB2	2.26	0.51
1:B:565:LYS:NZ	1:B:572:GLY:HA2	2.25	0.51
1:B:752:LEU:O	1:B:752:LEU:HD23	2.10	0.51
2:E:63:ILE:HD12	2:E:63:ILE:N	2.26	0.51
1:C:561:ASN:O	1:C:564:VAL:HG22	2.11	0.51
1:B:360:VAL:O	1:B:360:VAL:HG22	2.09	0.51
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.45	0.51
1:A:449:GLU:N	1:A:449:GLU:OE1	2.44	0.51
1:A:657:ILE:HD11	1:A:704:TYR:CG	2.46	0.51
1:B:760:VAL:HG11	1:B:773:PHE:HE2	1.75	0.51
1:C:504:ILE:HG21	1:C:625:LEU:HD22	1.93	0.51
1:C:747:ASN:HD22	1:C:750:GLN:NE2	2.09	0.51
1:A:456:LYS:HB2	1:A:470:ASN:HA	1.93	0.51
1:A:648:PRO:HA	1:A:651:LYS:CD	2.41	0.51
1:B:655:ASN:HB3	1:B:759:GLN:NE2	2.26	0.51
1:A:404:LYS:HE2	1:A:450:ASN:O	2.10	0.51
1:A:549:LEU:N	1:A:549:LEU:HD12	2.26	0.51
1:A:338:LEU:O	1:A:341:SER:HB3	2.11	0.51
1:A:478:ALA:HA	1:A:488:LEU:HG	1.92	0.51
1:A:781:ASN:HB3	1:A:789:ASN:CG	2.35	0.51
1:B:540:ARG:CZ	1:B:627:TYR:CE1	2.94	0.51
1:B:632:TYR:O	1:B:634:LYS:HG3	2.10	0.51
1:B:711:ILE:HG13	1:B:712:PHE:HD1	1.76	0.51
1:B:381:GLU:CG	1:B:465:LEU:HD21	2.40	0.50
2:E:47:GLU:HA	2:E:50:ASP:OD1	2.11	0.50
1:C:640:LYS:HE2	6:C:36:HOH:O	2.11	0.50
1:B:549:LEU:HD11	1:B:553:GLN:HB3	1.93	0.50
2:E:109:MET:C	2:E:111:ASN:H	2.20	0.50
1:C:339:ILE:HD13	1:C:492:TYR:CE1	2.44	0.50
1:C:521:ASN:HB2	1:C:524:GLU:HB2	1.94	0.50
2:F:64:ASP:OD1	2:F:67:GLU:HG3	2.11	0.50
1:A:664:ILE:C	1:A:666:ASN:N	2.69	0.50
1:B:730:ASN:ND2	1:B:734:ASN:N	2.58	0.50
1:B:773:PHE:O	1:B:777:TYR:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:THR:C	2:E:119:GLU:H	2.20	0.50
2:F:23:GLY:C	2:F:25:GLY:H	2.19	0.50
1:B:499:PRO:HD2	1:B:625:LEU:O	2.12	0.50
1:B:707:SER:C	1:B:709:ASN:H	2.18	0.50
1:B:743:PRO:O	1:B:747:ASN:CB	2.60	0.50
2:E:125:ILE:O	2:E:129:ASP:HB2	2.10	0.50
1:C:376:GLN:O	1:C:380:VAL:HG23	2.11	0.50
1:C:666:ASN:N	1:C:666:ASN:HD22	2.08	0.50
2:D:95:ASP:OD2	2:D:97:ASN:HB3	2.12	0.50
1:B:373:LYS:O	1:B:374:HIS:C	2.54	0.50
1:B:537:GLY:O	1:B:625:LEU:HD21	2.11	0.50
1:B:704:TYR:HD1	1:B:724:ARG:HB2	1.77	0.50
1:C:668:SER:O	1:C:671:ARG:HB3	2.11	0.50
1:A:406:ASP:O	1:A:410:ILE:HG12	2.11	0.50
2:E:87:GLU:O	2:E:91:VAL:HG23	2.11	0.50
1:C:523:LEU:HD11	2:F:144:MET:HG2	1.94	0.50
1:C:740:GLN:O	1:C:741:ILE:C	2.54	0.50
1:A:740:GLN:O	1:A:741:ILE:HG12	2.12	0.50
2:D:15:ALA:HA	2:D:18:LEU:HD12	1.94	0.50
2:D:20:ASP:C	2:D:22:ASP:H	2.18	0.50
1:B:424:LYS:HG2	1:B:433:TYR:CE2	2.47	0.50
1:B:605:THR:HG21	1:B:611:THR:OG1	2.11	0.50
1:A:299:GLU:O	1:A:303:LYS:HG3	2.12	0.50
1:B:332:ASN:HD22	1:B:333:LYS:N	2.10	0.50
1:C:387:ASN:O	1:C:391:ILE:HG12	2.12	0.50
1:A:294:ASP:O	1:A:610:MET:HE1	2.11	0.50
1:A:505:LYS:HE3	1:A:513:TRP:CD2	2.47	0.50
1:A:781:ASN:HB3	1:A:789:ASN:ND2	2.27	0.50
1:B:359:PRO:C	1:B:361:ALA:H	2.20	0.50
1:B:703:ASP:O	1:B:704:TYR:C	2.54	0.50
1:B:735:VAL:CG2	1:B:738:SER:HB2	2.42	0.50
1:C:712:PHE:HB3	1:C:716:LYS:HG2	1.93	0.50
2:F:83:GLU:O	2:F:87:GLU:HG3	2.11	0.50
1:A:440:GLN:C	1:A:458:LYS:HD3	2.37	0.49
1:A:782:PHE:O	1:A:783:THR:C	2.54	0.49
1:B:366:PHE:CD1	1:B:400:LYS:HD3	2.47	0.49
1:B:459:GLU:O	1:B:461:LYS:N	2.44	0.49
1:B:793:PHE:HA	1:B:796:ILE:HG12	1.94	0.49
1:C:657:ILE:CD1	1:C:759:GLN:HG2	2.42	0.49
1:A:321:GLU:HG2	1:A:322:LEU:HD23	1.94	0.49
2:D:24:ASP:O	2:D:65:PHE:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:LEU:O	1:B:776:LEU:HG	2.12	0.49
1:A:349:ASN:ND2	1:A:349:ASN:H	2.10	0.49
1:B:299:GLU:O	1:B:303:LYS:HG3	2.13	0.49
1:B:318:ILE:N	1:B:318:ILE:HD12	2.28	0.49
1:B:585:GLU:HB3	1:B:586:PHE:CE1	2.46	0.49
1:B:743:PRO:O	1:B:747:ASN:HB2	2.11	0.49
1:C:462:ILE:HD11	1:C:466:GLY:C	2.37	0.49
1:C:537:GLY:O	1:C:625:LEU:HD21	2.13	0.49
1:A:392:THR:HG21	1:C:635:ILE:HG13	1.93	0.49
1:B:302:LEU:C	1:B:304:ALA:H	2.20	0.49
1:B:653:LYS:O	1:B:755:ARG:HD3	2.13	0.49
1:C:744:GLU:C	1:C:747:ASN:H	2.20	0.49
1:A:694:VAL:HG12	1:A:696:LYS:HB2	1.95	0.49
1:A:706:ASN:C	1:A:708:ALA:H	2.20	0.49
2:D:48:LEU:O	2:D:52:ILE:HG22	2.13	0.49
1:C:791:GLU:H	1:C:791:GLU:CD	2.17	0.49
1:B:300:LYS:HA	1:B:303:LYS:NZ	2.28	0.49
1:B:730:ASN:HD21	1:B:734:ASN:N	2.10	0.49
1:C:304:ALA:HB3	1:C:604:LEU:HD13	1.95	0.49
1:C:364:ILE:HB	1:C:477:MET:HB2	1.95	0.49
1:C:376:GLN:HB2	1:C:379:ALA:HB3	1.93	0.49
2:F:38:SER:C	2:F:39:LEU:HD23	2.38	0.49
2:F:137:ASN:OD1	2:F:137:ASN:C	2.56	0.49
1:A:564:VAL:HG23	1:A:565:LYS:N	2.27	0.49
2:D:75:LYS:C	2:D:77:LYS:H	2.21	0.49
1:C:636:ALA:HB3	1:C:639:ASN:ND2	2.28	0.49
1:C:764:LEU:C	1:C:766:HIS:H	2.20	0.49
1:A:538:ILE:HD12	1:A:538:ILE:H	1.78	0.49
1:B:315:PHE:HE2	1:B:560:LEU:HB3	1.78	0.49
1:B:530:THR:C	1:B:532:LEU:N	2.70	0.49
1:C:523:LEU:HB2	2:F:127:GLU:OE2	2.13	0.49
1:C:657:ILE:HD12	1:C:704:TYR:CE1	2.48	0.49
1:A:346:LYS:HD3	1:A:364:ILE:HG12	1.94	0.49
1:A:349:ASN:N	1:A:349:ASN:ND2	2.61	0.49
1:B:296:LEU:O	1:B:603:ILE:HA	2.13	0.49
1:B:437:SER:C	1:B:439:ASN:H	2.21	0.49
2:E:19:PHE:CE2	2:E:34:THR:HG21	2.48	0.49
2:E:52:ILE:O	2:E:52:ILE:HG13	2.12	0.49
2:D:27:ILE:HB	2:D:31:GLU:CG	2.42	0.48
2:E:106:ARG:NH2	2:E:118:ASP:HA	2.27	0.48
1:C:451:ASN:N	1:C:451:ASN:HD22	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:O	1:C:466:GLY:N	2.34	0.48
1:C:550:SER:H	1:C:553:GLN:HE21	1.60	0.48
1:C:581:GLN:NE2	1:C:628:PHE:HA	2.27	0.48
1:C:667:LEU:HA	1:C:670:ILE:CG2	2.44	0.48
1:C:671:ARG:HD3	1:C:672:ARG:HH21	1.76	0.48
2:F:114:GLU:HG3	2:F:116:LEU:HD11	1.94	0.48
1:A:559:ARG:HH11	1:A:559:ARG:CB	2.24	0.48
1:B:368:GLN:HG3	1:B:384:ASN:N	2.28	0.48
2:E:37:ARG:HG2	2:E:42:ASN:HA	1.96	0.48
1:A:718:ARG:HG3	2:D:132:GLY:O	2.13	0.48
1:B:549:LEU:HD21	1:B:557:LEU:HD22	1.94	0.48
1:B:774:LYS:CG	1:B:774:LYS:O	2.62	0.48
1:C:655:ASN:N	1:C:655:ASN:ND2	2.60	0.48
1:B:460:GLY:HA2	1:B:468:LYS:NZ	2.28	0.48
1:B:499:PRO:HG2	1:B:504:ILE:HD11	1.94	0.48
1:B:526:GLN:HE21	2:E:124:MET:CE	2.19	0.48
2:E:62:THR:C	2:E:63:ILE:HD12	2.39	0.48
1:C:511:LYS:O	1:C:514:ASP:HB2	2.13	0.48
1:C:763:LEU:HD21	2:F:131:ASP:HB2	1.95	0.48
1:A:400:LYS:HE2	1:A:475:GLU:CD	2.39	0.48
1:A:508:ILE:HG23	1:A:532:LEU:HD22	1.96	0.48
1:B:350:VAL:CG2	1:B:398:ILE:HG12	2.43	0.48
1:C:712:PHE:HB3	1:C:716:LYS:CG	2.44	0.48
2:F:24:ASP:O	2:F:26:THR:HG23	2.13	0.48
2:F:102:ALA:CA	2:F:125:ILE:HG13	2.40	0.48
1:B:552:TRP:CD1	1:B:552:TRP:C	2.90	0.48
1:C:691:LYS:HE2	1:C:741:ILE:CD1	2.44	0.48
2:D:120:GLU:O	2:D:123:GLU:N	2.47	0.48
1:B:311:HIS:HD2	1:B:564:VAL:CB	2.23	0.48
1:B:339:ILE:HD11	1:B:490:ALA:O	2.13	0.48
1:C:753:LYS:NZ	1:C:753:LYS:HB3	2.29	0.48
2:F:13:LYS:HG3	2:F:65:PHE:CD2	2.49	0.48
2:D:33:GLY:C	2:D:35:VAL:H	2.22	0.48
1:B:377:GLN:O	1:B:381:GLU:HG3	2.14	0.48
1:B:704:TYR:HH	2:E:131:ASP:CG	2.21	0.48
1:C:691:LYS:O	1:C:694:VAL:HG22	2.13	0.48
1:C:693:SER:O	1:C:697:ILE:HG13	2.14	0.48
1:A:324:THR:CB	1:A:499:PRO:HA	2.44	0.48
1:A:368:GLN:HG3	1:A:383:GLY:CA	2.44	0.48
1:A:438:ASN:N	1:A:438:ASN:ND2	2.62	0.48
1:A:665:LYS:HG2	2:D:11:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:HB3	1:B:567:THR:CG2	2.44	0.48
2:E:105:LEU:O	2:E:109:MET:HG2	2.14	0.48
1:C:636:ALA:O	1:C:640:LYS:HA	2.14	0.48
1:C:723:PHE:HB2	1:C:793:PHE:CD2	2.49	0.48
2:E:71:MET:C	2:E:73:ALA:N	2.72	0.47
1:C:747:ASN:O	1:C:750:GLN:HG2	2.14	0.47
1:A:716:LYS:O	1:A:717:LYS:C	2.57	0.47
1:A:778:LYS:C	1:A:780:LEU:N	2.72	0.47
1:B:648:PRO:C	1:B:650:THR:N	2.72	0.47
2:E:6:GLU:C	2:E:8:GLN:N	2.69	0.47
1:C:664:ILE:CG2	2:F:15:ALA:HB2	2.44	0.47
1:C:597:ASN:HD21	1:C:601:GLU:HB2	1.78	0.47
1:A:735:VAL:C	1:A:737:LYS:N	2.73	0.47
1:B:470:ASN:CG	1:B:471:TRP:H	2.22	0.47
1:C:292:ARG:HH22	1:C:297:LYS:HZ1	1.58	0.47
2:F:92:PHE:HB2	2:F:100:ILE:HD12	1.96	0.47
1:A:512:GLU:O	1:A:516:VAL:HG23	2.15	0.47
1:A:604:LEU:O	1:A:604:LEU:HD23	2.14	0.47
1:B:355:SER:HB2	1:B:371:SER:HA	1.96	0.47
1:B:596:ILE:HG12	1:B:602:PHE:CD2	2.49	0.47
1:C:550:SER:O	1:C:554:LYS:HG3	2.13	0.47
1:A:345:THR:HB	1:A:491:ASP:HB3	1.96	0.47
1:A:775:LEU:H	1:A:775:LEU:CD1	2.20	0.47
2:D:93:ASP:OD2	2:D:96:GLY:N	2.47	0.47
1:B:550:SER:H	1:B:553:GLN:HE21	1.63	0.47
1:B:570:THR:O	1:B:572:GLY:N	2.48	0.47
2:E:9:ILE:C	2:E:11:GLU:N	2.73	0.47
1:C:292:ARG:HH12	1:C:297:LYS:HE2	1.80	0.47
1:C:434:LEU:N	1:C:434:LEU:HD22	2.30	0.47
1:C:587:PRO:HB2	1:C:643:ILE:CD1	2.43	0.47
1:C:597:ASN:ND2	1:C:601:GLU:HB2	2.29	0.47
1:C:763:LEU:O	1:C:766:HIS:HB2	2.15	0.47
2:E:132:GLY:C	2:E:134:GLY:H	2.21	0.47
1:C:292:ARG:HH22	1:C:297:LYS:CE	2.27	0.47
2:F:20:ASP:OD2	2:F:27:ILE:HG23	2.15	0.47
2:D:102:ALA:CA	2:D:125:ILE:HG13	2.45	0.47
1:B:308:VAL:HB	1:B:311:HIS:ND1	2.30	0.47
1:B:338:LEU:HD21	1:B:409:ARG:CZ	2.44	0.47
1:B:565:LYS:C	1:B:567:THR:N	2.73	0.47
1:B:649:ILE:HG22	1:B:649:ILE:O	2.15	0.47
1:B:722:ILE:O	1:B:726:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:PHE:HE2	2:E:108:VAL:HG11	1.79	0.47
1:C:622:LYS:HA	1:C:622:LYS:HD3	1.71	0.47
1:C:657:ILE:HG23	1:C:658:PRO:HD2	1.97	0.47
1:C:692:GLU:C	1:C:734:ASN:HD21	2.23	0.47
2:F:97:ASN:ND2	2:F:99:TYR:CD1	2.83	0.47
1:A:492:TYR:CD2	1:A:574:VAL:CG1	2.98	0.46
2:D:29:THR:O	2:D:29:THR:HG22	2.16	0.46
1:B:614:PHE:C	1:B:614:PHE:CD2	2.92	0.46
1:B:784:GLU:HG2	1:B:788:ASP:OD2	2.15	0.46
2:E:9:ILE:C	2:E:11:GLU:H	2.23	0.46
1:C:739:LYS:C	1:C:741:ILE:N	2.73	0.46
2:F:99:TYR:CD2	2:F:137:ASN:HB3	2.50	0.46
1:A:728:ALA:C	1:A:730:ASN:H	2.23	0.46
1:B:401:ILE:HG22	1:B:485:LEU:HD23	1.97	0.46
1:B:723:PHE:HB2	1:B:793:PHE:CE2	2.50	0.46
2:E:63:ILE:HG21	2:E:71:MET:CE	2.42	0.46
1:C:713:SER:OG	1:C:715:GLU:HG2	2.15	0.46
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.50	0.46
1:B:353:LYS:HE2	1:B:353:LYS:HA	1.97	0.46
1:C:546:LYS:CB	1:C:549:LEU:HD21	2.46	0.46
1:A:581:GLN:NE2	1:A:629:ASN:H	2.14	0.46
1:A:694:VAL:HG11	1:A:731:GLU:CG	2.45	0.46
1:B:589:LYS:HE2	1:B:608:TRP:CD1	2.51	0.46
1:B:709:ASN:OD1	1:B:717:LYS:HG2	2.15	0.46
2:E:20:ASP:CG	2:E:27:ILE:HG22	2.41	0.46
1:C:655:ASN:N	1:C:655:ASN:HD22	2.13	0.46
1:C:697:ILE:HD11	1:C:735:VAL:HG21	1.96	0.46
2:F:47:GLU:HA	2:F:50:ASP:HB3	1.96	0.46
1:A:359:PRO:HB2	1:A:405:LEU:HD11	1.97	0.46
1:A:723:PHE:HB2	1:A:793:PHE:CE2	2.50	0.46
1:A:754:GLU:HG2	1:A:758:ASN:HD21	1.81	0.46
1:A:760:VAL:C	1:A:762:LEU:H	2.23	0.46
1:B:346:LYS:HD3	1:B:364:ILE:HD11	1.97	0.46
1:B:530:THR:HG22	2:E:92:PHE:CZ	2.51	0.46
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.49	0.46
1:A:456:LYS:HA	1:A:469:PHE:CE1	2.50	0.46
1:A:711:ILE:HG13	1:A:712:PHE:N	2.31	0.46
2:F:92:PHE:HB2	2:F:100:ILE:CD1	2.45	0.46
1:A:434:LEU:HD23	1:A:435:LEU:N	2.30	0.46
1:A:470:ASN:O	1:A:471:TRP:C	2.59	0.46
1:A:768:LYS:HB2	1:A:797:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ARG:HA	2:D:138:TYR:CE1	2.50	0.46
1:B:338:LEU:HD21	1:B:409:ARG:NE	2.29	0.46
1:B:415:GLU:C	1:B:417:GLY:H	2.23	0.46
1:C:437:SER:O	1:C:439:ASN:N	2.48	0.46
1:A:587:PRO:HB2	1:A:643:ILE:CD1	2.46	0.46
1:A:664:ILE:HD12	2:D:39:LEU:HD13	1.97	0.46
2:D:79:THR:C	2:D:81:SER:N	2.73	0.46
1:B:650:THR:O	1:B:651:LYS:C	2.59	0.46
1:C:455:TYR:HB3	1:C:474:ILE:HD11	1.97	0.46
1:A:329:ARG:HB3	1:A:330:PRO:CD	2.46	0.46
1:B:368:GLN:HG3	1:B:383:GLY:CA	2.46	0.46
1:B:723:PHE:O	1:B:727:GLN:N	2.44	0.46
1:C:406:ASP:OD1	1:C:408:LEU:N	2.49	0.46
1:C:456:LYS:HA	1:C:469:PHE:HE1	1.81	0.46
1:A:359:PRO:O	1:A:405:LEU:HD11	2.16	0.46
1:A:360:VAL:O	1:A:361:ALA:C	2.57	0.46
1:A:540:ARG:NH2	2:D:87:GLU:CD	2.73	0.46
1:B:378:LEU:HB2	1:C:377:GLN:HE22	1.81	0.46
2:E:107:HIS:O	2:E:111:ASN:ND2	2.49	0.46
1:C:477:MET:HE2	1:C:477:MET:HA	1.97	0.46
1:C:742:ALA:O	1:C:743:PRO:C	2.58	0.46
1:A:344:ALA:O	1:A:489:THR:HG22	2.16	0.45
1:A:704:TYR:C	1:A:704:TYR:CD2	2.94	0.45
1:C:730:ASN:HD21	1:C:782:PHE:HB2	1.81	0.45
1:C:748:TYR:O	1:C:751:TYR:HB3	2.16	0.45
2:D:27:ILE:O	2:D:63:ILE:HB	2.17	0.45
1:C:368:GLN:HG3	1:C:383:GLY:C	2.42	0.45
1:C:520:PRO:HG2	1:C:521:ASN:H	1.80	0.45
1:A:299:GLU:HG3	1:A:303:LYS:CE	2.47	0.45
1:A:432:TYR:CD2	1:A:447:SER:HA	2.52	0.45
1:C:557:LEU:O	1:C:558:ASP:C	2.59	0.45
2:F:144:MET:SD	2:F:145:MET:HE2	2.56	0.45
1:A:438:ASN:ND2	1:A:438:ASN:H	2.15	0.45
1:A:695:LYS:HD2	2:D:18:LEU:HB3	1.99	0.45
1:B:501:LEU:HG	1:B:623:ASP:O	2.16	0.45
1:B:607:ASN:HD21	1:B:609:GLU:HB2	1.82	0.45
1:B:653:LYS:HE2	1:B:755:ARG:NH1	2.28	0.45
1:C:747:ASN:ND2	1:C:750:GLN:NE2	2.65	0.45
1:A:670:ILE:HG23	1:A:745:TYR:CZ	2.51	0.45
2:D:92:PHE:CE2	2:D:108:VAL:HG11	2.50	0.45
1:B:603:ILE:HD13	1:B:614:PHE:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:LYS:C	1:B:780:LEU:N	2.75	0.45
1:A:299:GLU:HG3	1:A:303:LYS:HE2	1.99	0.45
1:B:455:TYR:CD2	1:B:474:ILE:HG12	2.51	0.45
1:B:776:LEU:HD13	1:B:779:GLN:CD	2.41	0.45
1:B:792:VAL:HG12	1:B:796:ILE:HD11	1.98	0.45
1:C:344:ALA:O	1:C:489:THR:HG22	2.16	0.45
1:C:505:LYS:HE3	1:C:513:TRP:CE2	2.52	0.45
2:F:29:THR:OG1	2:F:52:ILE:HG12	2.16	0.45
1:A:364:ILE:HD12	1:A:364:ILE:N	2.31	0.45
1:B:456:LYS:HG3	1:B:457:THR:N	2.30	0.45
1:C:707:SER:C	1:C:709:ASN:H	2.24	0.45
2:E:117:THR:C	2:E:119:GLU:N	2.73	0.45
1:C:323:ASN:HD22	1:C:598:PRO:CB	2.29	0.45
1:C:375:GLY:HA2	1:C:464:VAL:HG11	1.99	0.45
1:C:450:ASN:CG	1:C:452:GLU:HG3	2.41	0.45
1:C:792:VAL:O	1:C:796:ILE:HG12	2.17	0.45
1:A:587:PRO:HG3	1:A:636:ALA:HB2	1.99	0.45
1:B:391:ILE:HD11	1:B:400:LYS:CG	2.45	0.45
1:B:785:ASN:OD1	1:B:788:ASP:HB2	2.17	0.45
1:B:793:PHE:HA	1:B:796:ILE:CG1	2.47	0.45
1:A:333:LYS:C	1:A:335:ALA:H	2.25	0.45
2:D:15:ALA:O	2:D:18:LEU:HB2	2.16	0.45
1:B:507:GLN:HG2	1:B:536:TYR:HB3	1.99	0.45
1:C:308:VAL:HG13	1:C:340:LYS:HD3	1.99	0.45
1:A:534:ILE:HA	1:A:538:ILE:CD1	2.47	0.44
1:B:322:LEU:HD11	1:B:559:ARG:HD3	1.97	0.44
1:B:744:GLU:OE2	1:B:748:TYR:HB2	2.18	0.44
2:E:29:THR:HA	2:E:32:LEU:HB2	1.99	0.44
1:C:403:LEU:HD13	1:C:476:VAL:HG11	1.99	0.44
1:C:669:SER:C	1:C:671:ARG:N	2.75	0.44
1:C:524:GLU:HA	1:C:524:GLU:OE1	2.17	0.44
1:C:648:PRO:O	1:C:649:ILE:C	2.60	0.44
2:F:115:LYS:HD3	2:F:116:LEU:N	2.33	0.44
2:D:33:GLY:C	2:D:35:VAL:N	2.76	0.44
2:D:136:VAL:HA	2:D:140:GLU:OE1	2.17	0.44
1:B:345:THR:HB	1:B:491:ASP:HB3	1.98	0.44
1:B:425:GLU:N	1:B:432:TYR:O	2.47	0.44
1:B:716:LYS:HA	1:B:719:LYS:HB3	2.00	0.44
1:B:733:GLU:C	1:B:735:VAL:N	2.70	0.44
2:E:129:ASP:OD1	2:E:132:GLY:N	2.37	0.44
1:C:462:ILE:HG13	1:C:463:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:THR:O	1:C:755:ARG:HD2	2.18	0.44
1:A:505:LYS:HE3	1:A:513:TRP:CG	2.52	0.44
1:A:700:TYR:CD1	1:A:727:GLN:HB3	2.53	0.44
1:B:302:LEU:C	1:B:304:ALA:N	2.75	0.44
1:B:470:ASN:CG	1:B:471:TRP:N	2.76	0.44
1:B:649:ILE:CD1	2:E:86:ARG:HG3	2.47	0.44
2:E:29:THR:HG23	2:E:32:LEU:CD2	2.48	0.44
2:E:89:PHE:HD1	2:E:100:ILE:HD11	1.83	0.44
1:C:385:LEU:O	1:C:385:LEU:HD22	2.18	0.44
1:C:581:GLN:O	1:C:629:ASN:HA	2.17	0.44
1:C:636:ALA:CB	1:C:639:ASN:HD21	2.30	0.44
1:A:742:ALA:C	1:A:744:GLU:H	2.25	0.44
2:D:51:MET:HB3	2:D:71:MET:HE2	1.99	0.44
2:D:80:ASP:C	2:D:82:GLU:N	2.75	0.44
1:B:376:GLN:O	1:B:379:ALA:N	2.49	0.44
1:A:423:LYS:O	1:A:423:LYS:HG2	2.17	0.44
1:A:523:LEU:HD13	2:D:127:GLU:HB3	1.99	0.44
1:A:697:ILE:HD13	1:A:732:ILE:CG1	2.37	0.44
1:A:781:ASN:O	1:A:783:THR:N	2.51	0.44
2:D:9:ILE:H	2:D:9:ILE:CD1	2.28	0.44
1:B:325:TYR:HB3	1:B:327:LEU:HD11	2.00	0.44
1:B:400:LYS:HA	1:B:476:VAL:O	2.17	0.44
1:B:613:ARG:O	1:B:616:GLU:HG2	2.18	0.44
1:B:764:LEU:HD22	1:B:768:LYS:HD3	2.00	0.44
2:F:35:VAL:C	2:F:37:ARG:N	2.75	0.44
1:A:728:ALA:C	1:A:730:ASN:N	2.74	0.44
2:D:10:ALA:O	2:D:14:GLU:HG2	2.18	0.44
2:D:117:THR:C	2:D:119:GLU:N	2.76	0.44
1:C:308:VAL:HB	1:C:311:HIS:CG	2.52	0.44
1:C:514:ASP:C	1:C:516:VAL:H	2.25	0.44
1:C:717:LYS:HA	1:C:720:ILE:HD11	1.99	0.44
1:A:426:ILE:HA	1:A:430:LYS:O	2.17	0.44
1:A:522:SER:OG	2:D:127:GLU:HG3	2.17	0.44
1:A:731:GLU:O	1:A:735:VAL:HG23	2.18	0.44
1:C:718:ARG:O	1:C:722:ILE:HG13	2.17	0.44
1:A:549:LEU:HD12	1:A:549:LEU:H	1.83	0.44
1:A:557:LEU:HG	1:A:575:VAL:HG12	1.99	0.44
2:D:47:GLU:O	2:D:51:MET:HG3	2.18	0.44
1:B:310:GLU:HB3	1:B:567:THR:HG21	2.00	0.44
2:F:117:THR:OG1	2:F:120:GLU:HG3	2.18	0.44
1:A:540:ARG:HD2	1:A:582:ASP:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ILE:O	1:A:701:LEU:HG	2.18	0.43
1:B:629:ASN:HB3	1:B:632:TYR:CE2	2.53	0.43
1:B:730:ASN:HD22	1:B:730:ASN:HA	1.62	0.43
1:B:776:LEU:HD23	1:B:776:LEU:HA	1.87	0.43
1:C:753:LYS:HZ2	1:C:753:LYS:CB	2.31	0.43
2:F:36:MET:O	2:F:41:GLN:HB2	2.18	0.43
1:A:549:LEU:HB2	1:A:553:GLN:HE21	1.83	0.43
1:A:636:ALA:HA	1:A:637:PRO:HD3	1.90	0.43
1:B:376:GLN:HE21	1:B:376:GLN:HB3	1.70	0.43
1:B:565:LYS:C	1:B:567:THR:H	2.26	0.43
2:E:85:ILE:O	2:E:88:ALA:HB3	2.17	0.43
1:C:465:LEU:HD23	1:C:465:LEU:N	2.33	0.43
1:C:629:ASN:HB3	1:C:632:TYR:CD2	2.53	0.43
1:A:373:LYS:HG2	1:A:379:ALA:HB1	2.00	0.43
1:A:700:TYR:CE1	1:A:727:GLN:HB3	2.54	0.43
2:D:66:PRO:O	2:D:70:THR:HB	2.19	0.43
1:B:648:PRO:C	1:B:650:THR:H	2.25	0.43
1:B:760:VAL:CG1	1:B:773:PHE:HE2	2.31	0.43
1:B:774:LYS:O	1:B:774:LYS:HG3	2.18	0.43
1:C:732:ILE:HD13	1:C:752:LEU:HD12	2.00	0.43
1:A:714:GLN:C	1:A:718:ARG:HH21	2.26	0.43
1:B:418:ILE:HG22	1:B:419:ILE:HG23	2.01	0.43
1:B:508:ILE:HG23	1:B:509:PRO:HD2	1.99	0.43
1:B:513:TRP:O	1:B:517:VAL:HG12	2.18	0.43
1:B:530:THR:HG22	2:E:92:PHE:HZ	1.82	0.43
1:B:543:ASP:OD2	1:B:554:LYS:HE2	2.18	0.43
1:B:737:LYS:O	1:B:738:SER:C	2.61	0.43
2:E:115:LYS:NZ	2:E:115:LYS:CB	2.81	0.43
1:C:318:ILE:HG23	1:C:322:LEU:HD12	2.01	0.43
2:F:78:ASP:C	2:F:80:ASP:H	2.25	0.43
2:F:114:GLU:HG3	2:F:116:LEU:HD13	1.98	0.43
1:A:376:GLN:HE22	1:B:466:GLY:HA3	1.80	0.43
1:A:505:LYS:O	1:A:508:ILE:N	2.51	0.43
1:A:651:LYS:O	1:A:654:ILE:HG22	2.18	0.43
1:A:742:ALA:O	1:A:744:GLU:N	2.52	0.43
1:A:760:VAL:C	1:A:762:LEU:N	2.77	0.43
2:D:118:ASP:O	2:D:122:ASP:OD1	2.36	0.43
1:B:547:GLY:HA3	4:B:903:3AT:N1	2.34	0.43
1:B:727:GLN:C	1:B:727:GLN:CD	2.86	0.43
1:C:657:ILE:HG23	1:C:756:ILE:CD1	2.48	0.43
1:A:437:SER:C	1:A:439:ASN:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ILE:HA	1:B:601:GLU:O	2.17	0.43
1:B:605:THR:HG22	1:B:607:ASN:H	1.84	0.43
1:B:657:ILE:HG12	1:B:658:PRO:CD	2.44	0.43
1:B:752:LEU:HD23	1:B:752:LEU:C	2.44	0.43
1:C:322:LEU:O	1:C:323:ASN:C	2.61	0.43
1:B:505:LYS:O	1:B:508:ILE:N	2.47	0.43
2:E:72:MET:HE3	2:E:76:MET:SD	2.58	0.43
1:C:635:ILE:O	1:C:636:ALA:C	2.62	0.43
2:F:7:GLU:O	2:F:11:GLU:HG3	2.19	0.43
1:A:444:PHE:C	1:A:445:ARG:HG2	2.43	0.43
1:A:478:ALA:HB1	1:A:486:LYS:O	2.18	0.43
1:A:581:GLN:O	1:A:629:ASN:HA	2.19	0.43
1:B:336:THR:HG23	1:B:337:ASN:N	2.34	0.43
1:B:435:LEU:HD11	1:B:446:ILE:HB	2.01	0.43
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.54	0.43
1:C:695:LYS:HB2	2:F:18:LEU:HD22	2.00	0.43
2:D:103:ALA:O	2:D:106:ARG:HB3	2.18	0.43
1:B:390:SER:O	1:B:394:HIS:HB2	2.19	0.43
1:C:329:ARG:HD3	1:C:580:GLU:HG2	2.00	0.43
1:C:549:LEU:HD12	1:C:549:LEU:N	2.27	0.43
1:C:584:GLU:OE2	1:C:630:ARG:HB2	2.19	0.43
1:C:714:GLN:CA	1:C:714:GLN:NE2	2.81	0.43
1:A:509:PRO:HG3	1:A:512:GLU:OE1	2.19	0.43
1:B:543:ASP:CG	1:B:544:SER:H	2.03	0.43
2:E:102:ALA:CA	2:E:125:ILE:HD11	2.45	0.43
1:C:431:LYS:HE3	1:C:448:ASP:CG	2.43	0.43
1:C:529:VAL:HB	2:F:109:MET:HE1	2.01	0.43
1:A:533:LEU:HG	1:A:538:ILE:CD1	2.49	0.42
1:B:322:LEU:O	1:B:503:GLU:HG3	2.18	0.42
1:B:538:ILE:HD11	1:B:625:LEU:HD11	2.01	0.42
1:B:550:SER:H	1:B:553:GLN:NE2	2.16	0.42
1:C:401:ILE:HG21	1:C:485:LEU:HB3	2.01	0.42
1:C:526:GLN:OE1	2:F:144:MET:HE2	2.19	0.42
1:C:609:GLU:CD	1:C:609:GLU:H	2.27	0.42
1:A:372:LYS:CE	4:A:902:3AT:O2G	2.67	0.42
1:A:780:LEU:HD13	1:A:782:PHE:CE1	2.53	0.42
1:C:437:SER:C	1:C:439:ASN:N	2.77	0.42
1:C:499:PRO:HG2	1:C:625:LEU:HB3	1.99	0.42
2:D:7:GLU:O	2:D:11:GLU:HG3	2.20	0.42
1:B:526:GLN:CD	1:B:526:GLN:H	2.26	0.42
2:F:71:MET:O	2:F:74:ARG:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:O	1:A:425:GLU:HB2	2.19	0.42
1:B:320:ARG:CG	1:B:321:GLU:H	2.27	0.42
1:B:773:PHE:C	1:B:775:LEU:N	2.77	0.42
1:C:391:ILE:HD12	1:C:399:GLY:HA2	2.01	0.42
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.83	0.42
1:A:538:ILE:HD12	1:A:538:ILE:N	2.33	0.42
1:A:764:LEU:C	1:A:766:HIS:H	2.27	0.42
1:B:633:ASN:C	1:B:634:LYS:HG3	2.45	0.42
1:B:751:TYR:HA	1:B:754:GLU:OE2	2.20	0.42
2:E:5:THR:CB	2:E:8:GLN:HB2	2.49	0.42
2:F:34:THR:HG22	2:F:34:THR:O	2.20	0.42
1:A:716:LYS:O	1:A:719:LYS:HB2	2.19	0.42
1:A:777:TYR:C	1:A:779:GLN:N	2.78	0.42
1:C:318:ILE:H	1:C:318:ILE:CD1	2.30	0.42
1:C:479:LYS:HG3	1:C:481:VAL:HG22	2.00	0.42
1:C:701:LEU:O	1:C:704:TYR:HB3	2.19	0.42
2:F:138:TYR:O	2:F:139:GLU:C	2.62	0.42
1:A:540:ARG:HD3	1:A:627:TYR:CZ	2.54	0.42
1:A:740:GLN:C	1:A:741:ILE:HG12	2.45	0.42
1:A:768:LYS:HB2	1:A:797:ILE:HD13	2.02	0.42
2:E:42:ASN:N	2:E:43:PRO:CD	2.82	0.42
1:C:385:LEU:HA	1:C:388:LYS:HE3	2.00	0.42
1:C:647:ASP:O	1:C:648:PRO:C	2.63	0.42
2:F:5:THR:N	2:F:8:GLN:HB3	2.35	0.42
2:F:74:ARG:C	2:F:76:MET:H	2.27	0.42
1:A:360:VAL:HG22	1:A:363:TYR:HB2	2.02	0.42
1:A:713:SER:O	1:A:717:LYS:N	2.47	0.42
1:A:776:LEU:H	1:A:776:LEU:CD1	2.14	0.42
2:E:15:ALA:C	2:E:17:SER:H	2.27	0.42
2:E:49:GLN:HA	2:E:52:ILE:CG2	2.40	0.42
1:A:787:THR:O	1:A:787:THR:HG22	2.20	0.42
1:B:718:ARG:O	1:B:722:ILE:HG13	2.19	0.42
1:B:727:GLN:HG2	1:B:786:GLU:CD	2.45	0.42
1:B:729:TYR:O	1:B:733:GLU:CD	2.62	0.42
1:B:774:LYS:HA	1:B:774:LYS:HD2	1.73	0.42
2:E:19:PHE:CE1	2:E:31:GLU:HB3	2.55	0.42
1:C:408:LEU:O	1:C:411:GLU:HB3	2.20	0.42
1:C:659:THR:C	1:C:661:ALA:N	2.77	0.42
1:A:494:LEU:HD21	1:A:497:LEU:HD21	2.00	0.42
2:D:51:MET:C	2:D:53:ASN:H	2.25	0.42
2:D:93:ASP:OD2	2:D:93:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:TYR:O	2:D:142:VAL:HG23	2.19	0.42
1:B:302:LEU:HD11	1:B:312:ALA:CB	2.50	0.42
1:B:327:LEU:N	1:B:327:LEU:CD1	2.83	0.42
1:A:320:ARG:HA	1:A:598:PRO:O	2.20	0.41
1:A:494:LEU:HB3	1:A:579:THR:HG22	2.02	0.41
1:A:719:LYS:HE2	1:A:797:ILE:HG21	2.02	0.41
2:D:72:MET:O	2:D:74:ARG:N	2.53	0.41
1:B:359:PRO:C	1:B:361:ALA:N	2.76	0.41
2:F:144:MET:SD	2:F:144:MET:C	3.03	0.41
1:A:426:ILE:HG22	1:A:427:ASP:N	2.34	0.41
2:D:110:THR:HG23	2:D:115:LYS:HD2	2.02	0.41
2:D:145:MET:HE2	2:D:145:MET:HB2	1.90	0.41
1:B:622:LYS:O	1:B:623:ASP:HB2	2.20	0.41
1:C:500:SER:O	1:C:503:GLU:HB3	2.19	0.41
1:C:540:ARG:HH12	1:C:630:ARG:NH2	2.18	0.41
1:A:323:ASN:ND2	1:A:624:TYR:CE2	2.88	0.41
1:A:629:ASN:HD21	1:A:631:SER:HB2	1.84	0.41
1:B:294:ASP:O	1:B:610:MET:HE1	2.21	0.41
1:B:505:LYS:O	1:B:506:LYS:C	2.62	0.41
1:B:540:ARG:CZ	1:B:627:TYR:HE1	2.33	0.41
2:E:65:PHE:N	2:E:66:PRO:CD	2.83	0.41
2:F:13:LYS:HG3	2:F:65:PHE:HD2	1.84	0.41
2:F:72:MET:C	2:F:74:ARG:H	2.28	0.41
1:B:374:HIS:HB3	6:B:14:HOH:O	2.20	0.41
1:B:459:GLU:C	1:B:461:LYS:H	2.29	0.41
1:B:717:LYS:NZ	2:E:126:ARG:HG3	2.35	0.41
1:B:731:GLU:HG3	1:B:732:ILE:H	1.84	0.41
1:B:764:LEU:O	1:B:768:LYS:HB2	2.20	0.41
1:C:657:ILE:HG13	1:C:759:GLN:HG2	2.01	0.41
2:F:44:THR:C	2:F:46:ALA:H	2.29	0.41
2:F:44:THR:HG22	2:F:47:GLU:OE1	2.20	0.41
1:A:323:ASN:ND2	1:A:598:PRO:HB3	2.35	0.41
1:A:401:ILE:O	1:A:476:VAL:HG22	2.20	0.41
1:A:586:PHE:HA	1:A:639:ASN:ND2	2.35	0.41
1:A:604:LEU:HD23	1:A:604:LEU:C	2.46	0.41
1:A:781:ASN:O	1:A:782:PHE:C	2.63	0.41
1:B:538:ILE:O	1:B:539:GLU:C	2.64	0.41
1:B:731:GLU:H	1:B:731:GLU:HG2	1.34	0.41
1:B:750:GLN:O	1:B:753:LYS:HB3	2.21	0.41
1:B:762:LEU:HA	1:B:765:THR:OG1	2.20	0.41
1:C:360:VAL:O	1:C:361:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:ALA:C	1:C:663:PHE:N	2.71	0.41
2:D:9:ILE:HA	2:D:12:PHE:CD2	2.55	0.41
1:B:366:PHE:CE1	1:B:391:ILE:HD12	2.55	0.41
1:B:565:LYS:O	1:B:567:THR:N	2.53	0.41
2:E:93:ASP:OD2	2:E:96:GLY:HA2	2.19	0.41
2:E:109:MET:HG3	2:E:116:LEU:CD1	2.50	0.41
1:C:370:LEU:HD11	1:C:455:TYR:CE1	2.55	0.41
1:C:479:LYS:O	1:C:485:LEU:HD12	2.20	0.41
1:C:517:VAL:HG13	1:C:518:ASN:N	2.35	0.41
1:C:757:THR:HG23	1:C:773:PHE:CD2	2.55	0.41
1:B:535:LYS:C	1:B:537:GLY:H	2.29	0.41
1:B:654:ILE:HA	1:B:755:ARG:HD2	2.01	0.41
2:E:89:PHE:CE1	2:E:100:ILE:HG13	2.54	0.41
1:A:607:ASN:ND2	1:A:609:GLU:HB2	2.36	0.41
1:A:629:ASN:HB3	1:A:632:TYR:CE2	2.56	0.41
1:A:709:ASN:HD21	1:A:724:ARG:HH12	1.69	0.41
1:A:718:ARG:HD2	1:A:767:GLN:HG3	2.03	0.41
2:D:129:ASP:OD1	2:D:133:ASP:N	2.53	0.41
1:B:323:ASN:OD1	1:B:500:SER:HB3	2.21	0.41
1:B:334:LEU:HD22	1:B:334:LEU:H	1.83	0.41
1:B:714:GLN:HB3	2:E:126:ARG:HD2	2.03	0.41
1:C:499:PRO:HD3	1:C:552:TRP:CH2	2.56	0.41
2:F:12:PHE:CE1	2:F:76:MET:HE3	2.56	0.41
1:A:384:ASN:O	1:A:388:LYS:HD3	2.21	0.41
1:A:472:ARG:HH11	1:A:472:ARG:HB2	1.86	0.41
1:B:465:LEU:O	1:B:466:GLY:C	2.64	0.41
1:B:603:ILE:HG21	1:B:614:PHE:CE1	2.56	0.41
1:B:648:PRO:O	1:B:650:THR:N	2.54	0.41
1:B:717:LYS:HZ2	2:E:126:ARG:CD	2.34	0.41
2:E:6:GLU:O	2:E:7:GLU:C	2.64	0.41
1:C:327:LEU:N	1:C:327:LEU:HD12	2.36	0.41
1:C:349:ASN:HD22	1:C:349:ASN:H	1.69	0.41
1:C:480:ASN:C	1:C:480:ASN:HD22	2.28	0.41
2:F:15:ALA:O	2:F:18:LEU:HB2	2.21	0.41
2:F:44:THR:C	2:F:46:ALA:N	2.77	0.41
1:A:730:ASN:C	1:A:732:ILE:H	2.29	0.41
1:B:524:GLU:HG3	1:B:524:GLU:O	2.21	0.41
1:B:551:ASN:ND2	1:B:551:ASN:H	2.19	0.41
1:B:628:PHE:CD2	1:B:645:TRP:CD1	3.09	0.41
1:C:526:GLN:NE2	2:F:144:MET:HE1	2.27	0.41
1:C:636:ALA:HA	1:C:637:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:GLU:OE1	1:C:747:ASN:HB2	2.21	0.41
1:A:323:ASN:C	1:A:323:ASN:ND2	2.77	0.40
1:A:331:VAL:HG21	1:A:492:TYR:HD1	1.85	0.40
2:D:52:ILE:HD12	2:D:52:ILE:HA	1.95	0.40
1:B:458:LYS:O	1:B:459:GLU:C	2.64	0.40
1:B:470:ASN:O	1:B:471:TRP:C	2.64	0.40
2:E:36:MET:O	2:E:41:GLN:HB2	2.21	0.40
1:C:692:GLU:O	1:C:734:ASN:ND2	2.55	0.40
1:C:709:ASN:N	1:C:709:ASN:HD22	2.18	0.40
1:C:747:ASN:C	1:C:750:GLN:HG2	2.46	0.40
2:F:105:LEU:HD12	2:F:125:ILE:HD13	2.03	0.40
1:A:764:LEU:C	1:A:766:HIS:N	2.78	0.40
2:E:71:MET:O	2:E:73:ALA:N	2.54	0.40
2:E:92:PHE:HA	2:E:108:VAL:HG21	2.02	0.40
1:C:331:VAL:O	1:C:332:ASN:C	2.65	0.40
1:C:407:HIS:CD2	1:C:407:HIS:H	2.35	0.40
1:A:355:SER:CB	1:A:360:VAL:HG13	2.51	0.40
1:A:527:LYS:HG3	2:D:145:MET:SD	2.61	0.40
1:A:724:ARG:O	1:A:727:GLN:HB2	2.21	0.40
1:B:472:ARG:HB3	1:B:473:ASN:H	1.53	0.40
2:E:109:MET:C	2:E:111:ASN:N	2.78	0.40
1:C:404:LYS:HA	1:C:451:ASN:O	2.22	0.40
1:C:755:ARG:O	1:C:756:ILE:C	2.64	0.40
1:A:369:ASP:OD1	1:A:442:TYR:OH	2.31	0.40
1:B:529:VAL:HG21	2:E:109:MET:SD	2.61	0.40
1:B:722:ILE:HD13	1:B:764:LEU:CD2	2.52	0.40
2:E:106:ARG:HE	2:E:121:VAL:HG21	1.85	0.40
1:C:359:PRO:HB2	1:C:405:LEU:HD11	2.04	0.40
1:C:413:LEU:HB3	1:C:419:ILE:HG12	2.03	0.40
1:C:753:LYS:NZ	1:C:753:LYS:CB	2.85	0.40
1:A:360:VAL:HA	1:A:403:LEU:HD21	2.02	0.40
1:A:717:LYS:O	1:A:718:ARG:C	2.64	0.40
1:C:736:LEU:HD21	1:C:749:PHE:CB	2.51	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	479/510 (94%)	411 (86%)	52 (11%)	16 (3%)	3	5
1	B	457/510 (90%)	364 (80%)	66 (14%)	27 (6%)	1	1
1	C	499/510 (98%)	423 (85%)	60 (12%)	16 (3%)	3	5
2	D	141/148 (95%)	111 (79%)	24 (17%)	6 (4%)	2	3
2	E	141/148 (95%)	107 (76%)	29 (21%)	5 (4%)	3	5
2	F	141/148 (95%)	116 (82%)	23 (16%)	2 (1%)	9	17
All	All	1858/1974 (94%)	1532 (82%)	254 (14%)	72 (4%)	2	4

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	739	LYS
2	D	64	ASP
1	B	466	GLY
2	E	73	ALA
1	C	520	PRO
1	C	694	VAL
1	C	741	ILE
2	F	40	GLY
1	A	294	ASP
1	A	471	TRP
1	A	578	GLY
1	A	707	SER
2	D	73	ALA
2	D	74	ARG
2	D	93	ASP
1	B	460	GLY
1	B	464	VAL
1	B	537	GLY
1	B	547	GLY

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Mol	Chain	Res	Type
1	B	571	GLY
1	B	732	ILE
1	B	776	LEU
2	E	93	ASP
1	C	438	ASN
1	C	510	GLN
1	C	675	ASN
1	A	424	LYS
1	A	782	PHE
2	D	65	PHE
1	B	702	SER
1	B	734	ASN
2	E	72	MET
1	C	332	ASN
1	C	743	PRO
2	F	24	ASP
1	A	376	GLN
1	A	425	GLU
1	A	665	LYS
1	A	743	PRO
1	A	783	THR
2	D	76	MET
1	B	406	ASP
1	B	566	TYR
1	B	794	GLN
2	E	133	ASP
1	C	662	GLU
1	C	677	GLY
1	C	740	GLN
1	A	510	GLN
1	A	736	LEU
1	A	742	ALA
1	B	438	ASN
1	B	459	GLU
1	B	535	LYS
1	B	694	VAL
1	B	704	TYR
1	B	708	ALA
1	B	713	SER
1	B	774	LYS
1	C	294	ASP
1	B	303	LYS

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Mol	Chain	Res	Type
1	B	377	GLN
1	C	708	ALA
1	C	765	THR
1	C	578	GLY
1	B	743	PRO
2	E	27	ILE
1	C	537	GLY
1	B	309	PRO
1	B	657	ILE
1	B	295	VAL

5.3.2 Protein sidechains [i](#)

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	433/455 (95%)	410 (95%)	23 (5%)	20	39
1	B	414/455 (91%)	380 (92%)	34 (8%)	10	20
1	C	448/455 (98%)	420 (94%)	28 (6%)	16	30
2	D	121/126 (96%)	116 (96%)	5 (4%)	27	49
2	E	121/126 (96%)	118 (98%)	3 (2%)	42	64
2	F	121/126 (96%)	114 (94%)	7 (6%)	18	34
All	All	1658/1743 (95%)	1558 (94%)	100 (6%)	17	32

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	323	ASN
1	A	349	ASN
1	A	382	LYS
1	A	385	LEU
1	A	388	LYS
1	A	404	LYS
1	A	406	ASP

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Mol	Chain	Res	Type
1	A	409	ARG
1	A	426	ILE
1	A	438	ASN
1	A	450	ASN
1	A	455	TYR
1	A	485	LEU
1	A	494	LEU
1	A	523	LEU
1	A	549	LEU
1	A	574	VAL
1	A	620	THR
1	A	622	LYS
1	A	646	THR
1	A	670	ILE
1	A	775	LEU
2	D	64	ASP
2	D	75	LYS
2	D	87	GLU
2	D	105	LEU
2	D	123	GLU
1	B	307	LEU
1	B	320	ARG
1	B	332	ASN
1	B	353	LYS
1	B	391	ILE
1	B	397	GLU
1	B	398	ILE
1	B	415	GLU
1	B	426	ILE
1	B	428	ASN
1	B	440	GLN
1	B	485	LEU
1	B	510	GLN
1	B	518	ASN
1	B	529	VAL
1	B	532	LEU
1	B	539	GLU
1	B	544	SER
1	B	545	THR
1	B	552	TRP
1	B	557	LEU
1	B	585	GLU

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Mol	Chain	Res	Type
1	B	611	THR
1	B	620	THR
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	714	GLN
1	B	730	ASN
1	B	731	GLU
1	B	743	PRO
1	B	744	GLU
1	B	775	LEU
1	B	784	GLU
2	E	75	LYS
2	E	94	LYS
2	E	115	LYS
1	C	320	ARG
1	C	341	SER
1	C	349	ASN
1	C	377	GLN
1	C	381	GLU
1	C	385	LEU
1	C	455	TYR
1	C	465	LEU
1	C	481	VAL
1	C	485	LEU
1	C	508	ILE
1	C	517	VAL
1	C	533	LEU
1	C	535	LYS
1	C	540	ARG
1	C	549	LEU
1	C	557	LEU
1	C	565	LYS
1	C	574	VAL
1	C	629	ASN
1	C	639	ASN
1	C	694	VAL
1	C	714	GLN
1	C	715	GLU
1	C	734	ASN
1	C	743	PRO
1	C	775	LEU

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Mol	Chain	Res	Type
1	C	791	GLU
2	F	14	GLU
2	F	21	LYS
2	F	83	GLU
2	F	105	LEU
2	F	123	GLU
2	F	127	GLU
2	F	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	337	ASN
1	A	349	ASN
1	A	351	HIS
1	A	376	GLN
1	A	394	HIS
1	A	407	HIS
1	A	416	ASN
1	A	438	ASN
1	A	439	ASN
1	A	440	GLN
1	A	507	GLN
1	A	510	GLN
1	A	518	ASN
1	A	526	GLN
1	A	531	ASN
1	A	553	GLN
1	A	576	ASN
1	A	581	GLN
1	A	607	ASN
1	A	629	ASN
1	A	633	ASN
1	A	706	ASN
1	A	710	HIS
1	A	714	GLN
1	A	727	GLN
1	A	734	ASN
1	A	758	ASN
1	A	789	ASN
1	A	794	GLN

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Mol	Chain	Res	Type
2	D	41	GLN
2	D	42	ASN
1	B	332	ASN
1	B	368	GLN
1	B	376	GLN
1	B	377	GLN
1	B	394	HIS
1	B	407	HIS
1	B	428	ASN
1	B	439	ASN
1	B	451	ASN
1	B	507	GLN
1	B	518	ASN
1	B	551	ASN
1	B	553	GLN
1	B	555	GLN
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	709	ASN
1	B	727	GLN
1	B	730	ASN
1	B	734	ASN
1	B	750	GLN
1	B	759	GLN
1	B	761	GLN
1	B	794	GLN
2	E	107	HIS
2	E	135	GLN
2	E	143	GLN
1	C	323	ASN
1	C	349	ASN
1	C	351	HIS
1	C	376	GLN
1	C	377	GLN
1	C	407	HIS
1	C	440	GLN
1	C	451	ASN
1	C	480	ASN
1	C	507	GLN
1	C	518	ASN
1	C	553	GLN

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Mol	Chain	Res	Type
1	C	555	GLN
1	C	581	GLN
1	C	629	ASN
1	C	639	ASN
1	C	655	ASN
1	C	666	ASN
1	C	709	ASN
1	C	714	GLN
1	C	734	ASN
1	C	747	ASN
1	C	758	ASN
1	C	789	ASN
1	C	794	GLN
2	F	111	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3AT	A	902	3	30,32,32	1.99	5 (16%)	42,50,50	1.07	3 (7%)
4	3AT	C	904	3	30,32,32	1.57	7 (23%)	42,50,50	1.05	3 (7%)
4	3AT	B	903	3	30,32,32	1.96	6 (20%)	42,50,50	1.08	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3AT	A	902	3	-	8/22/34/34	0/3/3/3
4	3AT	C	904	3	-	8/22/34/34	0/3/3/3
4	3AT	B	903	3	-	6/22/34/34	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	3AT	PB-O3B	5.86	1.65	1.59
4	B	903	3AT	PB-O3A	-5.74	1.53	1.59
4	A	902	3AT	PB-O3B	5.62	1.65	1.59
4	A	902	3AT	PB-O3A	-5.19	1.53	1.59
4	A	902	3AT	PA-O3A	-4.85	1.54	1.59
4	C	904	3AT	PB-O3A	-4.51	1.54	1.59
4	B	903	3AT	PA-O3A	-4.02	1.55	1.59
4	C	904	3AT	PB-O3B	3.32	1.63	1.59
4	A	902	3AT	PG-O2G	-2.96	1.43	1.54
4	B	903	3AT	PG-O2G	-2.54	1.45	1.54
4	B	903	3AT	C4-N3	2.48	1.39	1.34
4	C	904	3AT	PG-O3G	-2.44	1.45	1.54
4	C	904	3AT	C4-N3	2.37	1.38	1.34
4	C	904	3AT	PG-O2G	-2.32	1.46	1.54
4	C	904	3AT	PB-O2B	-2.31	1.44	1.55
4	B	903	3AT	PB-O2B	-2.27	1.44	1.55
4	A	902	3AT	PB-O2B	-2.09	1.45	1.55
4	C	904	3AT	PA-O3A	-2.03	1.57	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	904	3AT	O3G-PG-O2G	2.63	117.65	107.80
4	B	903	3AT	O3G-PG-O2G	2.59	117.51	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	3AT	O3G-PG-O2G	2.55	117.38	107.80
4	B	903	3AT	O2B-PB-O3A	2.13	113.03	107.27
4	C	904	3AT	O2G-PG-O3B	-2.10	97.60	104.64
4	A	902	3AT	O2B-PB-O3A	2.02	112.74	107.27
4	A	902	3AT	C3'-C4'-C5'	2.01	117.45	113.30
4	C	904	3AT	O2B-PB-O3A	2.01	112.70	107.27

There are no chirality outliers.

All (22) torsion outliers are listed below:

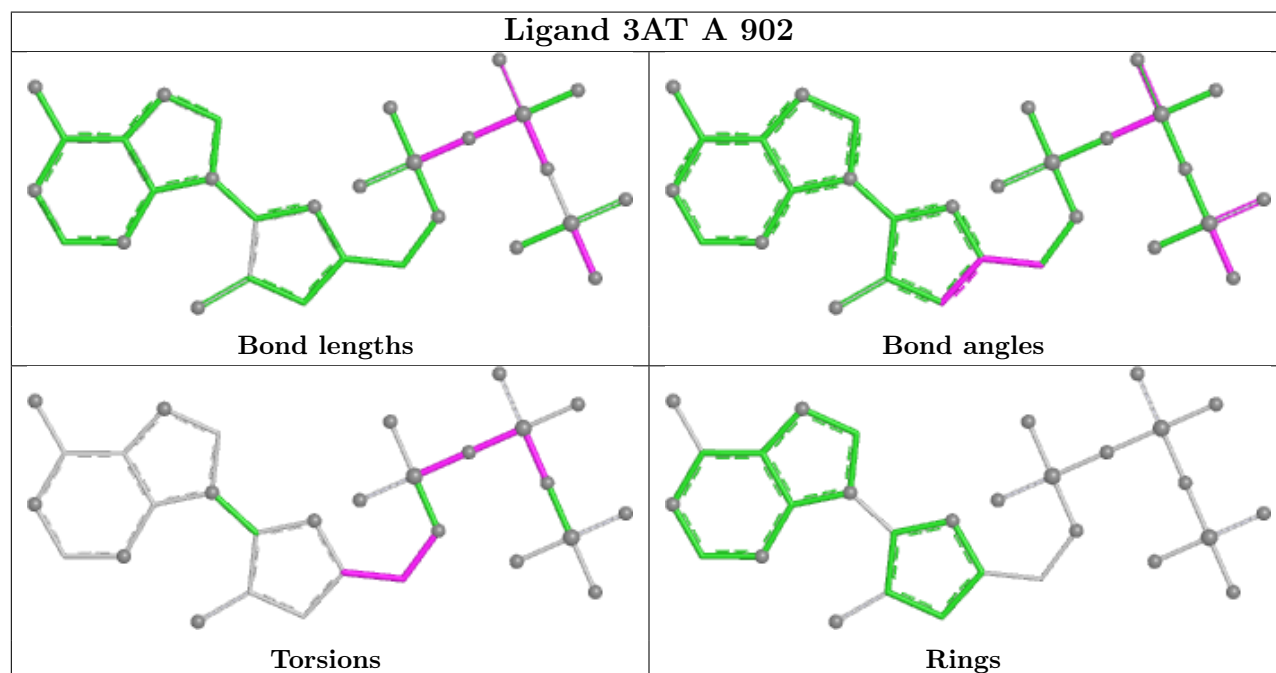
Mol	Chain	Res	Type	Atoms
4	A	902	3AT	O4'-C4'-C5'-O5'
4	A	902	3AT	C3'-C4'-C5'-O5'
4	B	903	3AT	O4'-C4'-C5'-O5'
4	B	903	3AT	C3'-C4'-C5'-O5'
4	C	904	3AT	O4'-C4'-C5'-O5'
4	C	904	3AT	C3'-C4'-C5'-O5'
4	B	903	3AT	PG-O3B-PB-O2B
4	C	904	3AT	PG-O3B-PB-O2B
4	A	902	3AT	PG-O3B-PB-O1B
4	A	902	3AT	PG-O3B-PB-O2B
4	A	902	3AT	C4'-C5'-O5'-PA
4	B	903	3AT	PG-O3B-PB-O1B
4	B	903	3AT	PB-O3A-PA-O1A
4	C	904	3AT	PG-O3B-PB-O1B
4	B	903	3AT	C4'-C5'-O5'-PA
4	C	904	3AT	C4'-C5'-O5'-PA
4	A	902	3AT	PB-O3A-PA-O1A
4	C	904	3AT	PB-O3A-PA-O1A
4	A	902	3AT	PA-O3A-PB-O1B
4	A	902	3AT	PB-O3A-PA-O2A
4	C	904	3AT	PA-O3A-PB-O1B
4	C	904	3AT	PB-O3A-PA-O2A

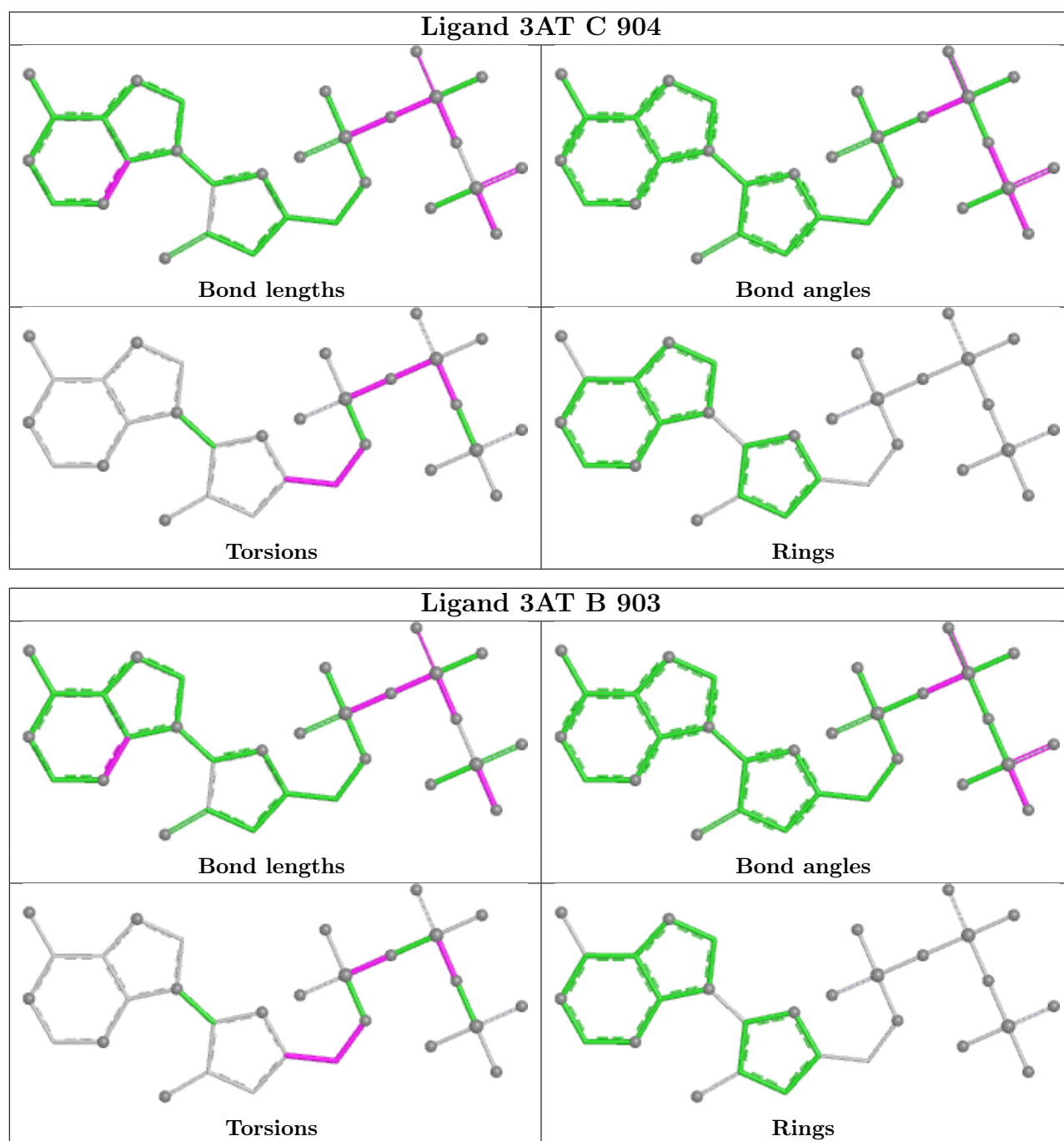
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	3AT	2	0
4	B	903	3AT	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	485/510 (95%)	0.20	25 (5%)	33 32	21, 61, 145, 174	16 (3%)
1	B	457/510 (89%)	0.76	55 (12%)	9 7	16, 78, 172, 191	12 (2%)
1	C	491/510 (96%)	0.20	23 (4%)	36 36	17, 60, 146, 177	19 (3%)
2	D	143/148 (96%)	0.87	22 (15%)	5 4	39, 134, 185, 193	0
2	E	143/148 (96%)	1.44	39 (27%)	1 1	61, 159, 199, 199	0
2	F	143/148 (96%)	0.92	25 (17%)	4 3	43, 145, 188, 198	0
All	All	1862/1974 (94%)	0.54	189 (10%)	12 11	16, 75, 181, 199	47 (2%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ILE	18.1
2	D	18	LEU	6.9
1	B	736	LEU	6.5
1	B	704	TYR	6.4
2	D	57	ALA	5.8
2	E	18	LEU	5.3
1	B	782	PHE	5.1
2	F	55	VAL	5.1
2	E	19	PHE	5.0
1	A	445	ARG	4.9
1	B	731	GLU	4.7
1	B	658	PRO	4.6
1	B	773	PHE	4.6
1	B	732	ILE	4.6
1	B	793	PHE	4.4
2	D	19	PHE	4.2
1	B	713	SER	4.2
1	A	793	PHE	4.2
2	F	102	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	775	LEU	4.2
2	D	75	LYS	4.1
1	B	434	LEU	3.9
2	E	62	THR	3.8
2	F	39	LEU	3.8
2	E	15	ALA	3.8
2	D	55	VAL	3.7
2	E	51	MET	3.7
2	D	16	PHE	3.7
2	E	12	PHE	3.7
2	E	72	MET	3.6
1	C	694	VAL	3.6
1	C	787	THR	3.5
1	B	728	ALA	3.5
1	B	752	LEU	3.5
1	C	741	ILE	3.5
2	F	57	ALA	3.5
1	B	712	PHE	3.5
1	A	792	VAL	3.5
1	B	777	TYR	3.4
1	A	434	LEU	3.4
2	F	43	PRO	3.4
2	F	19	PHE	3.4
2	E	80	ASP	3.4
1	B	549	LEU	3.3
2	E	147	ALA	3.3
1	B	780	LEU	3.3
2	E	52	ILE	3.3
1	B	462	ILE	3.3
1	B	792	VAL	3.3
2	F	76	MET	3.2
1	B	751	TYR	3.2
2	E	63	ILE	3.1
2	E	99	TYR	3.1
2	E	68	PHE	3.1
2	E	131	ASP	3.1
2	F	62	THR	3.1
1	B	721	SER	3.1
1	A	744	GLU	3.0
2	E	14	GLU	3.0
2	F	56	ASP	3.0
1	C	767	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	61	GLY	3.0
1	A	694	VAL	3.0
2	D	9	ILE	3.0
2	E	71	MET	3.0
2	D	23	GLY	3.0
1	B	735	VAL	3.0
2	F	12	PHE	3.0
1	B	702	SER	2.9
1	B	779	GLN	2.9
2	D	69	LEU	2.9
1	A	781	ASN	2.9
1	A	440	GLN	2.9
1	B	748	TYR	2.9
1	C	780	LEU	2.9
1	C	792	VAL	2.9
1	B	738	SER	2.8
1	C	748	TYR	2.8
1	A	782	PHE	2.8
1	C	745	TYR	2.8
2	E	112	LEU	2.8
1	C	798	ASP	2.8
1	C	691	LYS	2.8
1	B	720	ILE	2.8
1	A	471	TRP	2.8
1	C	693	SER	2.8
1	B	776	LEU	2.8
1	B	654	ILE	2.7
1	B	657	ILE	2.7
2	D	58	ASP	2.7
2	E	55	VAL	2.7
1	B	743	PRO	2.7
1	A	779	GLN	2.6
2	D	15	ALA	2.6
2	D	66	PRO	2.6
2	F	65	PHE	2.6
2	E	135	GLN	2.6
2	D	78	ASP	2.6
1	B	516	VAL	2.6
2	F	36	MET	2.6
2	D	48	LEU	2.6
1	B	705	TYR	2.6
1	B	724	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	717	LYS	2.6
1	A	736	LEU	2.5
2	F	48	LEU	2.5
1	B	568	GLY	2.5
2	F	9	ILE	2.5
1	A	735	VAL	2.5
1	B	783	THR	2.5
2	D	5	THR	2.5
2	E	79	THR	2.5
1	B	744	GLU	2.5
1	A	432	TYR	2.5
1	A	723	PHE	2.5
2	F	38	SER	2.5
1	A	798	ASP	2.5
1	B	656	THR	2.4
2	D	59	GLY	2.4
1	B	710	HIS	2.4
2	F	71	MET	2.4
1	A	797	ILE	2.4
1	B	711	ILE	2.4
1	B	759	GLN	2.4
1	C	793	PHE	2.4
2	E	57	ALA	2.4
1	C	664	ILE	2.4
2	D	32	LEU	2.4
2	F	5	THR	2.3
1	A	431	LYS	2.3
1	B	737	LYS	2.3
2	E	102	ALA	2.3
2	F	15	ALA	2.3
2	F	21	LYS	2.3
1	B	578	GLY	2.3
2	D	65	PHE	2.3
1	A	695	LYS	2.3
2	E	13	LYS	2.3
1	C	749	PHE	2.3
1	C	763	LEU	2.3
2	E	69	LEU	2.3
1	B	649	ILE	2.3
2	F	79	THR	2.3
1	A	768	LYS	2.2
1	B	545	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	785	ASN	2.2
1	C	514	ASP	2.2
2	E	130	ILE	2.2
1	C	775	LEU	2.2
2	D	38	SER	2.2
2	D	68	PHE	2.2
1	B	709	ASN	2.2
2	F	75	LYS	2.2
1	A	776	LEU	2.2
1	B	427	ASP	2.2
2	E	76	MET	2.2
1	B	544	SER	2.2
2	F	63	ILE	2.2
2	E	116	LEU	2.1
2	D	24	ASP	2.1
1	A	738	SER	2.1
2	E	17	SER	2.1
2	E	35	VAL	2.1
2	E	121	VAL	2.1
2	E	136	VAL	2.1
1	B	749	PHE	2.1
2	D	79	THR	2.1
2	E	5	THR	2.1
1	C	768	LYS	2.1
1	B	508	ILE	2.1
1	A	790	PHE	2.1
1	C	742	ALA	2.1
2	E	115	LYS	2.1
2	F	13	LYS	2.1
1	C	743	PRO	2.1
2	F	42	ASN	2.1
1	C	729	TYR	2.1
2	E	32	LEU	2.1
2	E	59	GLY	2.1
1	C	796	ILE	2.1
2	E	8	GLN	2.0
2	E	33	GLY	2.0
2	F	33	GLY	2.0
1	B	536	TYR	2.0
1	B	729	TYR	2.0
1	C	790	PHE	2.0
2	E	56	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	513	TRP	2.0
1	B	620	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

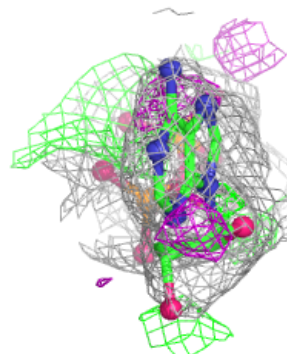
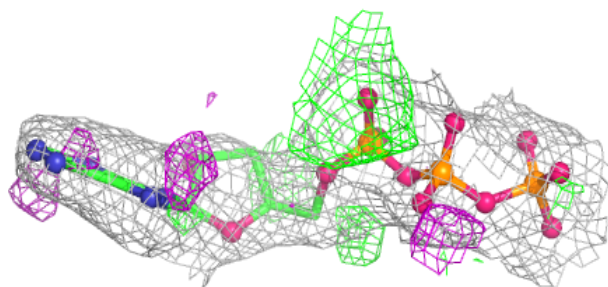
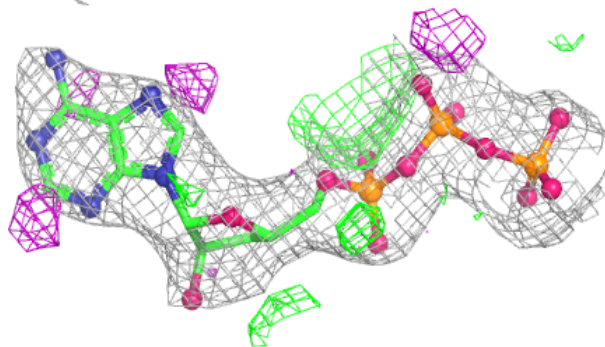
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	3AT	A	902	30/30	0.96	0.10	23,44,55,55	0
4	3AT	B	903	30/30	0.96	0.11	43,54,61,65	0
4	3AT	C	904	30/30	0.96	0.09	28,44,53,58	0
5	CA	E	802	1/1	0.96	0.04	105,105,105,105	0
5	CA	D	800	1/1	0.97	0.04	53,53,53,53	0
5	CA	D	801	1/1	0.98	0.05	59,59,59,59	0
5	CA	E	803	1/1	0.98	0.03	83,83,83,83	0
5	CA	F	804	1/1	0.98	0.04	67,67,67,67	0
3	YB	B	902	1/1	0.99	0.06	47,47,47,47	0
5	CA	F	805	1/1	0.99	0.02	63,63,63,63	0
3	YB	C	903	1/1	1.00	0.05	38,38,38,38	0
3	YB	A	901	1/1	1.00	0.06	38,38,38,38	0

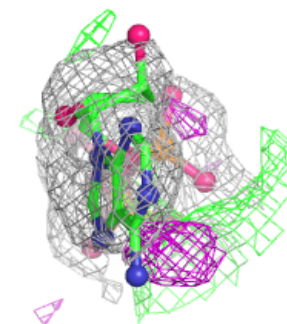
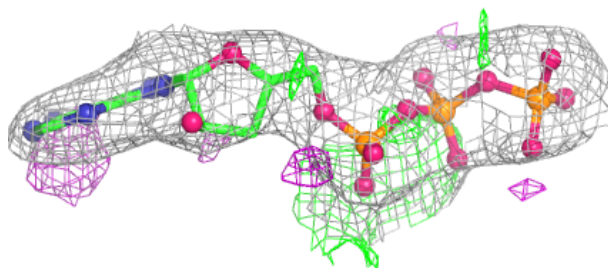
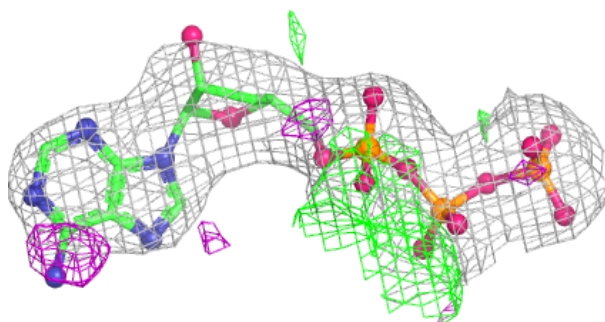
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3AT A 902:

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

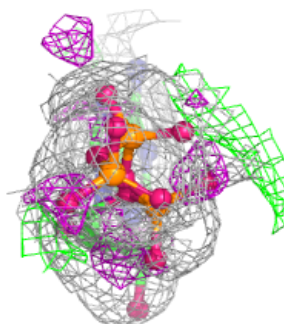
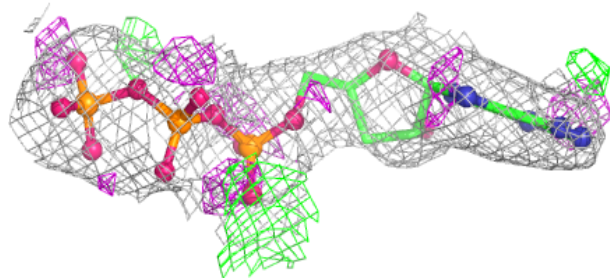
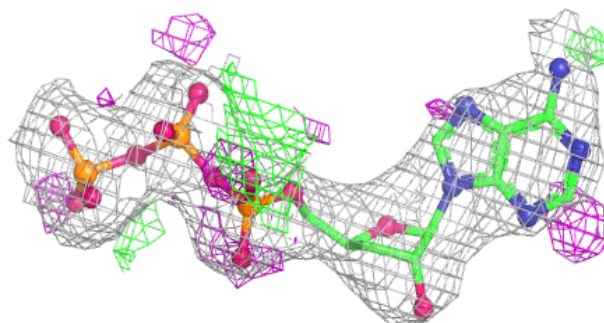
**Electron density around 3AT B 903:**

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



Electron density around 3AT C 904:

$2mF_o-DF_c$ (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.