



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:47 PM UTC

PDB ID : 1KWO / pdb_00001kwo
Title : SCALLOP MYOSIN S1-ATPgammaS-p-PDM IN THE ACTIN-DETACHED CONFORMATION
Authors : Himmel, D.M.; Gourinath, S.; Reshetnikova, L.; Shen, Y.; Szent-Gyorgyi, G.; Cohen, C.
Deposited on : 2002-01-30
Resolution : 3.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

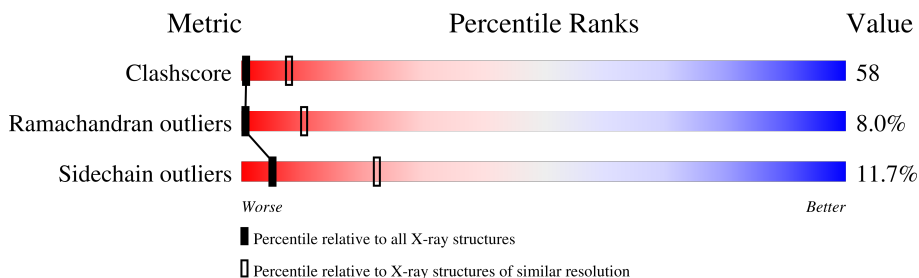
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	835	29% 50% 13% 7%
2	B	156	28% 52% 10% 9%
3	C	156	35% 49% 13% 2%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PDM	A	900	X	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8108 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 MYOSIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	1	0	0
			5867	3725	1009	1100	33			

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	3	0	0
			1032	646	165	214	7			

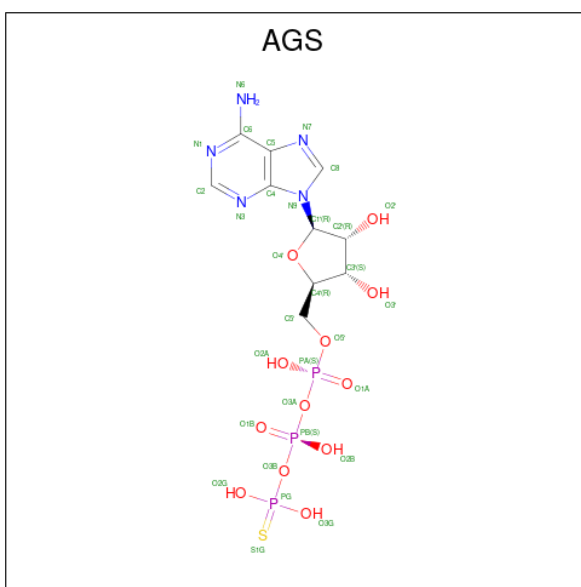
- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1148	722	183	236	7			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

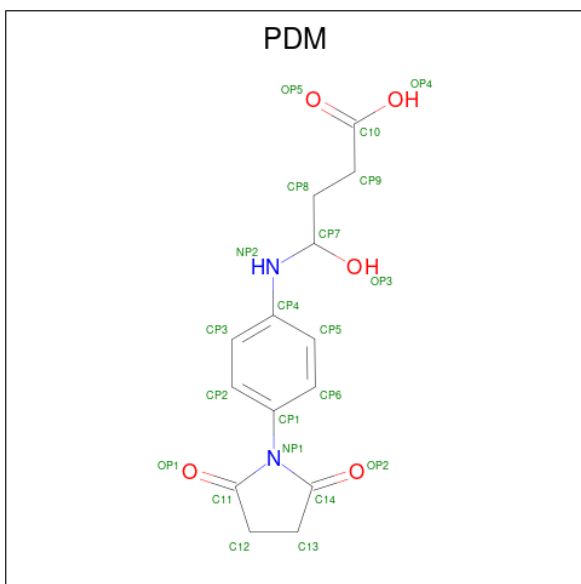
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 6 is 4-[4-(2,5-DIOXO-PYRROLIDIN-1-YL)-PHENYLAMINO]-4-HYDROXY-BUTYRIC ACID (CCD ID: PDM) (formula: $C_{14}H_{16}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			21	14	2	5		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Ca 1	0	0

- Molecule 8 is water.

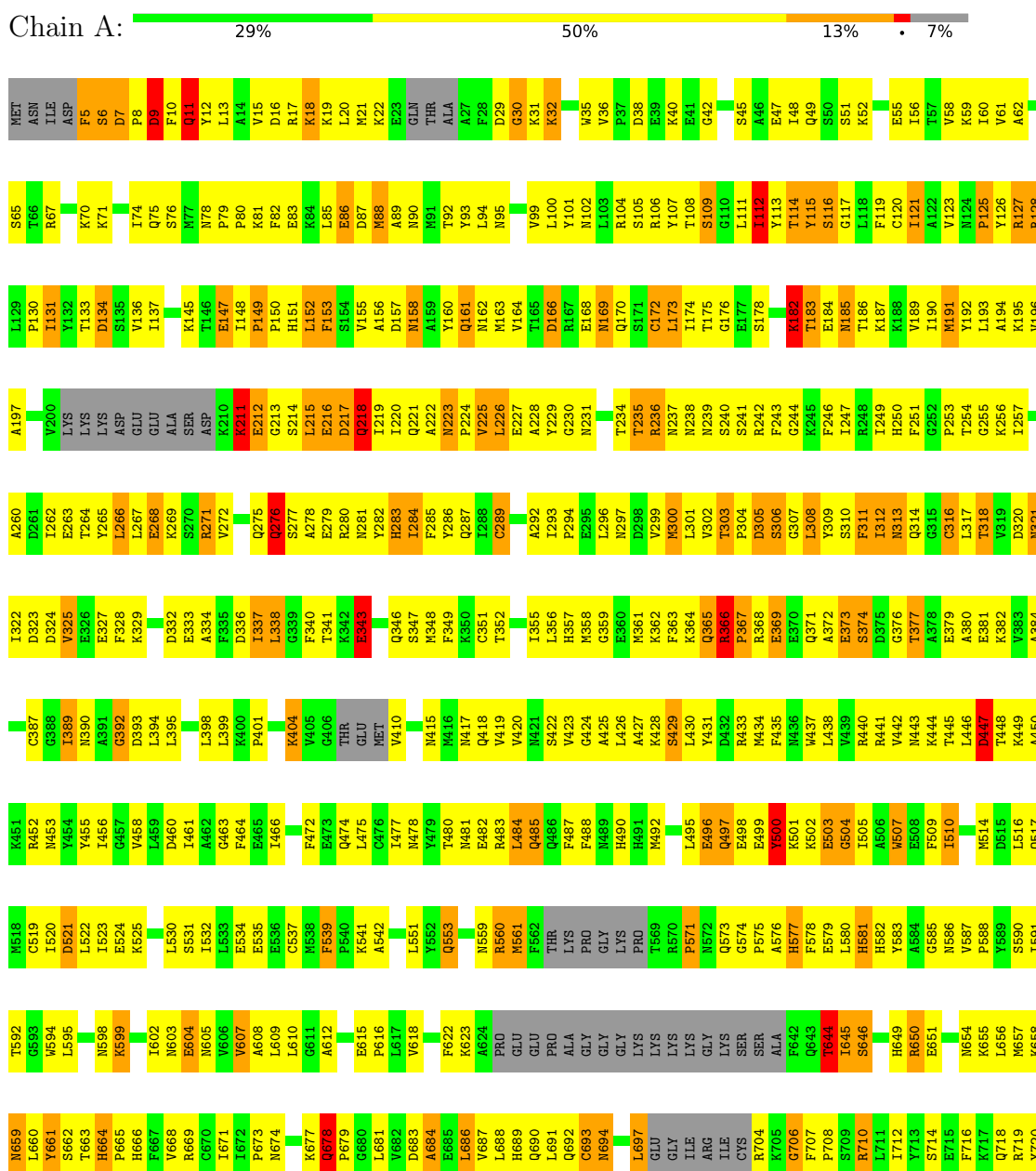
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total 3	O 3	0	0
8	B	1	Total 1	O 1	0	0
8	C	2	Total 2	O 2	0	0

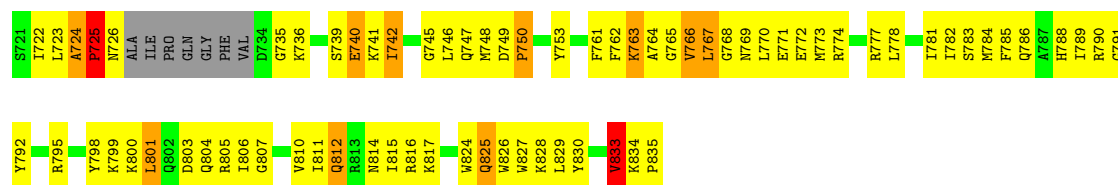
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

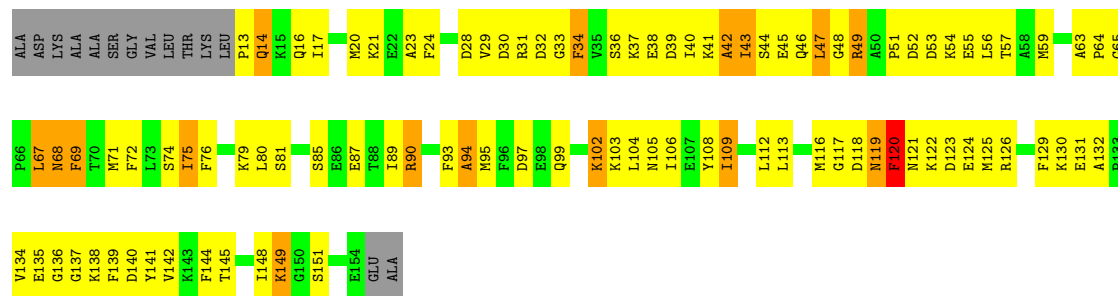
Note EDS was not executed.

• Molecule 1: MYOSIN HEAVY CHAIN

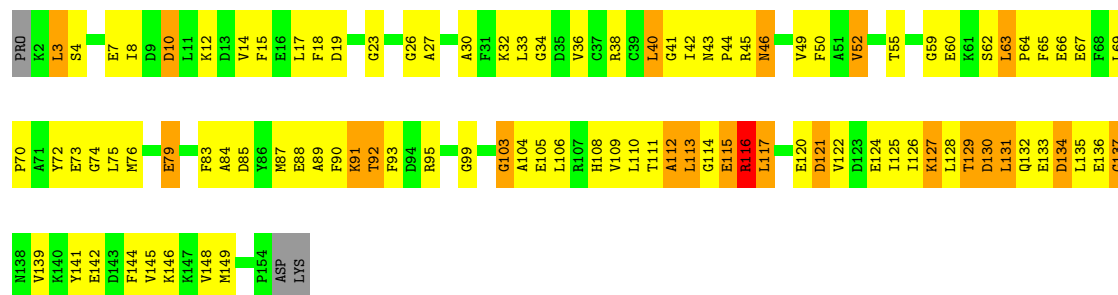




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 57.03Å 151.71Å 95.16° 96.45° 100.93°	Depositor
Resolution (Å)	36.87 – 3.80	Depositor
% Data completeness (in resolution range)	78.8 (36.87-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.238 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8108	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PDM, AGS, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/5980	1.33	79/8106 (1.0%)
2	B	0.67	0/1048	1.15	7/1415 (0.5%)
3	C	0.61	0/1169	1.02	4/1582 (0.3%)
All	All	0.67	0/8197	1.27	90/11103 (0.8%)

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	SER	N-CA-C	-24.70	86.46	114.62
1	A	539	PHE	CA-CB-CG	18.84	132.64	113.80
1	A	320	ASP	N-CA-C	14.49	130.25	112.87
1	A	368	ARG	N-CA-C	-13.03	97.69	113.19
1	A	19	LYS	N-CA-C	-12.61	97.88	113.01
1	A	303	THR	CA-C-N	11.48	134.19	119.84
1	A	303	THR	C-N-CA	11.48	134.19	119.84
1	A	644	THR	N-CA-C	11.09	134.41	110.80
3	C	79	GLU	N-CA-C	10.93	126.37	110.42
1	A	574	GLY	CA-C-N	10.71	132.24	120.13
1	A	574	GLY	C-N-CA	10.71	132.24	120.13
1	A	21	MET	N-CA-C	10.44	126.43	112.13
1	A	371	GLN	N-CA-C	10.26	121.78	108.34
1	A	373	GLU	N-CA-C	10.10	126.56	108.69
1	A	16	ASP	N-CA-C	9.99	124.33	110.35
1	A	718	GLN	N-CA-C	9.78	123.17	111.82
1	A	372	ALA	N-CA-C	9.67	124.11	108.63
1	A	22	LYS	N-CA-C	9.62	131.29	110.80
1	A	212	GLU	N-CA-C	9.61	123.79	109.95
1	A	767	LEU	N-CA-C	-9.51	99.58	111.75
1	A	216	GLU	N-CA-C	-9.42	90.73	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	VAL	CB-CA-C	-9.05	102.05	110.91
2	B	120	PHE	N-CA-C	-8.69	97.15	110.10
1	A	303	THR	N-CA-C	-8.68	95.51	109.40
1	A	500	TYR	N-CA-C	-8.35	103.22	113.50
1	A	499	GLU	N-CA-C	-8.29	101.63	112.41
1	A	678	GLN	CA-C-N	7.72	127.65	119.85
1	A	678	GLN	C-N-CA	7.72	127.65	119.85
1	A	369	GLU	N-CA-C	-7.58	94.66	110.80
1	A	367	PRO	N-CA-CB	7.57	111.20	103.25
1	A	365	GLN	N-CA-C	-7.38	95.09	110.80
1	A	724	ALA	CA-C-N	-7.35	110.65	119.84
1	A	724	ALA	C-N-CA	-7.35	110.65	119.84
1	A	447	ASP	N-CA-C	-7.33	95.66	108.20
1	A	645	ILE	N-CA-C	7.21	124.34	109.34
1	A	17	ARG	N-CA-C	7.04	125.79	110.80
1	A	693	CYS	N-CA-C	-7.00	104.01	114.64
1	A	307	GLY	N-CA-C	-6.96	96.69	113.18
1	A	162	ASN	N-CA-C	-6.87	104.98	113.15
1	A	833	VAL	CB-CA-C	-6.73	100.26	111.29
2	B	34	PHE	N-CA-C	6.62	119.48	109.95
1	A	650	ARG	N-CA-C	-6.57	105.12	113.01
2	B	67	LEU	N-CA-C	6.57	118.61	109.15
1	A	311	PHE	N-CA-C	6.49	120.45	112.54
1	A	575	PRO	N-CA-C	6.45	121.07	110.55
1	A	301	LEU	N-CA-C	-6.44	105.00	112.86
3	C	116	ARG	CA-C-N	-6.43	112.92	122.56
3	C	116	ARG	C-N-CA	-6.43	112.92	122.56
2	B	69	PHE	N-CA-C	-6.36	107.37	114.62
1	A	366	ARG	N-CA-C	6.29	123.71	109.81
1	A	693	CYS	CA-C-N	-6.07	109.95	121.54
1	A	693	CYS	C-N-CA	-6.07	109.95	121.54
1	A	182	LYS	N-CA-C	-6.04	104.99	112.72
1	A	9	ASP	N-CA-C	-5.95	97.99	109.24
1	A	185	ASN	N-CA-C	-5.83	105.66	112.89
1	A	92	THR	N-CA-C	-5.83	105.06	111.82
1	A	706	GLY	N-CA-C	-5.77	99.50	113.18
1	A	577	HIS	N-CA-C	5.76	120.44	113.41
1	A	306	SER	N-CA-C	-5.74	104.00	111.74
1	A	503	GLU	N-CA-C	-5.71	105.51	112.88
1	A	376	GLY	N-CA-C	-5.71	99.65	113.18
1	A	300	MET	N-CA-C	-5.70	104.89	113.89
1	A	145	LYS	N-CA-C	5.52	120.89	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ASP	CA-C-N	5.47	126.67	119.84
1	A	7	ASP	C-N-CA	5.47	126.67	119.84
1	A	374	SER	CA-C-N	-5.45	112.36	122.60
1	A	374	SER	C-N-CA	-5.45	112.36	122.60
1	A	664	HIS	CA-C-N	5.42	125.72	119.92
1	A	664	HIS	C-N-CA	5.42	125.72	119.92
1	A	115	TYR	N-CA-C	-5.41	105.42	112.23
3	C	10	ASP	N-CA-C	-5.39	106.55	113.23
1	A	377	THR	N-CA-C	-5.39	108.48	114.62
1	A	211	LYS	N-CA-C	5.37	122.24	110.80
1	A	484	LEU	N-CA-C	-5.37	105.46	112.23
1	A	149	PRO	CA-C-N	5.32	125.57	119.83
1	A	149	PRO	C-N-CA	5.32	125.57	119.83
1	A	312	ILE	CB-CA-C	-5.29	105.46	110.70
1	A	644	THR	CA-C-N	5.25	131.42	121.97
1	A	644	THR	C-N-CA	5.25	131.42	121.97
1	A	553	GLN	N-CA-C	-5.24	106.57	113.17
1	A	5	PHE	N-CA-C	5.22	125.61	111.00
1	A	447	ASP	CA-C-N	-5.21	115.76	123.05
1	A	447	ASP	C-N-CA	-5.21	115.76	123.05
1	A	305	ASP	N-CA-C	-5.18	99.76	110.80
2	B	102	LYS	N-CA-C	-5.18	104.50	111.54
1	A	218	GLN	N-CA-C	-5.17	105.27	112.45
1	A	18	LYS	N-CA-C	5.12	118.57	111.55
1	A	321	ASN	N-CA-CB	-5.12	101.80	111.43
2	B	13	PRO	CA-C-N	-5.04	116.44	122.44
2	B	13	PRO	C-N-CA	-5.04	116.44	122.44

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	5867	0	5467	687	0
2	B	1032	0	907	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1148	0	1032	136	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	31	0	12	6	0
6	A	21	0	10	10	0
7	C	1	0	0	0	0
8	A	3	0	0	4	0
8	B	1	0	0	1	0
8	C	2	0	0	0	0
All	All	8108	0	7428	903	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 58.

All (903) 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:A:697:LEU:HA	1:A:704:ARG:HH21	1.02	1.12
1:A:187:LYS:HE2	1:A:223:ASN:HD22	1.13	1.11
1:A:693:CYS:HB2	6:A:900:PDM:OP3	1.48	1.11
1:A:644:THR:CG2	1:A:645:ILE:HG13	1.86	1.05
2:B:43:ILE:O	2:B:47:LEU:HB2	1.57	1.04
1:A:115:TYR:CE1	1:A:150:PRO:HB3	1.93	1.04
1:A:523:ILE:O	1:A:530:LEU:HD13	1.57	1.02
1:A:496:GLU:C	1:A:498:GLU:H	1.68	1.01
3:C:111:THR:HA	3:C:116:ARG:HA	1.39	1.01
1:A:644:THR:HG22	1:A:645:ILE:CG1	1.90	1.00
1:A:833:VAL:O	1:A:835:PRO:HD3	1.62	0.99
1:A:178:SER:OG	5:A:999:AGS:S1G	2.22	0.98
1:A:697:LEU:HB3	1:A:704:ARG:HE	1.24	0.97
1:A:78:ASN:HD21	1:A:93:TYR:H	0.99	0.97
1:A:482:GLU:HG2	1:A:520:ILE:HD11	1.49	0.95
1:A:581:HIS:HA	1:A:586:ASN:OD1	1.67	0.94
1:A:226:LEU:HD12	1:A:226:LEU:H	1.28	0.93
2:B:44:SER:O	2:B:48:GLY:N	2.02	0.92
1:A:644:THR:HG22	1:A:645:ILE:HG13	0.95	0.91
1:A:495:LEU:HD13	1:A:495:LEU:O	1.72	0.90
3:C:46:ASN:O	3:C:49:VAL:HG22	1.70	0.90
1:A:196:VAL:HG13	1:A:197:ALA:H	1.35	0.90
1:A:12:TYR:HB2	1:A:131:ILE:CG2	2.02	0.90
2:B:90:ARG:HB2	2:B:90:ARG:HH11	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:ARG:HH11	1:A:781:ILE:HD11	1.36	0.89
1:A:170:GLN:NE2	1:A:664:HIS:HB3	1.88	0.88
1:A:697:LEU:HA	1:A:704:ARG:NH2	1.88	0.88
1:A:78:ASN:ND2	1:A:93:TYR:H	1.71	0.88
1:A:764:ALA:O	1:A:766:VAL:HG23	1.73	0.88
3:C:42:ILE:HG22	3:C:44:PRO:HD3	1.57	0.87
2:B:129:PHE:HA	2:B:132:ALA:HB2	1.57	0.86
1:A:215:LEU:O	1:A:215:LEU:HD22	1.75	0.86
1:A:693:CYS:HA	6:A:900:PDM:HP3	1.56	0.86
1:A:833:VAL:O	1:A:835:PRO:CD	2.24	0.86
3:C:73:GLU:HA	3:C:76:MET:SD	2.16	0.85
1:A:560:ARG:H	1:A:561:MET:HE2	1.38	0.85
1:A:267:LEU:HD23	1:A:268:GLU:N	1.92	0.84
1:A:187:LYS:HE2	1:A:223:ASN:ND2	1.93	0.83
1:A:367:PRO:C	1:A:369:GLU:H	1.82	0.83
1:A:173:LEU:HD12	1:A:173:LEU:H	1.43	0.83
1:A:88:MET:HE3	1:A:102:ASN:HB3	1.61	0.82
1:A:88:MET:HB2	1:A:116:SER:OG	1.79	0.81
1:A:343:GLU:CD	1:A:343:GLU:H	1.86	0.81
1:A:289:CYS:HB2	1:A:306:SER:OG	1.80	0.81
1:A:242:ARG:HE	1:A:271:ARG:HH12	1.27	0.81
1:A:182:LYS:HG3	5:A:999:AGS:O2B	1.81	0.81
1:A:379:GLU:HA	1:A:382:LYS:HE2	1.62	0.80
1:A:85:LEU:H	1:A:102:ASN:HD21	1.26	0.80
1:A:100:LEU:HD12	1:A:688:LEU:HD21	1.63	0.80
1:A:78:ASN:HD21	1:A:93:TYR:N	1.78	0.80
1:A:169:ASN:HB3	1:A:663:THR:HG22	1.62	0.80
2:B:65:GLY:H	2:B:71:MET:HE3	1.44	0.80
2:B:106:ILE:HG22	2:B:137:GLY:O	1.81	0.80
2:B:145:THR:O	2:B:148:ILE:HG22	1.79	0.80
1:A:253:PRO:HD3	1:A:453:ASN:HD21	1.47	0.80
1:A:151:HIS:CE1	1:A:153:PHE:CD2	2.70	0.79
1:A:35:TRP:HB2	1:A:75:GLN:HB2	1.65	0.79
1:A:48:ILE:HA	1:A:58:VAL:HG12	1.65	0.79
1:A:125:PRO:O	1:A:679:PRO:HB3	1.81	0.79
1:A:750:PRO:HA	1:A:753:TYR:HE1	1.48	0.79
1:A:309:TYR:CD2	1:A:356:LEU:HG	2.18	0.78
1:A:496:GLU:C	1:A:498:GLU:N	2.39	0.78
3:C:114:GLY:C	3:C:115:GLU:HG2	2.07	0.78
1:A:189:VAL:O	1:A:193:LEU:HD23	1.83	0.78
1:A:720:TYR:HE1	1:A:770:LEU:HB3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:SER:HA	1:A:313:ASN:HD21	1.48	0.78
1:A:798:TYR:OH	3:C:14:VAL:HG22	1.83	0.78
1:A:812:GLN:NE2	2:B:118:ASP:OD1	2.18	0.77
1:A:112:ILE:HD11	1:A:123:VAL:N	2.00	0.76
1:A:60:ILE:HD11	1:A:67:ARG:NE	2.00	0.76
1:A:86:GLU:O	1:A:114:THR:HG22	1.84	0.76
3:C:128:LEU:C	3:C:130:ASP:H	1.93	0.76
1:A:215:LEU:O	1:A:215:LEU:CD2	2.34	0.76
1:A:223:ASN:HB2	1:A:224:PRO:HD3	1.67	0.76
3:C:122:VAL:O	3:C:125:ILE:HG22	1.86	0.76
1:A:602:ILE:HD12	1:A:607:VAL:HG22	1.68	0.76
1:A:85:LEU:HD21	1:A:90:ASN:HB2	1.68	0.75
1:A:542:ALA:HB1	1:A:595:LEU:HD13	1.69	0.75
2:B:34:PHE:HD2	2:B:68:ASN:HA	1.52	0.75
1:A:115:TYR:OH	1:A:150:PRO:HA	1.87	0.75
2:B:90:ARG:HB2	2:B:90:ARG:NH1	2.02	0.75
1:A:289:CYS:SG	1:A:306:SER:OG	2.45	0.75
3:C:111:THR:O	3:C:116:ARG:HB3	1.87	0.75
2:B:34:PHE:CD2	2:B:68:ASN:HA	2.23	0.74
1:A:507:TRP:HZ3	1:A:761:PHE:HB3	1.53	0.74
1:A:367:PRO:C	1:A:369:GLU:N	2.40	0.74
1:A:417:ASN:HA	1:A:420:VAL:HG12	1.69	0.74
1:A:660:LEU:C	1:A:662:SER:H	1.95	0.74
3:C:45:ARG:O	3:C:49:VAL:HG13	1.88	0.74
1:A:829:LEU:O	1:A:833:VAL:HG23	1.87	0.73
1:A:716:PHE:HD2	1:A:739:SER:HG	1.35	0.73
1:A:78:ASN:OD1	1:A:93:TYR:HB2	1.88	0.73
1:A:806:ILE:O	1:A:810:VAL:HG23	1.89	0.73
1:A:792:TYR:OH	3:C:129:THR:HG22	1.89	0.73
1:A:615:GLU:HB3	1:A:618:VAL:HG23	1.69	0.72
2:B:93:PHE:CD2	2:B:141:TYR:HB2	2.24	0.72
1:A:280:ARG:HH11	1:A:318:THR:HA	1.55	0.72
1:A:466:ILE:HG23	1:A:466:ILE:O	1.90	0.72
2:B:16:GLN:O	2:B:20:MET:HG2	1.88	0.72
1:A:719:ARG:HG2	1:A:774:ARG:NH1	2.04	0.71
1:A:212:GLU:C	1:A:337:ILE:HG22	2.14	0.71
1:A:112:ILE:HD13	1:A:123:VAL:HG22	1.72	0.71
1:A:361:MET:HG2	1:A:380:ALA:HB2	1.70	0.71
1:A:645:ILE:HG22	1:A:645:ILE:O	1.90	0.71
1:A:289:CYS:CB	1:A:306:SER:OG	2.38	0.71
1:A:214:SER:OG	1:A:217:ASP:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:C	1:A:425:ALA:H	1.99	0.70
1:A:447:ASP:CG	1:A:447:ASP:O	2.34	0.70
1:A:488:PHE:CE2	1:A:669:ARG:NH2	2.59	0.70
1:A:488:PHE:CE1	1:A:492:MET:HG3	2.26	0.70
1:A:674:ASN:HD21	1:A:678:GLN:H	1.38	0.70
3:C:40:LEU:HD13	3:C:72:TYR:CE1	2.26	0.70
1:A:268:GLU:OE1	1:A:271:ARG:NH1	2.25	0.70
1:A:559:ASN:HB3	1:A:561:MET:HE2	1.74	0.70
1:A:196:VAL:HG22	1:A:197:ALA:N	2.07	0.69
1:A:89:ALA:HB2	1:A:117:GLY:HA2	1.73	0.69
1:A:112:ILE:HD12	1:A:112:ILE:O	1.92	0.69
1:A:496:GLU:O	1:A:498:GLU:N	2.25	0.69
3:C:110:LEU:HD23	3:C:122:VAL:HG22	1.75	0.69
1:A:7:ASP:OD1	1:A:7:ASP:N	2.26	0.69
1:A:216:GLU:C	1:A:218:GLN:H	2.00	0.69
1:A:764:ALA:O	1:A:766:VAL:N	2.25	0.69
1:A:151:HIS:CE1	1:A:153:PHE:H	2.10	0.69
1:A:644:THR:HG22	1:A:645:ILE:N	2.03	0.69
3:C:27:ALA:HB1	3:C:62:SER:HB3	1.75	0.69
3:C:8:ILE:O	3:C:12:LYS:HG3	1.92	0.68
1:A:266:LEU:HD21	1:A:649:HIS:CE1	2.28	0.68
1:A:723:LEU:HD21	1:A:773:MET:O	1.93	0.68
3:C:74:GLY:C	3:C:76:MET:H	2.01	0.68
1:A:109:SER:HB2	1:A:111:LEU:HG	1.75	0.68
1:A:576:ALA:HA	1:A:590:SER:HB2	1.75	0.68
2:B:121:ASN:OD1	2:B:124:GLU:HB2	1.94	0.68
1:A:417:ASN:C	1:A:419:VAL:H	2.02	0.68
1:A:266:LEU:H	1:A:266:LEU:HD22	1.58	0.68
2:B:31:ARG:C	2:B:33:GLY:H	2.02	0.68
1:A:95:ASN:O	1:A:99:VAL:HG23	1.95	0.67
1:A:112:ILE:HD11	1:A:123:VAL:O	1.93	0.67
1:A:216:GLU:C	1:A:218:GLN:N	2.50	0.67
2:B:103:LYS:O	2:B:104:LEU:HD23	1.95	0.67
1:A:175:THR:HG22	1:A:176:GLY:H	1.60	0.67
1:A:231:ASN:HB3	1:A:239:ASN:ND2	2.10	0.67
1:A:355:ILE:HG23	1:A:427:ALA:HB1	1.77	0.67
1:A:395:LEU:O	1:A:399:LEU:HG	1.94	0.67
1:A:437:TRP:HA	1:A:440:ARG:HH11	1.59	0.67
1:A:795:ARG:HH22	3:C:42:ILE:N	1.93	0.67
1:A:300:MET:O	1:A:302:VAL:HG13	1.95	0.67
1:A:32:LYS:O	1:A:47:GLU:HA	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:O	1:A:163:MET:HB3	1.94	0.67
1:A:801:LEU:HD12	3:C:17:LEU:HD11	1.77	0.67
1:A:115:TYR:CZ	1:A:150:PRO:HA	2.30	0.66
1:A:183:THR:HG23	1:A:460:ASP:OD1	1.95	0.66
1:A:226:LEU:HD12	1:A:226:LEU:N	2.08	0.66
1:A:417:ASN:O	1:A:419:VAL:N	2.28	0.66
1:A:522:LEU:HA	1:A:525:LYS:HE3	1.75	0.66
1:A:437:TRP:HA	1:A:440:ARG:NH1	2.11	0.66
1:A:826:TRP:O	1:A:829:LEU:HB3	1.95	0.66
1:A:463:GLY:HA2	1:A:481:ASN:OD1	1.94	0.66
3:C:134:ASP:CG	3:C:136:GLU:H	2.04	0.66
1:A:253:PRO:CD	1:A:453:ASN:HD21	2.09	0.66
6:A:900:PDM:OP1	6:A:900:PDM:HP6	1.96	0.66
2:B:126:ARG:O	2:B:130:LYS:HG3	1.95	0.66
1:A:111:LEU:O	1:A:112:ILE:HG22	1.96	0.65
1:A:174:ILE:CG2	1:A:182:LYS:HB3	2.26	0.65
2:B:140:ASP:OD1	2:B:142:VAL:HB	1.96	0.65
1:A:693:CYS:CB	6:A:900:PDM:OP3	2.38	0.65
1:A:789:ILE:HG23	3:C:125:ILE:HD13	1.78	0.65
1:A:394:LEU:O	1:A:398:LEU:HB2	1.97	0.65
1:A:833:VAL:O	1:A:833:VAL:HG12	1.96	0.65
2:B:34:PHE:HB3	2:B:67:LEU:O	1.96	0.65
1:A:693:CYS:SG	6:A:900:PDM:HP3	2.36	0.64
1:A:598:ASN:HB3	1:A:599:LYS:HZ2	1.62	0.64
1:A:55:GLU:O	1:A:55:GLU:HG2	1.96	0.64
1:A:196:VAL:HG13	1:A:197:ALA:N	2.11	0.64
2:B:32:ASP:OD1	2:B:34:PHE:O	2.14	0.64
1:A:507:TRP:O	1:A:510:ILE:HD11	1.96	0.64
2:B:134:VAL:HG13	2:B:138:LYS:O	1.97	0.64
1:A:276:GLN:HG2	1:A:279:GLU:OE1	1.98	0.64
1:A:115:TYR:CE1	1:A:150:PRO:CB	2.77	0.64
1:A:657:MET:C	1:A:659:ASN:H	2.06	0.64
3:C:27:ALA:HA	3:C:63:LEU:O	1.97	0.64
3:C:30:ALA:O	3:C:33:LEU:HB3	1.97	0.64
1:A:297:ASN:ND2	1:A:302:VAL:O	2.29	0.63
1:A:788:HIS:HA	3:C:43:ASN:HB3	1.79	0.63
2:B:24:PHE:CE1	2:B:68:ASN:O	2.51	0.63
1:A:303:THR:CG2	1:A:304:PRO:HD2	2.28	0.63
2:B:40:ILE:C	2:B:42:ALA:H	2.07	0.63
1:A:94:LEU:HD23	1:A:94:LEU:O	1.98	0.63
1:A:185:ASN:O	1:A:189:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HA	1:A:218:GLN:CB	2.28	0.63
1:A:51:SER:HB2	3:C:95:ARG:HH21	1.64	0.63
1:A:537:CYS:C	1:A:539:PHE:H	2.06	0.62
1:A:719:ARG:HG2	1:A:774:ARG:CZ	2.29	0.62
1:A:338:LEU:HD21	1:A:442:VAL:HG13	1.81	0.62
1:A:429:SER:O	1:A:433:ARG:HD2	1.99	0.62
1:A:693:CYS:HB2	6:A:900:PDM:CP7	2.28	0.62
1:A:482:GLU:HG2	1:A:520:ILE:CD1	2.27	0.62
1:A:461:ILE:O	1:A:461:ILE:HG13	1.99	0.62
1:A:131:ILE:HB	8:A:1001:HOH:O	1.98	0.62
2:B:30:ASP:OD1	2:B:32:ASP:HB3	2.00	0.62
1:A:249:ILE:HD12	1:A:249:ILE:N	2.15	0.61
1:A:303:THR:HG22	1:A:304:PRO:HD2	1.82	0.61
1:A:30:GLY:C	1:A:31:LYS:HD2	2.24	0.61
1:A:363:PHE:HE2	1:A:399:LEU:HD21	1.64	0.61
1:A:475:LEU:HD22	1:A:594:TRP:HH2	1.66	0.61
1:A:310:SER:HA	1:A:313:ASN:ND2	2.16	0.61
1:A:784:MET:SD	3:C:79:GLU:HG2	2.40	0.61
1:A:786:GLN:HE22	3:C:115:GLU:H	1.46	0.61
1:A:106:ARG:O	1:A:111:LEU:HG	2.00	0.61
1:A:340:PHE:CZ	1:A:441:ARG:HG2	2.35	0.61
1:A:151:HIS:CD2	8:A:1001:HOH:O	2.53	0.61
1:A:461:ILE:HD11	1:A:484:LEU:HD11	1.82	0.61
3:C:92:THR:C	3:C:93:PHE:HD1	2.07	0.61
1:A:507:TRP:CZ3	1:A:761:PHE:HB3	2.36	0.61
1:A:708:PRO:HB3	1:A:762:PHE:O	2.00	0.61
3:C:8:ILE:HG22	3:C:12:LYS:HG3	1.82	0.61
1:A:169:ASN:HD21	1:A:455:TYR:N	1.99	0.61
2:B:56:LEU:O	2:B:59:MET:HB3	2.01	0.61
1:A:690:GLN:O	1:A:694:ASN:ND2	2.26	0.60
1:A:697:LEU:CB	1:A:704:ARG:HE	2.08	0.60
6:A:900:PDM:HP2	6:A:900:PDM:OP2	2.00	0.60
3:C:74:GLY:O	3:C:76:MET:N	2.29	0.60
3:C:128:LEU:O	3:C:130:ASP:N	2.33	0.60
1:A:170:GLN:HG3	1:A:666:HIS:NE2	2.16	0.60
1:A:216:GLU:O	1:A:219:ILE:N	2.34	0.60
1:A:192:TYR:O	1:A:196:VAL:HG12	2.01	0.60
1:A:228:ALA:HA	1:A:283:HIS:HB2	1.83	0.60
1:A:366:ARG:CB	1:A:373:GLU:CB	2.79	0.60
1:A:577:HIS:CE1	1:A:592:THR:HG23	2.36	0.60
1:A:748:MET:O	1:A:749:ASP:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:PRO:HA	1:A:753:TYR:CE1	2.32	0.60
1:A:795:ARG:HH12	3:C:41:GLY:H	1.49	0.60
1:A:815:ILE:HD11	2:B:144:PHE:CE2	2.37	0.60
1:A:126:TYR:CE1	1:A:677:LYS:HA	2.35	0.60
1:A:605:ASN:O	1:A:609:LEU:HB2	2.02	0.60
2:B:87:GLU:O	2:B:90:ARG:HG3	2.02	0.60
1:A:487:PHE:HD1	1:A:661:TYR:CE1	2.20	0.60
1:A:213:GLY:N	1:A:337:ILE:HG22	2.17	0.60
2:B:64:PRO:HD2	2:B:71:MET:SD	2.41	0.60
1:A:226:LEU:H	1:A:226:LEU:CD1	2.07	0.60
1:A:300:MET:C	1:A:302:VAL:HG13	2.27	0.60
1:A:152:LEU:O	1:A:155:VAL:HG23	2.02	0.59
1:A:275:GLN:OE1	1:A:314:GLN:HB2	2.02	0.59
1:A:466:ILE:HD13	1:A:587:VAL:HG22	1.84	0.59
1:A:542:ALA:CB	1:A:595:LEU:HD13	2.31	0.59
1:A:724:ALA:O	1:A:726:ASN:N	2.35	0.59
1:A:292:ALA:O	1:A:293:ILE:HD13	2.01	0.59
1:A:364:LYS:O	1:A:366:ARG:N	2.34	0.59
2:B:45:GLU:C	2:B:47:LEU:H	2.11	0.59
1:A:789:ILE:HG23	3:C:125:ILE:CD1	2.32	0.59
1:A:85:LEU:HD12	1:A:86:GLU:H	1.67	0.59
1:A:100:LEU:C	1:A:100:LEU:HD23	2.27	0.59
1:A:778:LEU:HA	1:A:781:ILE:HD13	1.83	0.59
1:A:811:ILE:HG12	2:B:93:PHE:CE1	2.38	0.59
3:C:83:PHE:N	3:C:149:MET:HE1	2.17	0.59
1:A:11:GLN:O	1:A:12:TYR:CD2	2.55	0.59
1:A:265:TYR:OH	1:A:656:LEU:HB2	2.02	0.59
1:A:366:ARG:O	1:A:367:PRO:C	2.45	0.59
3:C:105:GLU:O	3:C:109:VAL:HG23	2.02	0.59
1:A:152:LEU:HD11	1:A:189:VAL:CG2	2.33	0.59
1:A:212:GLU:HA	1:A:337:ILE:HA	1.83	0.59
1:A:644:THR:CG2	1:A:645:ILE:N	2.65	0.59
1:A:748:MET:O	1:A:750:PRO:N	2.35	0.59
2:B:39:ASP:O	2:B:42:ALA:HB3	2.03	0.59
2:B:49:ARG:NH2	8:B:157:HOH:O	2.35	0.59
1:A:106:ARG:CB	1:A:111:LEU:HD12	2.33	0.59
1:A:501:LYS:C	1:A:504:GLY:H	2.09	0.59
3:C:126:ILE:C	3:C:128:LEU:N	2.59	0.59
1:A:12:TYR:HB2	1:A:131:ILE:HG21	1.84	0.59
1:A:292:ALA:HB3	1:A:328:PHE:HD2	1.68	0.59
3:C:91:LYS:C	3:C:93:PHE:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:CG	1:A:111:LEU:HD12	2.33	0.59
1:A:293:ILE:HG22	1:A:296:LEU:HB2	1.85	0.58
1:A:519:CYS:SG	1:A:581:HIS:O	2.59	0.58
3:C:106:LEU:HD12	3:C:110:LEU:CD1	2.32	0.58
1:A:246:PHE:HB3	1:A:263:GLU:HB3	1.85	0.58
1:A:560:ARG:O	1:A:561:MET:SD	2.61	0.58
1:A:697:LEU:CA	1:A:704:ARG:HH21	1.95	0.58
1:A:712:ILE:HG22	1:A:714:SER:H	1.68	0.58
1:A:79:PRO:C	1:A:81:LYS:H	2.11	0.58
1:A:329:LYS:O	1:A:332:ASP:HB3	2.02	0.58
1:A:284:ILE:O	1:A:287:GLN:HG2	2.02	0.58
1:A:334:ALA:O	1:A:338:LEU:HB2	2.03	0.58
1:A:464:PHE:H	1:A:481:ASN:ND2	2.02	0.58
1:A:11:GLN:O	1:A:12:TYR:HD2	1.86	0.58
1:A:175:THR:HB	1:A:669:ARG:HD3	1.86	0.58
1:A:215:LEU:CD2	1:A:215:LEU:C	2.77	0.58
1:A:807:GLY:HA3	2:B:95:MET:SD	2.44	0.58
2:B:40:ILE:C	2:B:42:ALA:N	2.60	0.58
1:A:88:MET:HE3	1:A:102:ASN:CB	2.33	0.58
1:A:147:GLU:HG3	1:A:148:ILE:N	2.17	0.58
1:A:106:ARG:HG2	1:A:111:LEU:HD12	1.86	0.58
1:A:115:TYR:CD1	1:A:150:PRO:HB3	2.38	0.58
1:A:250:HIS:CD2	1:A:452:ARG:HG2	2.39	0.57
1:A:300:MET:CB	1:A:302:VAL:HG13	2.34	0.57
3:C:111:THR:HG23	3:C:116:ARG:HB2	1.86	0.57
2:B:40:ILE:O	2:B:42:ALA:N	2.37	0.57
1:A:151:HIS:ND1	1:A:153:PHE:N	2.48	0.57
1:A:161:GLN:C	1:A:163:MET:H	2.12	0.57
1:A:169:ASN:HD21	1:A:455:TYR:H	1.51	0.57
1:A:781:ILE:HG21	3:C:89:ALA:HB2	1.86	0.57
1:A:785:PHE:HE1	3:C:145:VAL:HG23	1.67	0.57
3:C:106:LEU:O	3:C:110:LEU:HD13	2.03	0.57
1:A:88:MET:HB2	1:A:116:SER:HG	1.69	0.57
1:A:287:GLN:HB2	1:A:328:PHE:HB2	1.85	0.57
1:A:313:ASN:C	1:A:313:ASN:HD22	2.13	0.57
3:C:42:ILE:CG2	3:C:44:PRO:HD3	2.32	0.57
3:C:106:LEU:HD12	3:C:110:LEU:HD13	1.85	0.57
2:B:64:PRO:HB2	2:B:71:MET:HE1	1.86	0.57
1:A:109:SER:HB2	1:A:111:LEU:CG	2.35	0.57
1:A:488:PHE:CD1	1:A:488:PHE:C	2.83	0.57
2:B:51:PRO:HG2	2:B:56:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLN:O	1:A:347:SER:C	2.48	0.56
1:A:363:PHE:CE2	1:A:419:VAL:HG11	2.40	0.56
3:C:65:PHE:C	3:C:67:GLU:H	2.11	0.56
1:A:799:LYS:O	1:A:803:ASP:HB2	2.05	0.56
1:A:215:LEU:HA	1:A:218:GLN:HB3	1.86	0.56
1:A:237:ASN:HD21	1:A:240:SER:N	2.03	0.56
1:A:254:THR:O	1:A:256:LYS:HG2	2.06	0.56
1:A:262:ILE:H	1:A:443:ASN:ND2	2.03	0.56
1:A:448:THR:O	1:A:450:ALA:N	2.35	0.56
1:A:484:LEU:O	1:A:487:PHE:HB3	2.04	0.56
2:B:36:SER:OG	2:B:39:ASP:OD2	2.19	0.56
2:B:145:THR:HA	2:B:148:ILE:HG22	1.85	0.56
1:A:235:THR:HG23	1:A:236:ARG:N	2.21	0.56
1:A:788:HIS:HD2	3:C:148:VAL:HG12	1.70	0.56
1:A:341:THR:HB	1:A:343:GLU:OE2	2.06	0.56
1:A:674:ASN:HD21	1:A:678:GLN:N	2.02	0.56
2:B:17:ILE:O	2:B:20:MET:HB2	2.05	0.56
3:C:4:SER:OG	3:C:7:GLU:HB2	2.04	0.56
3:C:111:THR:CA	3:C:116:ARG:HA	2.25	0.56
1:A:219:ILE:HD11	1:A:260:ALA:HB2	1.88	0.56
1:A:812:GLN:NE2	2:B:118:ASP:H	2.03	0.56
1:A:85:LEU:N	1:A:102:ASN:HD21	2.01	0.55
1:A:112:ILE:HD12	1:A:112:ILE:C	2.30	0.55
1:A:284:ILE:HA	1:A:287:GLN:NE2	2.20	0.55
1:A:127:ARG:O	1:A:128:ARG:C	2.48	0.55
1:A:338:LEU:HD23	1:A:445:THR:HG21	1.89	0.55
1:A:812:GLN:NE2	2:B:118:ASP:HB2	2.21	0.55
1:A:78:ASN:CG	1:A:93:TYR:HB2	2.32	0.55
1:A:231:ASN:HB3	1:A:239:ASN:HD22	1.71	0.55
1:A:716:PHE:HD2	1:A:739:SER:OG	1.88	0.55
1:A:786:GLN:HA	1:A:789:ILE:HD12	1.88	0.55
1:A:660:LEU:C	1:A:662:SER:N	2.64	0.55
2:B:109:ILE:O	2:B:113:LEU:HG	2.06	0.55
1:A:285:PHE:HB3	1:A:312:ILE:HG21	1.89	0.55
1:A:673:PRO:O	1:A:686:LEU:HD23	2.06	0.55
1:A:182:LYS:C	1:A:184:GLU:H	2.14	0.55
1:A:109:SER:HB2	1:A:111:LEU:CD2	2.38	0.54
1:A:152:LEU:O	1:A:153:PHE:C	2.50	0.54
3:C:32:LYS:O	3:C:36:VAL:HG23	2.07	0.54
1:A:322:ILE:HG23	1:A:327:GLU:HG3	1.88	0.54
1:A:811:ILE:H	1:A:811:ILE:HD12	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:GLN:NE2	2:B:14:GLN:C	2.66	0.54
3:C:15:PHE:C	3:C:17:LEU:H	2.15	0.54
1:A:423:VAL:C	1:A:425:ALA:N	2.66	0.54
1:A:442:VAL:O	1:A:445:THR:HG22	2.06	0.54
2:B:46:GLN:O	2:B:47:LEU:HD22	2.08	0.54
1:A:247:ILE:HG12	1:A:262:ILE:HG12	1.90	0.54
1:A:477:ILE:O	1:A:480:THR:HG22	2.07	0.54
1:A:674:ASN:ND2	1:A:678:GLN:H	2.05	0.54
1:A:51:SER:CB	3:C:95:ARG:HH21	2.21	0.54
1:A:74:ILE:HG22	1:A:75:GLN:N	2.22	0.54
1:A:173:LEU:H	1:A:173:LEU:CD1	2.18	0.54
1:A:266:LEU:HD11	1:A:649:HIS:CG	2.42	0.54
3:C:55:THR:HG21	3:C:60:GLU:HB2	1.88	0.54
1:A:361:MET:O	1:A:363:PHE:CD1	2.61	0.54
1:A:530:LEU:N	1:A:530:LEU:HD12	2.23	0.54
1:A:100:LEU:HD12	1:A:688:LEU:CD2	2.35	0.54
1:A:309:TYR:CG	1:A:356:LEU:HG	2.43	0.53
1:A:404:LYS:CB	1:A:410:VAL:N	2.71	0.53
1:A:152:LEU:HD11	1:A:189:VAL:HG23	1.89	0.53
1:A:361:MET:O	1:A:363:PHE:CE1	2.62	0.53
1:A:507:TRP:O	1:A:510:ILE:CG1	2.55	0.53
1:A:833:VAL:HG12	1:A:835:PRO:HD3	1.89	0.53
2:B:14:GLN:C	2:B:14:GLN:HE21	2.15	0.53
1:A:348:MET:SD	1:A:434:MET:HE2	2.48	0.53
1:A:438:LEU:O	1:A:442:VAL:HG23	2.08	0.53
1:A:237:ASN:CG	1:A:238:ASN:N	2.63	0.53
3:C:65:PHE:C	3:C:67:GLU:N	2.65	0.53
3:C:70:PRO:O	3:C:73:GLU:HB3	2.09	0.53
3:C:111:THR:O	3:C:116:ARG:CB	2.56	0.53
1:A:70:LYS:O	1:A:71:LYS:C	2.52	0.53
1:A:269:LYS:O	1:A:272:VAL:HG23	2.09	0.53
1:A:783:SER:HA	1:A:786:GLN:OE1	2.08	0.53
1:A:60:ILE:HD11	1:A:67:ARG:CZ	2.38	0.53
1:A:687:VAL:HG23	1:A:688:LEU:H	1.72	0.53
1:A:213:GLY:HA2	1:A:337:ILE:HG22	1.90	0.53
1:A:215:LEU:HA	1:A:218:GLN:HB2	1.89	0.53
1:A:262:ILE:HB	1:A:443:ASN:HD21	1.72	0.53
3:C:122:VAL:O	3:C:126:ILE:HG13	2.09	0.53
1:A:12:TYR:HB2	1:A:131:ILE:HG23	1.89	0.53
1:A:275:GLN:O	1:A:276:GLN:C	2.52	0.53
3:C:105:GLU:O	3:C:108:HIS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:CD1	1:A:123:VAL:N	2.70	0.53
1:A:517:GLN:OE1	1:A:520:ILE:HB	2.09	0.53
1:A:693:CYS:HA	6:A:900:PDM:CP3	2.32	0.53
3:C:121:ASP:O	3:C:124:GLU:N	2.39	0.53
3:C:128:LEU:C	3:C:128:LEU:HD12	2.34	0.53
1:A:722:ILE:HB	3:C:88:GLU:HG3	1.91	0.52
1:A:85:LEU:HD23	1:A:88:MET:HA	1.91	0.52
1:A:507:TRP:O	1:A:510:ILE:HG13	2.09	0.52
1:A:792:TYR:CD1	1:A:792:TYR:C	2.87	0.52
1:A:277:SER:O	1:A:279:GLU:HG3	2.09	0.52
1:A:387:CYS:O	1:A:618:VAL:HG21	2.08	0.52
1:A:571:PRO:C	1:A:573:GLN:H	2.17	0.52
3:C:27:ALA:CB	3:C:62:SER:HB3	2.38	0.52
1:A:266:LEU:N	1:A:266:LEU:HD13	2.24	0.52
1:A:507:TRP:CZ3	1:A:708:PRO:HB3	2.44	0.52
2:B:68:ASN:OD1	2:B:68:ASN:N	2.33	0.52
1:A:30:GLY:O	1:A:31:LYS:HD2	2.09	0.52
1:A:317:LEU:N	1:A:317:LEU:HD12	2.24	0.52
1:A:615:GLU:OE1	1:A:616:PRO:HD2	2.10	0.52
1:A:693:CYS:CA	6:A:900:PDM:HP3	2.33	0.52
2:B:85:SER:O	2:B:89:ILE:HG13	2.10	0.52
2:B:106:ILE:HD12	2:B:134:VAL:HG11	1.92	0.52
3:C:72:TYR:O	3:C:76:MET:HG2	2.09	0.52
3:C:126:ILE:C	3:C:128:LEU:H	2.16	0.52
1:A:423:VAL:O	1:A:425:ALA:N	2.42	0.52
1:A:671:ILE:HG23	1:A:690:GLN:CD	2.35	0.52
3:C:74:GLY:C	3:C:76:MET:N	2.67	0.52
1:A:249:ILE:HB	1:A:456:ILE:HG22	1.92	0.52
1:A:358:MET:SD	1:A:427:ALA:HB2	2.49	0.52
1:A:531:SER:HA	1:A:650:ARG:HH22	1.74	0.52
1:A:683:ASP:O	1:A:686:LEU:HB3	2.09	0.52
1:A:237:ASN:ND2	1:A:239:ASN:H	2.07	0.52
1:A:507:TRP:C	1:A:509:PHE:H	2.18	0.52
1:A:113:TYR:CG	1:A:151:HIS:HA	2.45	0.52
1:A:213:GLY:CA	1:A:337:ILE:HG22	2.40	0.52
1:A:770:LEU:HD23	1:A:773:MET:HE3	1.91	0.52
1:A:160:TYR:O	1:A:164:VAL:HG23	2.10	0.51
1:A:423:VAL:HG23	1:A:424:GLY:N	2.25	0.51
1:A:603:ASN:O	1:A:605:ASN:N	2.43	0.51
3:C:115:GLU:O	3:C:116:ARG:C	2.52	0.51
1:A:773:MET:O	1:A:777:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ILE:CG2	3:C:125:ILE:HD13	2.41	0.51
3:C:49:VAL:HG23	3:C:50:PHE:CD2	2.46	0.51
1:A:184:GLU:HG3	5:A:999:AGS:H3'	1.91	0.51
1:A:377:THR:HG23	1:A:381:GLU:OE1	2.10	0.51
3:C:55:THR:HB	3:C:60:GLU:HG3	1.92	0.51
2:B:93:PHE:O	2:B:95:MET:N	2.44	0.51
3:C:95:ARG:NH1	3:C:95:ARG:HB2	2.26	0.51
1:A:812:GLN:HE22	2:B:118:ASP:N	2.08	0.51
1:A:18:LYS:C	1:A:20:LEU:N	2.60	0.51
1:A:56:ILE:HD12	1:A:74:ILE:HD12	1.92	0.51
1:A:86:GLU:O	1:A:114:THR:CG2	2.57	0.51
1:A:644:THR:CG2	1:A:645:ILE:H	2.24	0.51
1:A:766:VAL:C	1:A:768:GLY:N	2.63	0.51
3:C:84:ALA:O	3:C:85:ASP:C	2.52	0.51
3:C:113:LEU:HD23	3:C:114:GLY:H	1.76	0.51
1:A:13:LEU:CB	8:A:1001:HOH:O	2.59	0.51
1:A:284:ILE:HA	1:A:287:GLN:HE21	1.75	0.51
1:A:480:THR:HB	1:A:649:HIS:HE1	1.76	0.51
1:A:535:GLU:C	1:A:537:CYS:H	2.17	0.51
1:A:12:TYR:HD1	1:A:130:PRO:HD2	1.77	0.50
1:A:45:SER:O	1:A:61:VAL:HG12	2.11	0.50
1:A:169:ASN:O	1:A:664:HIS:N	2.44	0.50
1:A:284:ILE:N	1:A:287:GLN:HE21	2.08	0.50
1:A:537:CYS:SG	1:A:599:LYS:HE2	2.51	0.50
2:B:55:GLU:O	2:B:59:MET:HB2	2.10	0.50
1:A:475:LEU:HD22	1:A:594:TRP:CH2	2.46	0.50
1:A:477:ILE:HG23	1:A:478:ASN:N	2.26	0.50
1:A:507:TRP:O	1:A:510:ILE:CD1	2.57	0.50
2:B:145:THR:C	2:B:148:ILE:HG22	2.35	0.50
1:A:88:MET:N	1:A:116:SER:HA	2.27	0.50
1:A:267:LEU:HD23	1:A:267:LEU:C	2.36	0.50
1:A:579:GLU:HG2	1:A:588:PRO:HA	1.93	0.50
2:B:71:MET:O	2:B:75:ILE:HG13	2.12	0.50
2:B:132:ALA:HB1	2:B:134:VAL:HG23	1.93	0.50
3:C:65:PHE:O	3:C:67:GLU:N	2.44	0.50
3:C:113:LEU:CD2	3:C:114:GLY:H	2.25	0.50
1:A:157:ASP:HB2	1:A:192:TYR:OH	2.11	0.50
1:A:182:LYS:HB2	1:A:460:ASP:OD2	2.10	0.50
1:A:244:GLY:O	1:A:264:THR:HA	2.11	0.50
1:A:399:LEU:C	1:A:401:PRO:HD3	2.35	0.50
1:A:463:GLY:HA2	1:A:481:ASN:CG	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:HB1	1:A:287:GLN:HE22	1.76	0.50
1:A:343:GLU:O	1:A:347:SER:N	2.40	0.50
3:C:15:PHE:C	3:C:17:LEU:N	2.69	0.50
1:A:341:THR:OG1	1:A:343:GLU:HG2	2.11	0.50
1:A:501:LYS:O	1:A:504:GLY:N	2.41	0.50
1:A:272:VAL:O	1:A:281:ASN:OD1	2.30	0.50
1:A:297:ASN:C	1:A:299:VAL:H	2.19	0.50
1:A:707:PHE:HB3	1:A:708:PRO:CD	2.41	0.50
2:B:145:THR:HA	2:B:148:ILE:CG2	2.41	0.50
1:A:217:ASP:O	1:A:221:GLN:CB	2.60	0.50
2:B:74:SER:C	2:B:76:PHE:H	2.20	0.50
3:C:69:LEU:HB3	3:C:70:PRO:HD3	1.93	0.50
1:A:417:ASN:HA	1:A:420:VAL:CG1	2.40	0.49
1:A:591:ILE:HG22	1:A:594:TRP:CE3	2.46	0.49
1:A:673:PRO:HG2	1:A:674:ASN:H	1.77	0.49
1:A:112:ILE:O	1:A:112:ILE:HG23	2.11	0.49
1:A:234:THR:O	1:A:236:ARG:N	2.45	0.49
1:A:693:CYS:HB3	1:A:694:ASN:HD22	1.76	0.49
3:C:17:LEU:O	3:C:17:LEU:HD22	2.12	0.49
1:A:280:ARG:NH1	1:A:318:THR:HA	2.24	0.49
2:B:122:LYS:O	2:B:125:MET:HB2	2.12	0.49
2:B:145:THR:CA	2:B:148:ILE:HG22	2.42	0.49
1:A:85:LEU:HG	1:A:86:GLU:N	2.27	0.49
1:A:657:MET:C	1:A:659:ASN:N	2.71	0.49
2:B:131:GLU:O	2:B:132:ALA:C	2.56	0.49
1:A:59:LYS:O	1:A:59:LYS:HG3	2.12	0.49
1:A:152:LEU:O	1:A:155:VAL:N	2.45	0.49
1:A:266:LEU:HD11	1:A:649:HIS:CD2	2.47	0.49
1:A:292:ALA:C	1:A:293:ILE:HD13	2.38	0.49
2:B:93:PHE:C	2:B:95:MET:H	2.20	0.49
3:C:19:ASP:OD1	3:C:27:ALA:O	2.30	0.49
1:A:323:ASP:OD1	1:A:325:VAL:HB	2.13	0.49
1:A:571:PRO:C	1:A:573:GLN:N	2.71	0.49
1:A:361:MET:HG2	1:A:380:ALA:CB	2.39	0.49
1:A:655:LYS:O	1:A:656:LEU:C	2.54	0.49
1:A:739:SER:O	1:A:740:GLU:C	2.55	0.49
1:A:766:VAL:O	1:A:770:LEU:N	2.43	0.49
1:A:216:GLU:N	1:A:218:GLN:H	2.10	0.49
1:A:243:PHE:CD2	1:A:264:THR:HG22	2.48	0.49
1:A:603:ASN:C	1:A:605:ASN:N	2.70	0.49
1:A:276:GLN:O	1:A:277:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLN:O	1:A:807:GLY:N	2.46	0.49
3:C:7:GLU:O	3:C:10:ASP:HB2	2.13	0.49
1:A:87:ASP:O	1:A:89:ALA:N	2.46	0.48
1:A:107:TYR:HD1	1:A:123:VAL:CG2	2.26	0.48
1:A:151:HIS:ND1	1:A:152:LEU:N	2.61	0.48
1:A:173:LEU:O	1:A:174:ILE:HD13	2.13	0.48
1:A:687:VAL:O	1:A:688:LEU:C	2.55	0.48
3:C:40:LEU:O	3:C:42:ILE:HG13	2.13	0.48
1:A:151:HIS:HD2	8:A:1001:HOH:O	1.91	0.48
1:A:223:ASN:CB	1:A:224:PRO:HD3	2.38	0.48
1:A:815:ILE:C	1:A:817:LYS:H	2.20	0.48
2:B:74:SER:C	2:B:76:PHE:N	2.71	0.48
1:A:253:PRO:C	1:A:255:GLY:H	2.21	0.48
1:A:349:PHE:O	1:A:352:THR:HB	2.13	0.48
1:A:363:PHE:CE2	1:A:399:LEU:HD21	2.47	0.48
1:A:485:GLN:HG3	1:A:583:TYR:CE1	2.48	0.48
1:A:812:GLN:HE22	2:B:118:ASP:H	1.61	0.48
2:B:102:LYS:HA	2:B:141:TYR:OH	2.12	0.48
2:B:112:LEU:HD12	2:B:116:MET:HG3	1.96	0.48
1:A:112:ILE:CD1	1:A:123:VAL:H	2.26	0.48
2:B:93:PHE:C	2:B:95:MET:N	2.69	0.48
3:C:111:THR:C	3:C:116:ARG:HB3	2.38	0.48
3:C:126:ILE:O	3:C:128:LEU:N	2.46	0.48
1:A:262:ILE:HG22	1:A:263:GLU:N	2.29	0.48
1:A:12:TYR:CB	1:A:131:ILE:CG2	2.86	0.48
1:A:807:GLY:O	1:A:811:ILE:HD12	2.12	0.48
2:B:31:ARG:C	2:B:33:GLY:N	2.71	0.48
3:C:63:LEU:N	3:C:63:LEU:HD22	2.29	0.48
3:C:141:TYR:O	3:C:142:GLU:C	2.56	0.48
1:A:170:GLN:HG3	1:A:666:HIS:CD2	2.48	0.48
1:A:561:MET:HB3	1:A:580:LEU:HD12	1.96	0.48
1:A:772:GLU:C	1:A:774:ARG:N	2.71	0.48
2:B:43:ILE:O	2:B:47:LEU:N	2.47	0.48
3:C:19:ASP:O	3:C:23:GLY:O	2.32	0.48
1:A:477:ILE:C	1:A:480:THR:HG22	2.39	0.48
1:A:800:LYS:HA	1:A:803:ASP:HB3	1.96	0.48
2:B:37:LYS:HE3	2:B:38:GLU:OE2	2.13	0.48
1:A:29:ASP:C	1:A:31:LYS:H	2.20	0.48
1:A:107:TYR:OH	1:A:679:PRO:HA	2.14	0.48
1:A:660:LEU:O	1:A:662:SER:N	2.45	0.48
1:A:827:TRP:O	1:A:828:LYS:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ALA:O	3:C:92:THR:N	2.44	0.48
3:C:111:THR:O	3:C:116:ARG:CA	2.62	0.48
3:C:131:LEU:HD11	3:C:139:VAL:HB	1.95	0.48
1:A:134:ASP:HA	1:A:137:ILE:HD12	1.96	0.47
1:A:300:MET:C	1:A:302:VAL:N	2.71	0.47
1:A:477:ILE:CG2	1:A:478:ASN:N	2.77	0.47
1:A:483:ARG:O	1:A:657:MET:HE2	2.14	0.47
1:A:560:ARG:C	1:A:561:MET:SD	2.97	0.47
1:A:687:VAL:HG23	1:A:688:LEU:N	2.28	0.47
1:A:687:VAL:O	1:A:691:LEU:HG	2.14	0.47
1:A:348:MET:HE1	1:A:437:TRP:CZ3	2.49	0.47
1:A:500:TYR:OH	1:A:708:PRO:HG2	2.15	0.47
1:A:778:LEU:C	1:A:778:LEU:HD23	2.38	0.47
1:A:158:ASN:C	1:A:160:TYR:H	2.20	0.47
1:A:377:THR:O	1:A:381:GLU:HG3	2.15	0.47
3:C:90:PHE:HB3	3:C:141:TYR:CD1	2.49	0.47
1:A:745:GLY:C	1:A:747:GLN:H	2.20	0.47
1:A:804:GLN:HA	2:B:95:MET:SD	2.54	0.47
2:B:17:ILE:HA	2:B:20:MET:CG	2.44	0.47
2:B:105:ASN:O	2:B:108:TYR:HB3	2.15	0.47
1:A:237:ASN:HD21	1:A:239:ASN:C	2.23	0.47
1:A:532:ILE:HD12	1:A:551:LEU:HD12	1.96	0.47
1:A:230:GLY:O	1:A:242:ARG:HB2	2.15	0.47
1:A:305:ASP:HB3	1:A:308:LEU:HB2	1.96	0.47
1:A:708:PRO:HA	1:A:763:LYS:O	2.13	0.47
1:A:786:GLN:O	1:A:790:ARG:HG3	2.15	0.47
1:A:815:ILE:HD11	2:B:144:PHE:CZ	2.50	0.47
2:B:119:ASN:O	2:B:120:PHE:C	2.56	0.47
3:C:89:ALA:O	3:C:90:PHE:C	2.57	0.47
1:A:222:ALA:HA	1:A:338:LEU:HD11	1.97	0.47
1:A:244:GLY:HA2	1:A:461:ILE:HG22	1.96	0.47
1:A:271:ARG:CG	1:A:271:ARG:HH11	2.28	0.47
1:A:503:GLU:O	1:A:505:ILE:HG23	2.13	0.47
1:A:722:ILE:HB	3:C:88:GLU:CG	2.45	0.47
2:B:45:GLU:C	2:B:47:LEU:N	2.72	0.47
2:B:118:ASP:O	2:B:120:PHE:N	2.47	0.47
3:C:42:ILE:HG22	3:C:43:ASN:N	2.30	0.47
3:C:73:GLU:C	3:C:76:MET:HG2	2.39	0.47
1:A:5:PHE:HB2	1:A:6:SER:H	1.22	0.47
1:A:178:SER:CB	5:A:999:AGS:S1G	3.03	0.47
1:A:417:ASN:C	1:A:419:VAL:N	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLN:O	1:A:521:ASP:HB2	2.15	0.47
2:B:72:PHE:O	2:B:75:ILE:CD1	2.63	0.47
3:C:133:GLU:HA	3:C:139:VAL:CG1	2.45	0.47
1:A:9:ASP:OD2	1:A:11:GLN:NE2	2.48	0.47
1:A:229:TYR:HA	1:A:431:TYR:OH	2.15	0.47
1:A:343:GLU:CD	1:A:343:GLU:N	2.65	0.47
1:A:392:GLY:O	1:A:393:ASP:C	2.56	0.47
1:A:812:GLN:NE2	2:B:118:ASP:CB	2.78	0.47
1:A:815:ILE:C	1:A:817:LYS:N	2.72	0.47
1:A:234:THR:O	1:A:235:THR:C	2.58	0.47
2:B:21:LYS:O	2:B:24:PHE:N	2.41	0.47
3:C:19:ASP:OD2	3:C:26:GLY:N	2.45	0.47
3:C:33:LEU:HD23	3:C:34:GLY:N	2.30	0.47
1:A:169:ASN:CB	1:A:663:THR:HG22	2.40	0.46
1:A:741:LYS:O	1:A:742:ILE:C	2.58	0.46
1:A:389:ILE:HD12	1:A:389:ILE:O	2.14	0.46
1:A:580:LEU:HD23	1:A:582:HIS:NE2	2.31	0.46
1:A:777:ARG:NH1	1:A:781:ILE:HD11	2.18	0.46
1:A:785:PHE:O	1:A:789:ILE:HG13	2.14	0.46
1:A:791:GLY:O	1:A:795:ARG:NE	2.48	0.46
2:B:72:PHE:HA	2:B:75:ILE:HD11	1.97	0.46
1:A:12:TYR:CB	1:A:131:ILE:HG21	2.44	0.46
1:A:174:ILE:HG22	1:A:182:LYS:HB3	1.97	0.46
1:A:464:PHE:N	1:A:481:ASN:ND2	2.62	0.46
1:A:211:LYS:H	1:A:211:LYS:HG2	1.27	0.46
3:C:89:ALA:O	3:C:92:THR:HG23	2.14	0.46
1:A:127:ARG:HG2	1:A:127:ARG:HH11	1.80	0.46
1:A:795:ARG:HH12	3:C:41:GLY:N	2.11	0.46
2:B:132:ALA:C	2:B:134:VAL:H	2.24	0.46
3:C:120:GLU:O	3:C:121:ASP:C	2.59	0.46
1:A:85:LEU:CD1	1:A:86:GLU:H	2.28	0.46
1:A:166:ASP:HB3	1:A:168:GLU:HG2	1.96	0.46
1:A:243:PHE:HD2	1:A:264:THR:HG22	1.79	0.46
1:A:285:PHE:CB	1:A:312:ILE:HG21	2.46	0.46
1:A:313:ASN:ND2	1:A:313:ASN:C	2.74	0.46
1:A:472:PHE:HA	1:A:594:TRP:CZ2	2.51	0.46
1:A:112:ILE:HG23	1:A:113:TYR:CD2	2.50	0.46
1:A:357:HIS:C	1:A:359:GLY:N	2.71	0.46
2:B:28:ASP:OD2	2:B:31:ARG:HA	2.16	0.46
2:B:113:LEU:O	2:B:120:PHE:HB2	2.15	0.46
1:A:120:CYS:O	1:A:120:CYS:SG	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:CA	1:A:287:GLN:HE21	2.29	0.46
1:A:615:GLU:HB3	1:A:618:VAL:CG2	2.42	0.46
1:A:795:ARG:HG2	1:A:795:ARG:HH11	1.80	0.46
2:B:40:ILE:HD12	2:B:40:ILE:N	2.31	0.46
3:C:40:LEU:HD22	3:C:72:TYR:OH	2.15	0.46
3:C:88:GLU:O	3:C:92:THR:HG23	2.16	0.46
3:C:114:GLY:O	3:C:115:GLU:HG2	2.16	0.46
1:A:81:LYS:C	1:A:83:GLU:H	2.24	0.45
1:A:152:LEU:O	1:A:155:VAL:CG2	2.64	0.45
1:A:217:ASP:O	1:A:221:GLN:HB2	2.15	0.45
1:A:221:GLN:HG2	1:A:337:ILE:HD12	1.97	0.45
1:A:824:TRP:O	1:A:825:GLN:C	2.59	0.45
1:A:107:TYR:HD1	1:A:123:VAL:HG21	1.81	0.45
1:A:109:SER:HB2	1:A:111:LEU:HD21	1.98	0.45
1:A:178:SER:HA	5:A:999:AGS:O3G	2.16	0.45
1:A:580:LEU:O	1:A:582:HIS:N	2.49	0.45
1:A:694:ASN:ND2	1:A:694:ASN:N	2.62	0.45
2:B:57:THR:C	2:B:59:MET:H	2.25	0.45
2:B:94:ALA:HA	2:B:97:ASP:HB3	1.98	0.45
1:A:51:SER:HB2	3:C:95:ARG:NH2	2.32	0.45
1:A:281:ASN:HD22	1:A:282:TYR:H	1.65	0.45
1:A:379:GLU:O	1:A:380:ALA:C	2.59	0.45
2:B:79:LYS:O	2:B:80:LEU:HG	2.16	0.45
1:A:153:PHE:HD1	1:A:192:TYR:CG	2.34	0.45
1:A:161:GLN:C	1:A:163:MET:N	2.73	0.45
1:A:237:ASN:CG	1:A:238:ASN:H	2.23	0.45
1:A:683:ASP:O	1:A:684:ALA:C	2.60	0.45
1:A:785:PHE:CE1	3:C:145:VAL:HG23	2.50	0.45
1:A:161:GLN:HE21	1:A:161:GLN:HB3	1.51	0.45
1:A:767:LEU:HA	1:A:770:LEU:HD12	1.97	0.45
1:A:770:LEU:O	1:A:773:MET:N	2.50	0.45
1:A:125:PRO:O	1:A:126:TYR:HB2	2.17	0.45
1:A:766:VAL:O	1:A:769:ASN:N	2.49	0.45
1:A:78:ASN:ND2	1:A:93:TYR:N	2.51	0.45
1:A:151:HIS:ND1	1:A:151:HIS:C	2.75	0.45
1:A:296:LEU:O	1:A:299:VAL:HB	2.15	0.45
3:C:108:HIS:O	3:C:112:ALA:N	2.49	0.45
1:A:152:LEU:O	1:A:155:VAL:CB	2.65	0.45
1:A:231:ASN:HA	1:A:240:SER:O	2.17	0.45
1:A:474:GLN:O	1:A:477:ILE:HG22	2.17	0.45
3:C:18:PHE:CG	3:C:36:VAL:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PHE:CE2	1:A:257:ILE:HG12	2.51	0.45
1:A:283:HIS:O	1:A:284:ILE:C	2.60	0.45
1:A:726:ASN:OD1	1:A:726:ASN:O	2.34	0.45
3:C:103:GLY:O	3:C:104:ALA:C	2.60	0.45
1:A:29:ASP:OD2	1:A:31:LYS:HB2	2.17	0.45
1:A:79:PRO:C	1:A:81:LYS:N	2.74	0.45
1:A:777:ARG:O	1:A:781:ILE:HD12	2.17	0.45
1:A:782:ILE:O	1:A:786:GLN:HG2	2.17	0.45
2:B:51:PRO:HG2	2:B:56:LEU:CD2	2.47	0.45
1:A:119:PHE:CD1	1:A:119:PHE:N	2.85	0.44
1:A:186:THR:O	1:A:190:ILE:HG12	2.18	0.44
1:A:433:ARG:HD3	1:A:622:PHE:CE1	2.52	0.44
1:A:707:PHE:HB3	1:A:708:PRO:HD2	1.97	0.44
1:A:174:ILE:HD13	1:A:668:VAL:HB	1.98	0.44
1:A:241:SER:OG	5:A:999:AGS:O2G	2.35	0.44
1:A:578:PHE:CD1	1:A:578:PHE:N	2.84	0.44
1:A:671:ILE:HA	1:A:690:GLN:OE1	2.17	0.44
1:A:722:ILE:HA	3:C:88:GLU:HG2	1.98	0.44
2:B:52:ASP:O	2:B:56:LEU:HD12	2.17	0.44
1:A:262:ILE:CB	1:A:443:ASN:HD21	2.29	0.44
1:A:293:ILE:O	1:A:294:PRO:C	2.60	0.44
1:A:603:ASN:O	1:A:604:GLU:C	2.60	0.44
1:A:646:SER:O	1:A:650:ARG:HB2	2.18	0.44
3:C:14:VAL:O	3:C:17:LEU:HB3	2.18	0.44
1:A:18:LYS:C	1:A:20:LEU:H	2.16	0.44
1:A:215:LEU:C	1:A:215:LEU:HD23	2.42	0.44
1:A:216:GLU:H	1:A:218:GLN:H	1.64	0.44
1:A:286:TYR:CE2	1:A:317:LEU:HA	2.53	0.44
2:B:104:LEU:HG	2:B:141:TYR:HD2	1.83	0.44
3:C:67:GLU:C	3:C:70:PRO:HD2	2.43	0.44
1:A:6:SER:HB2	1:A:7:ASP:H	1.38	0.44
1:A:182:LYS:C	1:A:184:GLU:N	2.76	0.44
1:A:216:GLU:O	1:A:218:GLN:N	2.51	0.44
1:A:271:ARG:NH1	1:A:271:ARG:HG2	2.32	0.44
1:A:804:GLN:O	1:A:805:ARG:C	2.59	0.44
2:B:24:PHE:CZ	2:B:68:ASN:O	2.70	0.44
3:C:50:PHE:C	3:C:52:VAL:H	2.25	0.44
1:A:377:THR:C	1:A:381:GLU:OE1	2.61	0.44
1:A:466:ILE:CD1	1:A:587:VAL:HG22	2.47	0.44
2:B:136:GLY:C	2:B:138:LYS:H	2.23	0.44
1:A:111:LEU:N	1:A:111:LEU:HD23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:MET:O	1:A:659:ASN:N	2.51	0.43
1:A:191:MET:HA	1:A:220:ILE:HD11	2.00	0.43
1:A:311:PHE:CD1	1:A:359:GLY:HA3	2.52	0.43
1:A:485:GLN:C	1:A:487:PHE:N	2.75	0.43
1:A:490:HIS:C	1:A:492:MET:H	2.25	0.43
1:A:766:VAL:O	1:A:767:LEU:C	2.59	0.43
2:B:36:SER:O	2:B:39:ASP:N	2.48	0.43
1:A:38:ASP:HB3	1:A:42:GLY:O	2.18	0.43
1:A:227:GLU:C	1:A:229:TYR:H	2.27	0.43
1:A:338:LEU:CD2	1:A:442:VAL:HG13	2.47	0.43
1:A:583:TYR:C	1:A:585:GLY:H	2.26	0.43
1:A:761:PHE:CD1	1:A:761:PHE:N	2.87	0.43
2:B:112:LEU:HD12	2:B:112:LEU:HA	1.76	0.43
3:C:134:ASP:OD1	3:C:137:GLY:N	2.50	0.43
1:A:112:ILE:C	1:A:112:ILE:CD1	2.90	0.43
1:A:428:LYS:O	1:A:429:SER:C	2.61	0.43
1:A:772:GLU:C	1:A:774:ARG:H	2.26	0.43
1:A:783:SER:O	1:A:786:GLN:HG2	2.18	0.43
1:A:152:LEU:C	1:A:155:VAL:HG23	2.44	0.43
3:C:18:PHE:CD1	3:C:36:VAL:HG22	2.54	0.43
1:A:52:LYS:O	1:A:52:LYS:HG2	2.19	0.43
1:A:120:CYS:O	1:A:121:ILE:C	2.62	0.43
1:A:293:ILE:CG2	1:A:296:LEU:HB2	2.48	0.43
1:A:801:LEU:HD13	1:A:801:LEU:O	2.18	0.43
3:C:106:LEU:HD12	3:C:110:LEU:HD11	2.00	0.43
1:A:771:GLU:O	1:A:774:ARG:HB3	2.19	0.43
2:B:72:PHE:O	2:B:75:ILE:HD12	2.18	0.43
1:A:137:ILE:HG23	1:A:192:TYR:CD1	2.53	0.43
1:A:260:ALA:HB3	1:A:446:LEU:HD13	2.00	0.43
1:A:294:PRO:C	1:A:296:LEU:H	2.26	0.43
3:C:133:GLU:HA	3:C:139:VAL:HG12	2.01	0.43
1:A:85:LEU:CG	1:A:86:GLU:N	2.82	0.43
1:A:152:LEU:O	1:A:155:VAL:HB	2.19	0.43
1:A:174:ILE:CD1	1:A:668:VAL:HB	2.49	0.43
1:A:442:VAL:C	1:A:444:LYS:H	2.26	0.43
1:A:684:ALA:O	1:A:688:LEU:HD23	2.19	0.43
2:B:118:ASP:O	2:B:119:ASN:C	2.61	0.43
3:C:50:PHE:C	3:C:52:VAL:N	2.73	0.43
1:A:74:ILE:CG2	1:A:75:GLN:N	2.81	0.42
1:A:100:LEU:HD21	1:A:104:ARG:NE	2.34	0.42
1:A:530:LEU:N	1:A:530:LEU:CD1	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ILE:HG12	2:B:59:MET:HE1	2.00	0.42
2:B:69:PHE:O	2:B:72:PHE:HB3	2.19	0.42
3:C:111:THR:HA	3:C:116:ARG:CA	2.28	0.42
3:C:117:LEU:CD1	3:C:121:ASP:CB	2.97	0.42
1:A:649:HIS:C	1:A:651:GLU:N	2.76	0.42
3:C:91:LYS:C	3:C:93:PHE:N	2.77	0.42
1:A:169:ASN:HD22	1:A:169:ASN:HA	1.58	0.42
1:A:275:GLN:HB3	1:A:279:GLU:HB2	1.99	0.42
1:A:311:PHE:CE1	1:A:359:GLY:HA3	2.55	0.42
1:A:29:ASP:C	1:A:31:LYS:N	2.77	0.42
3:C:132:GLN:HE21	3:C:132:GLN:HA	1.84	0.42
1:A:112:ILE:HD13	1:A:112:ILE:HA	1.67	0.42
1:A:379:GLU:O	1:A:382:LYS:N	2.45	0.42
1:A:390:ASN:ND2	1:A:392:GLY:H	2.16	0.42
1:A:428:LYS:O	1:A:430:LEU:N	2.53	0.42
2:B:40:ILE:HG12	2:B:59:MET:CE	2.49	0.42
2:B:106:ILE:HG22	2:B:137:GLY:C	2.43	0.42
1:A:152:LEU:HA	1:A:155:VAL:CG2	2.49	0.42
1:A:496:GLU:OE2	1:A:710:ARG:NH2	2.46	0.42
1:A:816:ARG:NH2	2:B:120:PHE:HA	2.34	0.42
2:B:28:ASP:OD1	2:B:34:PHE:O	2.37	0.42
2:B:54:LYS:O	2:B:54:LYS:HD3	2.18	0.42
3:C:18:PHE:CD2	3:C:36:VAL:HG22	2.54	0.42
3:C:92:THR:C	3:C:93:PHE:CD1	2.93	0.42
3:C:99:GLY:O	3:C:141:TYR:CE2	2.73	0.42
1:A:35:TRP:CZ2	1:A:101:TYR:HB2	2.55	0.42
1:A:325:VAL:CG1	1:A:329:LYS:HE2	2.50	0.42
1:A:492:MET:CE	1:A:697:LEU:HD21	2.49	0.42
1:A:516:LEU:O	1:A:520:ILE:HD13	2.19	0.42
1:A:582:HIS:HB2	1:A:585:GLY:O	2.20	0.42
1:A:686:LEU:HG	1:A:690:GLN:HE21	1.85	0.42
1:A:795:ARG:NH1	3:C:38:ARG:O	2.52	0.42
1:A:814:ASN:ND2	2:B:89:ILE:CD1	2.83	0.42
2:B:148:ILE:O	2:B:149:LYS:HB2	2.19	0.42
3:C:84:ALA:O	3:C:87:MET:N	2.53	0.42
1:A:59:LYS:HE3	1:A:59:LYS:HB2	1.81	0.42
1:A:172:CYS:HB3	1:A:458:VAL:HG22	2.01	0.42
1:A:598:ASN:HD22	1:A:599:LYS:NZ	2.18	0.42
1:A:664:HIS:HA	1:A:665:PRO:HD2	1.90	0.42
1:A:514:MET:O	1:A:517:GLN:N	2.48	0.42
1:A:786:GLN:HE22	3:C:115:GLU:N	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:LEU:HD12	3:C:3:LEU:N	2.33	0.42
1:A:137:ILE:HG23	1:A:192:TYR:HD1	1.85	0.42
1:A:474:GLN:O	1:A:475:LEU:C	2.62	0.42
1:A:792:TYR:HE1	3:C:128:LEU:CD2	2.32	0.42
1:A:303:THR:HA	1:A:304:PRO:HD3	1.73	0.41
1:A:328:PHE:O	1:A:329:LYS:C	2.63	0.41
1:A:348:MET:CE	1:A:437:TRP:HZ3	2.33	0.41
1:A:689:HIS:C	1:A:691:LEU:N	2.78	0.41
2:B:121:ASN:OD1	2:B:121:ASN:C	2.63	0.41
1:A:105:SER:O	1:A:109:SER:OG	2.38	0.41
1:A:415:ASN:OD1	1:A:417:ASN:N	2.54	0.41
1:A:472:PHE:HB2	1:A:594:TRP:CE2	2.55	0.41
1:A:582:HIS:HB3	1:A:583:TYR:H	1.54	0.41
1:A:691:LEU:C	1:A:693:CYS:H	2.28	0.41
1:A:735:GLY:O	1:A:736:LYS:C	2.63	0.41
3:C:111:THR:HG23	3:C:116:ARG:CB	2.49	0.41
1:A:89:ALA:HB2	1:A:117:GLY:CA	2.44	0.41
1:A:112:ILE:O	1:A:113:TYR:CG	2.72	0.41
1:A:285:PHE:HB3	1:A:312:ILE:HD13	2.01	0.41
1:A:791:GLY:O	1:A:795:ARG:HG3	2.20	0.41
1:A:795:ARG:HH22	3:C:42:ILE:H	1.67	0.41
1:A:815:ILE:O	1:A:817:LYS:N	2.53	0.41
2:B:20:MET:O	2:B:23:ALA:N	2.54	0.41
1:A:272:VAL:HA	1:A:281:ASN:HD21	1.85	0.41
1:A:278:ALA:HA	1:A:316:CYS:HB2	2.01	0.41
1:A:607:VAL:O	1:A:608:ALA:C	2.62	0.41
1:A:827:TRP:O	1:A:830:TYR:N	2.53	0.41
2:B:21:LYS:O	2:B:24:PHE:HB3	2.20	0.41
1:A:36:VAL:HG11	1:A:58:VAL:HG21	2.03	0.41
1:A:60:ILE:HB	1:A:65:SER:OG	2.21	0.41
1:A:86:GLU:N	1:A:86:GLU:CD	2.78	0.41
1:A:107:TYR:CD1	1:A:123:VAL:HG21	2.56	0.41
1:A:349:PHE:N	1:A:349:PHE:CD1	2.87	0.41
1:A:522:LEU:HA	1:A:525:LYS:CE	2.47	0.41
1:A:673:PRO:HB2	1:A:681:LEU:O	2.21	0.41
1:A:722:ILE:O	1:A:725:PRO:HD3	2.20	0.41
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.69	0.41
2:B:139:PHE:CD1	2:B:139:PHE:C	2.99	0.41
1:A:348:MET:HE1	1:A:437:TRP:HZ3	1.85	0.41
1:A:466:ILE:O	1:A:466:ILE:CG2	2.60	0.41
1:A:507:TRP:CZ3	1:A:708:PRO:CB	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:TRP:C	1:A:509:PHE:N	2.78	0.41
2:B:36:SER:C	2:B:38:GLU:N	2.75	0.41
1:A:137:ILE:HG12	1:A:153:PHE:CZ	2.56	0.41
1:A:351:CYS:HB2	1:A:434:MET:CE	2.50	0.41
1:A:693:CYS:CB	6:A:900:PDM:CP7	2.93	0.41
2:B:121:ASN:OD1	2:B:121:ASN:O	2.38	0.41
2:B:129:PHE:CA	2:B:132:ALA:HB2	2.39	0.41
3:C:117:LEU:CD1	3:C:121:ASP:HB3	2.51	0.41
2:B:36:SER:O	2:B:37:LYS:C	2.62	0.41
1:A:156:ALA:HB3	1:A:192:TYR:CD2	2.56	0.41
1:A:384:ALA:O	1:A:389:ILE:O	2.39	0.41
1:A:442:VAL:C	1:A:444:LYS:N	2.78	0.41
1:A:535:GLU:C	1:A:537:CYS:N	2.79	0.41
1:A:591:ILE:HG22	1:A:594:TRP:CD2	2.56	0.41
1:A:610:LEU:C	1:A:612:ALA:H	2.27	0.41
1:A:742:ILE:O	1:A:746:LEU:HG	2.21	0.41
1:A:814:ASN:ND2	2:B:89:ILE:HG12	2.36	0.41
2:B:105:ASN:O	2:B:108:TYR:N	2.42	0.41
3:C:145:VAL:O	3:C:149:MET:HG3	2.21	0.41
1:A:125:PRO:HG2	1:A:126:TYR:N	2.36	0.41
1:A:217:ASP:O	1:A:221:GLN:HB3	2.20	0.41
1:A:377:THR:OG1	1:A:381:GLU:CD	2.64	0.41
1:A:422:SER:O	1:A:425:ALA:HB3	2.21	0.41
1:A:532:ILE:C	1:A:534:GLU:N	2.79	0.41
1:A:559:ASN:CB	1:A:561:MET:HE2	2.47	0.41
1:A:815:ILE:HD11	2:B:144:PHE:HE2	1.83	0.41
1:A:826:TRP:CZ2	2:B:59:MET:HE3	2.56	0.41
2:B:63:ALA:HA	2:B:64:PRO:HD3	1.94	0.41
3:C:126:ILE:O	3:C:127:LYS:C	2.64	0.41
3:C:144:PHE:C	3:C:146:LYS:N	2.79	0.41
1:A:88:MET:C	1:A:90:ASN:N	2.79	0.40
1:A:148:ILE:O	1:A:149:PRO:C	2.64	0.40
1:A:151:HIS:O	1:A:152:LEU:C	2.64	0.40
1:A:364:LYS:C	1:A:366:ARG:N	2.80	0.40
1:A:686:LEU:HG	1:A:690:GLN:NE2	2.35	0.40
1:A:693:CYS:HB3	1:A:694:ASN:ND2	2.36	0.40
3:C:91:LYS:O	3:C:93:PHE:N	2.53	0.40
1:A:87:ASP:OD1	1:A:115:TYR:HB2	2.21	0.40
1:A:133:THR:OG1	1:A:136:VAL:HG23	2.21	0.40
1:A:324:ASP:HA	1:A:327:GLU:HB2	2.04	0.40
1:A:483:ARG:HG2	1:A:657:MET:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:HD12	1:A:580:LEU:HA	1.76	0.40
1:A:580:LEU:HD23	1:A:582:HIS:CD2	2.56	0.40
1:A:434:MET:O	1:A:435:PHE:C	2.64	0.40
1:A:539:PHE:C	1:A:541:LYS:H	2.29	0.40
2:B:93:PHE:CE2	2:B:141:TYR:HB2	2.56	0.40
2:B:112:LEU:HA	2:B:116:MET:CG	2.52	0.40
3:C:4:SER:O	3:C:7:GLU:N	2.54	0.40
1:A:112:ILE:CD1	1:A:123:VAL:O	2.65	0.40
1:A:186:THR:HG23	1:A:458:VAL:HG11	2.02	0.40
1:A:223:ASN:C	1:A:225:VAL:N	2.79	0.40
1:A:516:LEU:HD13	1:A:520:ILE:HD13	2.04	0.40
1:A:786:GLN:NE2	3:C:115:GLU:O	2.55	0.40
1:A:79:PRO:O	1:A:81:LYS:N	2.55	0.40
1:A:192:TYR:C	1:A:194:ALA:N	2.80	0.40
1:A:537:CYS:C	1:A:539:PHE:N	2.73	0.40
1:A:599:LYS:HD2	1:A:599:LYS:N	2.36	0.40
2:B:14:GLN:O	2:B:17:ILE:N	2.54	0.40
3:C:134:ASP:CG	3:C:135:LEU:N	2.79	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	764/835 (92%)	505 (66%)	197 (26%)	62 (8%)	1	10
2	B	140/156 (90%)	90 (64%)	40 (29%)	10 (7%)	1	12
3	C	151/156 (97%)	98 (65%)	41 (27%)	12 (8%)	1	10
All	All	1055/1147 (92%)	693 (66%)	278 (26%)	84 (8%)	1	10

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	MET
1	A	235	THR
1	A	389	ILE
1	A	418	GLN
1	A	607	VAL
1	A	8	PRO
1	A	11	GLN
1	A	127	ARG
1	A	153	PHE
1	A	283	HIS
1	A	325	VAL
1	A	366	ARG
1	A	497	GLN
1	A	504	GLY
1	A	604	GLU
1	A	623	LYS
1	A	644	THR
1	A	661	TYR
1	A	684	ALA
1	A	706	GLY
1	A	742	ILE
1	A	765	GLY
2	B	81	SER
2	B	149	LYS
3	C	75	LEU
3	C	112	ALA
3	C	129	THR
3	C	134	ASP
3	C	137	GLY
1	A	62	ALA
1	A	116	SER
1	A	195	LYS
1	A	211	LYS
1	A	236	ARG
1	A	276	GLN
1	A	362	LYS
1	A	404	LYS
1	A	449	LYS
1	A	658	LYS
1	A	763	LYS
1	A	825	GLN
1	A	834	LYS
2	B	41	LYS

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Mol	Chain	Res	Type
2	B	94	ALA
2	B	119	ASN
3	C	59	GLY
3	C	92	THR
1	A	40	LYS
1	A	82	PHE
1	A	343	GLU
1	A	581	HIS
1	A	725	PRO
1	A	740	GLU
1	A	750	PRO
2	B	42	ALA
2	B	53	ASP
3	C	64	PRO
3	C	66	GLU
3	C	121	ASP
1	A	128	ARG
1	A	131	ILE
1	A	223	ASN
1	A	225	VAL
1	A	336	ASP
1	A	686	LEU
1	A	692	GLN
2	B	117	GLY
2	B	151	SER
3	C	127	LYS
1	A	365	GLN
1	A	426	LEU
1	A	429	SER
1	A	812	GLN
1	A	833	VAL
1	A	30	GLY
2	B	29	VAL
1	A	15	VAL
1	A	80	PRO
1	A	121	ILE
1	A	125	PRO
1	A	284	ILE
1	A	112	ILE
3	C	103	GLY
1	A	392	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/728 (79%)	509 (88%)	68 (12%)	5	22
2	B	98/133 (74%)	86 (88%)	12 (12%)	5	21
3	C	114/132 (86%)	102 (90%)	12 (10%)	6	26
All	All	789/993 (80%)	697 (88%)	92 (12%)	5	22

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	9	ASP
1	A	10	PHE
1	A	11	GLN
1	A	32	LYS
1	A	49	GLN
1	A	76	SER
1	A	86	GLU
1	A	108	THR
1	A	109	SER
1	A	112	ILE
1	A	114	THR
1	A	134	ASP
1	A	147	GLU
1	A	152	LEU
1	A	158	ASN
1	A	161	GLN
1	A	166	ASP
1	A	169	ASN
1	A	172	CYS
1	A	173	LEU
1	A	182	LYS
1	A	183	THR
1	A	191	MET
1	A	211	LYS
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	217	ASP
1	A	218	GLN
1	A	226	LEU
1	A	266	LEU
1	A	268	GLU
1	A	271	ARG
1	A	276	GLN
1	A	289	CYS
1	A	308	LEU
1	A	313	ASN
1	A	316	CYS
1	A	318	THR
1	A	321	ASN
1	A	333	GLU
1	A	337	ILE
1	A	338	LEU
1	A	343	GLU
1	A	374	SER
1	A	447	ASP
1	A	485	GLN
1	A	496	GLU
1	A	497	GLN
1	A	500	TYR
1	A	502	LYS
1	A	507	TRP
1	A	510	ILE
1	A	521	ASP
1	A	524	GLU
1	A	553	GLN
1	A	560	ARG
1	A	561	MET
1	A	571	PRO
1	A	599	LYS
1	A	644	THR
1	A	654	ASN
1	A	659	ASN
1	A	678	GLN
1	A	694	ASN
1	A	697	LEU
1	A	710	ARG
1	A	725	PRO
1	A	801	LEU

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Mol	Chain	Res	Type
2	B	14	GLN
2	B	43	ILE
2	B	47	LEU
2	B	49	ARG
2	B	68	ASN
2	B	75	ILE
2	B	90	ARG
2	B	99	GLN
2	B	109	ILE
2	B	120	PHE
2	B	123	ASP
2	B	135	GLU
3	C	3	LEU
3	C	40	LEU
3	C	46	ASN
3	C	52	VAL
3	C	63	LEU
3	C	91	LYS
3	C	113	LEU
3	C	115	GLU
3	C	116	ARG
3	C	117	LEU
3	C	130	ASP
3	C	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	75	GLN
1	A	78	ASN
1	A	102	ASN
1	A	161	GLN
1	A	169	ASN
1	A	185	ASN
1	A	223	ASN
1	A	239	ASN
1	A	250	HIS
1	A	281	ASN
1	A	287	GLN
1	A	313	ASN
1	A	390	ASN

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Mol	Chain	Res	Type
1	A	436	ASN
1	A	443	ASN
1	A	453	ASN
1	A	481	ASN
1	A	485	GLN
1	A	486	GLN
1	A	577	HIS
1	A	582	HIS
1	A	598	ASN
1	A	649	HIS
1	A	654	ASN
1	A	674	ASN
1	A	678	GLN
1	A	694	ASN
1	A	814	ASN
1	A	823	ASN
2	B	91	ASN
3	C	5	GLN
3	C	132	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
6	PDM	A	900	1	21,22,22	2.86	8 (38%)	29,30,30	2.08	6 (20%)
5	AGS	A	999	4	32,33,33	2.00	8 (25%)	45,52,52	1.27	3 (6%)

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
6	PDM	A	900	1	1/1/5/6	9/13/26/26	0/2/2/2
5	AGS	A	999	4	-	0/21/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	900	PDM	CP7-NP2	-6.91	1.34	1.43
6	A	900	PDM	OP3-CP7	-5.66	1.24	1.40
5	A	999	AGS	PB-O3A	-5.32	1.53	1.59
5	A	999	AGS	PG-S1G	4.64	2.00	1.90
5	A	999	AGS	O5'-C5'	-4.57	1.27	1.44
6	A	900	PDM	C13-C12	-4.52	1.41	1.52
6	A	900	PDM	C13-C14	-3.83	1.40	1.51
6	A	900	PDM	C12-C11	-3.75	1.40	1.51
6	A	900	PDM	C14-NP1	-3.67	1.35	1.40
6	A	900	PDM	C11-NP1	-3.56	1.35	1.40
5	A	999	AGS	PB-O3B	3.23	1.63	1.59
5	A	999	AGS	PA-O5'	-3.19	1.46	1.59
5	A	999	AGS	C4-N3	2.84	1.39	1.34
6	A	900	PDM	CP6-CP5	2.12	1.42	1.38
5	A	999	AGS	C1'-N9	2.06	1.52	1.46
5	A	999	AGS	PB-O2B	-2.06	1.45	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	900	PDM	CP4-NP2-CP7	6.27	132.27	123.19
6	A	900	PDM	CP8-CP7-NP2	5.08	116.89	110.30
6	A	900	PDM	OP3-CP7-CP8	5.03	121.14	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	AGS	O4'-C4'-C5'	4.15	122.61	109.33
5	A	999	AGS	O3G-PG-O3B	3.33	115.77	104.64
6	A	900	PDM	OP5-C10-CP9	-2.37	115.59	123.09
6	A	900	PDM	C12-C13-C14	2.13	107.43	105.24
5	A	999	AGS	O2B-PB-O3A	2.01	112.69	107.27
6	A	900	PDM	C13-C12-C11	2.00	107.29	105.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	900	PDM	CP7

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	900	PDM	NP2-CP7-CP8-CP9
6	A	900	PDM	CP6-CP1-NP1-C11
6	A	900	PDM	CP2-CP1-NP1-C14
6	A	900	PDM	CP2-CP1-NP1-C11
6	A	900	PDM	CP6-CP1-NP1-C14
6	A	900	PDM	OP3-CP7-CP8-CP9
6	A	900	PDM	OP4-C10-CP9-CP8
6	A	900	PDM	OP5-C10-CP9-CP8
6	A	900	PDM	CP8-CP7-NP2-CP4

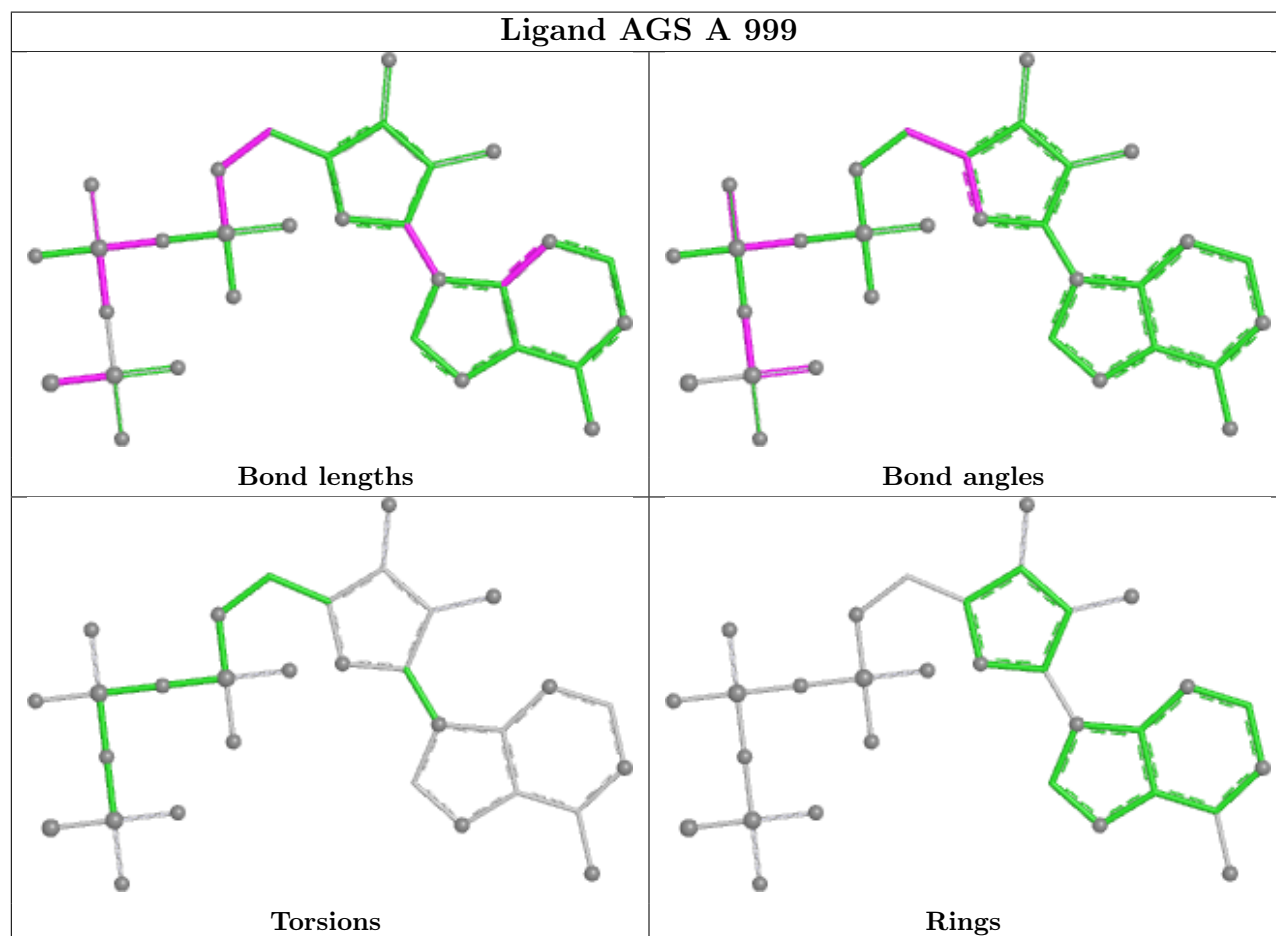
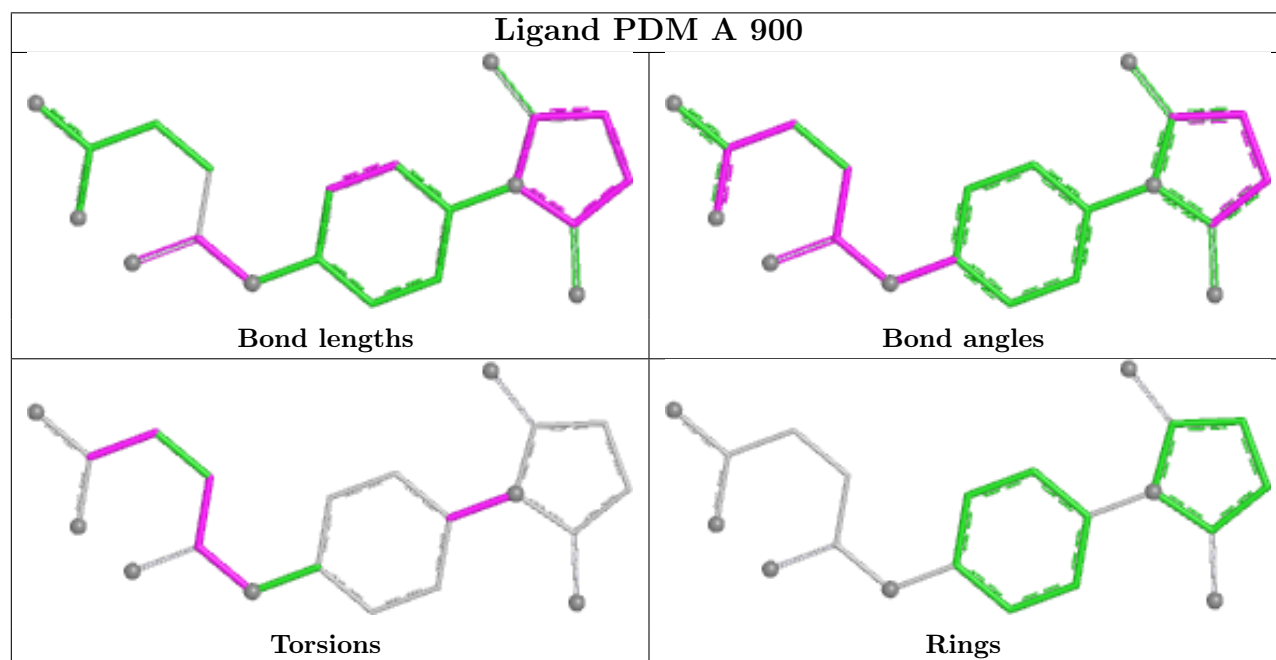
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	PDM	10	0
5	A	999	AGS	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.