



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:55 AM UTC

PDB ID : 2MYS / pdb_00002mys
Title : MYOSIN SUBFRAGMENT-1, ALPHA CARBON COORDINATES ONLY
FOR THE TWO LIGHT CHAINS
Authors : Rayment, I.; Holden, H.M.
Deposited on : 1996-06-27
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

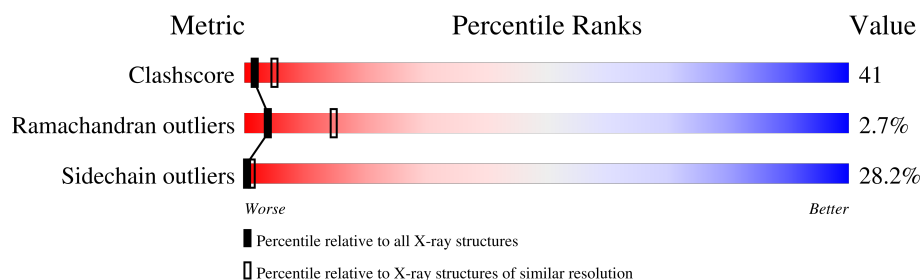
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	843	
2	B	166	
3	C	149	

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
4	SO4	A	5000	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6788 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	800	Total	C	N	O	S	0	0	0
			6510	4206	1081	1187	36			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MLY	LYS	modified residue	UNP P13538
A	30	MLY	LYS	modified residue	UNP P13538
A	35	MLY	LYS	modified residue	UNP P13538
A	45	GLN	GLU	conflict	UNP P13538
A	49	MLY	LYS	modified residue	UNP P13538
A	55	MLY	LYS	modified residue	UNP P13538
A	59	MLY	LYS	modified residue	UNP P13538
A	63	MLY	LYS	modified residue	UNP P13538
A	84	MLY	LYS	modified residue	UNP P13538
A	87	MLY	LYS	modified residue	UNP P13538
A	107	MLY	LYS	modified residue	UNP P13538
A	130	MLY	LYS	modified residue	UNP P13538
A	138	MLY	GLU	conflict	UNP P13538
A	190	MLY	LYS	modified residue	UNP P13538
A	236	MLY	LYS	modified residue	UNP P13538
A	248	MLY	LYS	modified residue	UNP P13538
A	272	MLY	LYS	modified residue	UNP P13538
A	295	MLY	LYS	modified residue	UNP P13538
A	296	MLY	LYS	modified residue	UNP P13538
A	317	GLU	GLN	conflict	UNP P13538
A	348	MLY	LYS	modified residue	UNP P13538
A	353	MLY	LYS	modified residue	UNP P13538
A	367	MLY	LYS	modified residue	UNP P13538
A	369	MLY	LYS	modified residue	UNP P13538
A	385	MLY	LYS	modified residue	UNP P13538
A	407	GLY	LYS	conflict	UNP P13538
A	412	ALA	PHE	conflict	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
A	415	MLY	LYS	modified residue	UNP P13538
A	417	GLU	GLN	conflict	UNP P13538
A	421	GLU	GLN	conflict	UNP P13538
A	431	MLY	LYS	modified residue	UNP P13538
A	436	MLY	LYS	modified residue	UNP P13538
A	486	MLY	LYS	modified residue	UNP P13538
A	504	MLY	LYS	modified residue	UNP P13538
A	505	MLY	LYS	modified residue	UNP P13538
A	528	MLY	LYS	modified residue	UNP P13538
A	551	MLY	LYS	modified residue	UNP P13538
A	553	MLY	LYS	modified residue	UNP P13538
A	557	GLU	GLN	conflict	UNP P13538
A	598	MLY	LYS	modified residue	UNP P13538
A	600	MLY	LYS	modified residue	UNP P13538
A	613	MLY	LYS	modified residue	UNP P13538
A	617	MLY	LYS	modified residue	UNP P13538
A	659	MLY	LYS	modified residue	UNP P13538
A	681	MLY	LYS	modified residue	UNP P13538
A	750	GLY	SER	conflict	UNP P13538
A	751	GLY	ILE	conflict	UNP P13538
A	759	ALA	ARG	conflict	UNP P13538
A	764	MLY	LYS	modified residue	UNP P13538
A	768	MLY	LYS	modified residue	UNP P13538
A	782	MLY	LYS	modified residue	UNP P13538
A	789	ALA	ARG	conflict	UNP P13538
A	805	ALA	ARG	conflict	UNP P13538
A	827	MLY	LYS	modified residue	UNP P13538
A	833	MLY	LYS	modified residue	UNP P13538
A	837	MLY	LYS	modified residue	UNP P13538
A	839	MLY	LYS	modified residue	UNP P13538

- Molecule 2 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	138	Total C 138 138	0	0	138

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	GLU	GLN	conflict	UNP P02609
B	23	GLU	GLN	conflict	UNP P02609

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLU	GLN	conflict	UNP P02609
B	26	ASP	GLU	conflict	UNP P02609
B	38	ALA	ARG	conflict	UNP P02609
B	124	GLY	GLN	conflict	UNP P02609
B	125	GLY	CYS	conflict	UNP P02609
B	126	GLY	ASP	conflict	UNP P02609
B	163	ALA	LYS	conflict	UNP P02609

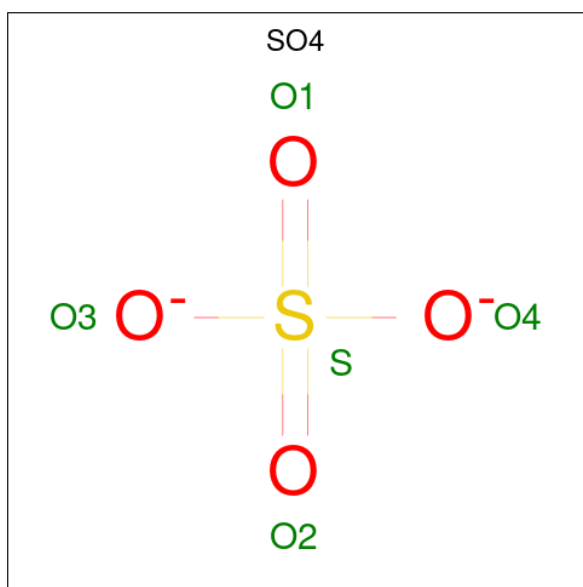
- Molecule 3 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	134	Total C 134 134	0	0	134

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	LYS	PRO	conflict	UNP P02605
C	5	ALA	ASP	conflict	UNP P02605
C	6	ALA	GLN	conflict	UNP P02605
C	7	ALA	ILE	conflict	UNP P02605
C	27	ALA	LEU	conflict	UNP P02605
C	34	ALA	VAL	conflict	UNP P02605
C	61	ALA	LYS	conflict	UNP P02605
C	62	ALA	LYS	conflict	UNP P02605

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

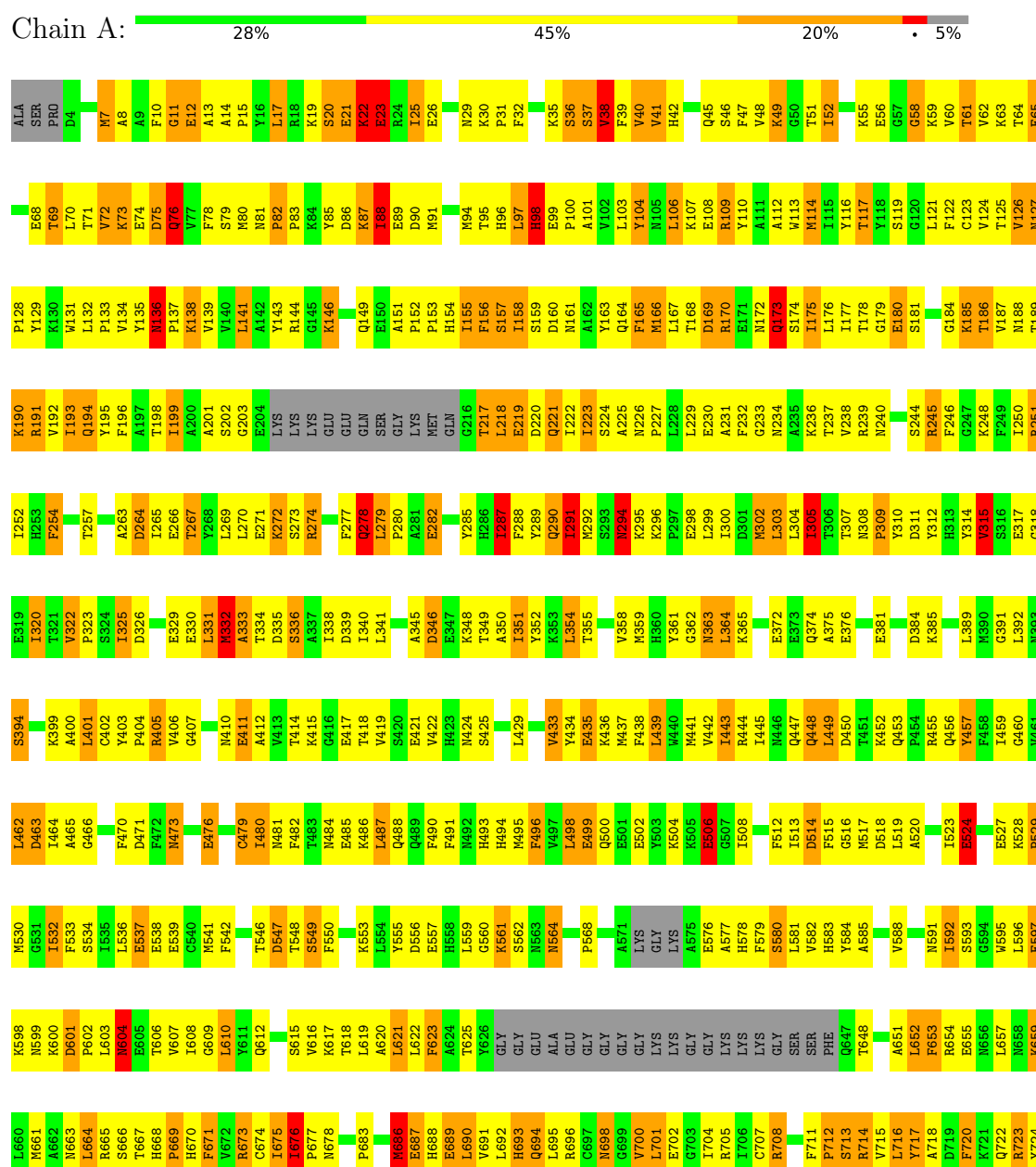
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

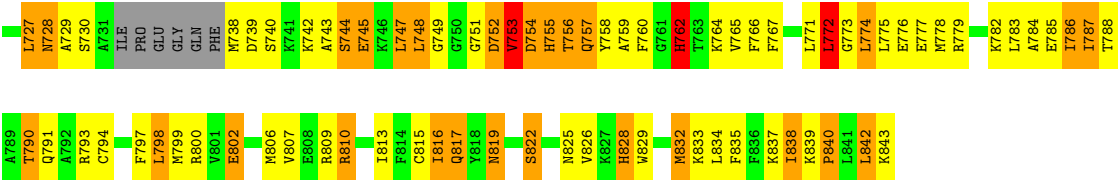
3 Residue-property plots

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.

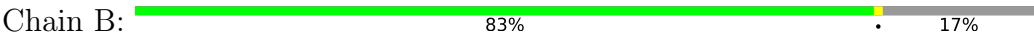
Note EDS was not executed.

• Molecule 1: MYOSIN

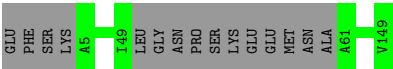
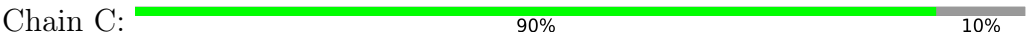




• Molecule 2: MYOSIN



• Molecule 3: MYOSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.40Å 124.20Å 274.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.223 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6788	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: SO4, MLY, 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	1.49	19/6156 (0.3%)	1.77	114/8350 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	PHE	C-N	-7.13	1.25	1.33
1	A	288	PHE	CA-C	-6.92	1.44	1.52
1	A	177	ILE	C-O	-6.76	1.16	1.24
1	A	496	PHE	C-O	-6.43	1.16	1.24
1	A	523	ILE	CA-CB	-6.39	1.47	1.54
1	A	514	ASP	C-O	-5.80	1.17	1.23
1	A	358	VAL	C-O	-5.78	1.17	1.24
1	A	434	TYR	CA-CB	-5.72	1.44	1.53
1	A	233	GLY	C-O	-5.43	1.20	1.24
1	A	340	ILE	CA-C	-5.41	1.45	1.52
1	A	482	PHE	C-O	-5.27	1.18	1.24
1	A	671	PHE	C-O	-5.24	1.17	1.23
1	A	476	GLU	CD-OE1	5.24	1.35	1.25
1	A	309	PRO	CA-CB	-5.23	1.46	1.53
1	A	576	GLU	CD-OE1	5.20	1.35	1.25
1	A	104	TYR	C-O	-5.19	1.17	1.24
1	A	252	ILE	CA-C	-5.15	1.47	1.52
1	A	177	ILE	CA-CB	-5.13	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	619	LEU	CA-C	-5.12	1.46	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	HIS	CB-CA-C	-11.85	87.28	111.22
1	A	320	ILE	CB-CA-C	-10.49	100.63	110.91
1	A	653	PHE	CA-CB-CG	-10.19	103.61	113.80
1	A	693	HIS	CA-CB-CG	-9.67	104.13	113.80
1	A	604	ASN	CA-CB-CG	9.33	121.93	112.60
1	A	264	ASP	CB-CA-C	-8.76	100.57	111.43
1	A	752	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	784	ALA	N-CA-C	-8.51	101.97	111.07
1	A	264	ASP	N-CA-CB	-8.31	98.06	110.86
1	A	752	ASP	CB-CA-C	8.30	121.44	111.22
1	A	141	LEU	CB-CA-C	-8.24	97.88	110.90
1	A	756	THR	N-CA-CB	-8.24	97.70	110.39
1	A	315	VAL	N-CA-C	8.23	119.98	112.17
1	A	75	ASP	N-CA-CB	8.20	122.93	110.79
1	A	473	ASN	CA-CB-CG	-7.93	104.67	112.60
1	A	800	ARG	NE-CZ-NH2	-7.86	112.13	119.20
1	A	547	ASP	N-CA-C	-7.84	102.68	111.07
1	A	447	GLN	N-CA-CB	7.71	121.45	110.12
1	A	698	ASN	CB-CA-C	-7.54	98.12	110.79
1	A	506	GLU	CA-C-N	-7.28	112.58	122.63
1	A	506	GLU	C-N-CA	-7.28	112.58	122.63
1	A	76	GLN	N-CA-C	-7.25	102.74	113.61
1	A	652	LEU	O-C-N	7.02	130.25	122.11
1	A	686	MET	CA-C-N	-6.96	111.47	121.42
1	A	686	MET	C-N-CA	-6.96	111.47	121.42
1	A	529	PRO	CA-C-N	-6.88	111.65	122.65
1	A	529	PRO	C-N-CA	-6.88	111.65	122.65
1	A	676	ILE	CA-C-N	6.84	128.39	119.84
1	A	676	ILE	C-N-CA	6.84	128.39	119.84
1	A	623	PHE	CA-CB-CG	6.82	120.62	113.80
1	A	146	LYS	N-CA-C	6.71	119.46	108.52
1	A	156	PHE	N-CA-C	-6.51	104.60	112.54
1	A	82	PRO	N-CA-CB	6.44	109.33	103.08
1	A	604	ASN	CA-C-O	6.42	128.40	121.02
1	A	340	ILE	O-C-N	6.37	128.30	121.87
1	A	755	HIS	CA-CB-CG	6.33	120.14	113.80
1	A	47	PHE	CB-CA-C	-6.33	100.99	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ILE	N-CA-C	6.33	117.01	110.36
1	A	688	HIS	CA-CB-CG	-6.32	107.48	113.80
1	A	524	GLU	N-CA-CB	6.27	119.47	110.06
1	A	443	ILE	CB-CA-C	-6.21	103.94	111.88
1	A	599	ASN	OD1-CG-ND2	-6.17	116.44	122.60
1	A	341	LEU	CB-CA-C	6.14	122.18	110.27
1	A	22	LYS	N-CA-C	-6.13	106.40	114.31
1	A	279	LEU	CA-C-N	6.12	126.02	119.28
1	A	279	LEU	C-N-CA	6.12	126.02	119.28
1	A	363	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	A	686	MET	N-CA-CB	-6.07	100.57	110.59
1	A	165	PHE	N-CA-CB	-6.06	100.25	110.49
1	A	352	TYR	N-CA-CB	6.04	120.76	110.50
1	A	231	ALA	O-C-N	6.03	129.69	122.27
1	A	136	ASN	CA-C-O	6.01	124.76	119.71
1	A	308	ASN	CA-C-N	6.01	125.63	119.56
1	A	308	ASN	C-N-CA	6.01	125.63	119.56
1	A	180	GLU	N-CA-CB	5.99	118.59	110.38
1	A	479	CYS	N-CA-CB	5.98	118.85	109.94
1	A	747	LEU	N-CA-CB	5.96	118.82	109.94
1	A	136	ASN	O-C-N	5.95	126.26	121.38
1	A	717	TYR	N-CA-C	5.94	121.17	111.37
1	A	753	VAL	N-CA-C	5.94	118.50	109.12
1	A	592	ILE	CA-C-N	-5.92	113.58	122.47
1	A	592	ILE	C-N-CA	-5.92	113.58	122.47
1	A	88	ILE	CB-CG1-CD1	-5.86	101.49	113.80
1	A	687	GLU	N-CA-CB	5.83	118.86	110.06
1	A	790	THR	CA-C-O	5.80	126.51	119.31
1	A	278	GLN	OE1-CD-NE2	5.79	128.39	122.60
1	A	786	ILE	CB-CA-C	-5.79	104.46	112.04
1	A	463	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	23	GLU	N-CA-C	-5.78	105.06	111.71
1	A	718	ALA	O-C-N	5.75	128.71	122.15
1	A	433	VAL	N-CA-C	5.69	115.88	110.42
1	A	22	LYS	CB-CA-C	5.67	118.55	109.02
1	A	828	HIS	CA-C-N	5.66	129.12	121.20
1	A	828	HIS	C-N-CA	5.66	129.12	121.20
1	A	755	HIS	CA-C-N	5.63	129.53	121.71
1	A	755	HIS	C-N-CA	5.63	129.53	121.71
1	A	346	ASP	N-CA-CB	-5.61	101.29	109.82
1	A	351	ILE	CB-CA-C	-5.61	104.71	111.88
1	A	196	PHE	CA-CB-CG	-5.57	108.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	THR	N-CA-C	-5.57	104.90	110.97
1	A	333	ALA	CA-C-O	5.55	126.84	120.90
1	A	309	PRO	CB-CA-C	-5.55	103.58	111.68
1	A	671	PHE	N-CA-C	5.49	118.76	109.76
1	A	173	GLN	N-CA-CB	-5.42	102.92	111.05
1	A	305	ILE	CB-CA-C	-5.41	103.77	111.34
1	A	447	GLN	CB-CA-C	5.33	119.63	110.79
1	A	654	ARG	CA-C-N	5.30	127.39	120.28
1	A	654	ARG	C-N-CA	5.30	127.39	120.28
1	A	329	GLU	CA-C-O	5.30	126.04	120.42
1	A	291	ILE	CB-CA-C	-5.30	105.10	111.88
1	A	592	ILE	N-CA-CB	-5.27	102.53	111.23
1	A	720	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	564	ASN	CA-CB-CG	-5.25	107.36	112.60
1	A	267	THR	OG1-CB-CG2	5.23	119.77	109.30
1	A	669	PRO	N-CA-CB	5.23	107.98	103.27
1	A	772	LEU	N-CA-C	-5.21	105.08	111.75
1	A	157	SER	O-C-N	5.20	127.70	122.09
1	A	401	LEU	CD1-CG-CD2	-5.20	99.37	110.80
1	A	201	ALA	N-CA-C	5.19	118.68	109.96
1	A	38	VAL	N-CA-CB	-5.18	102.68	111.23
1	A	663	ASN	N-CA-C	-5.15	105.85	111.82
1	A	601	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	694	GLN	CA-C-O	5.10	126.13	120.63
1	A	652	LEU	CB-CA-C	-5.08	102.48	110.86
1	A	322	VAL	O-C-N	5.08	125.56	120.59
1	A	332	MET	CB-CA-C	-5.07	102.23	110.85
1	A	332	MET	CG-SD-CE	-5.06	89.77	100.90
1	A	254	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	76	GLN	CA-C-O	5.05	125.14	119.18
1	A	172	ASN	N-CA-CB	5.05	118.12	110.45
1	A	425	SER	N-CA-CB	5.04	117.62	110.16
1	A	424	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	165	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	621	LEU	N-CA-C	5.03	116.45	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	HIS	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6510	0	6507	547	1
2	B	138	0	0	1	0
3	C	134	0	0	0	0
4	A	5	0	0	2	0
5	B	1	0	0	0	0
All	All	6788	0	6507	547	1

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 41.

All (547) 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:72:VAL:HG13	1:A:76:GLN:HB3	1.36	1.03
1:A:98:HIS:HB3	1:A:100:PRO:HD2	1.42	0.99
1:A:56:GLU:HB2	1:A:59:MLY:HB3	1.40	0.99
1:A:174:SER:HB3	1:A:667:THR:HG21	1.44	0.97
1:A:292:MET:HE1	1:A:309:PRO:HA	1.47	0.96
1:A:546:THR:HG22	1:A:548:THR:H	1.32	0.94
1:A:278:GLN:HG2	1:A:317:GLU:HB2	1.52	0.92
1:A:508:ILE:HD11	1:A:766:PHE:CD1	2.07	0.90
1:A:107:MLY:HB3	1:A:686:MET:HE2	1.54	0.89
1:A:292:MET:HE1	1:A:309:PRO:CA	2.05	0.86
1:A:755:HIS:HA	1:A:758:TYR:CE1	2.10	0.86
1:A:310:TYR:CZ	1:A:320:ILE:HD11	2.11	0.85
1:A:72:VAL:CG1	1:A:76:GLN:HB3	2.05	0.85
1:A:724:TYR:CE1	1:A:775:LEU:HB3	2.12	0.85
1:A:91:MET:HE3	1:A:119:SER:HB2	1.57	0.84
1:A:648:THR:CG2	1:A:651:ALA:HB2	2.08	0.83
1:A:418:THR:HB	1:A:421:GLU:HG3	1.59	0.83
1:A:127:ASN:HD22	1:A:128:PRO:HD2	1.44	0.82
1:A:279:LEU:HB2	1:A:282:GLU:HG3	1.60	0.82
1:A:648:THR:HG22	1:A:651:ALA:HB2	1.62	0.82
1:A:232:PHE:CZ	1:A:287:ILE:HD13	2.16	0.80
1:A:374:GLN:HG3	1:A:375:ALA:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:HG22	1:A:481:ASN:HD22	1.45	0.80
1:A:291:ILE:HA	1:A:331:LEU:HD11	1.64	0.80
1:A:166:MET:HE1	1:A:254:PHE:CD2	2.19	0.78
1:A:51:THR:O	1:A:62:VAL:HG13	1.84	0.78
1:A:174:SER:CB	1:A:667:THR:HG21	2.13	0.78
1:A:290:GLN:C	1:A:331:LEU:HD12	2.09	0.78
1:A:496:PHE:CD2	1:A:514:ASP:HA	2.19	0.77
1:A:407:GLY:HA2	1:A:412:ALA:HA	1.65	0.77
1:A:116:TYR:O	1:A:153:PRO:HB2	1.85	0.77
1:A:131:TRP:C	1:A:132:LEU:HD12	2.09	0.77
1:A:94:MET:CE	1:A:101:ALA:HB1	2.15	0.77
1:A:664:LEU:O	1:A:667:THR:HB	1.86	0.76
1:A:578:HIS:HD2	1:A:591:ASN:HA	1.51	0.75
1:A:295:MLY:HG3	1:A:332:MET:HE2	1.69	0.75
1:A:310:TYR:CE2	1:A:320:ILE:HD11	2.22	0.74
1:A:481:ASN:HD22	1:A:481:ASN:N	1.82	0.74
1:A:486:MLY:HH13	1:A:527:GLU:OE1	1.88	0.74
1:A:272:MLY:HH13	1:A:435:GLU:OE1	1.87	0.74
1:A:21:GLU:O	1:A:25:ILE:HG13	1.89	0.73
1:A:350:ALA:O	1:A:354:LEU:HB2	1.87	0.73
1:A:441:MET:O	1:A:445:ILE:HG13	1.88	0.73
1:A:487:LEU:O	1:A:490:PHE:HB3	1.89	0.73
1:A:237:THR:HG22	1:A:239:ARG:H	1.54	0.73
1:A:802:GLU:O	1:A:806:MET:HG3	1.89	0.73
1:A:295:MLY:HG3	1:A:332:MET:CE	2.19	0.72
1:A:536:LEU:HD13	1:A:550:PHE:CZ	2.24	0.72
1:A:190:MLY:HE3	1:A:230:GLU:OE2	1.89	0.72
1:A:519:LEU:HD12	1:A:519:LEU:N	2.04	0.72
1:A:546:THR:HG22	1:A:548:THR:N	2.05	0.72
1:A:176:LEU:N	1:A:176:LEU:HD12	2.05	0.72
1:A:36:SER:O	1:A:52:ILE:HG12	1.90	0.72
1:A:245:ARG:HD3	1:A:271:GLU:OE1	1.90	0.71
1:A:14:ALA:HB3	1:A:15:PRO:HD3	1.72	0.71
1:A:486:MLY:HH22	1:A:527:GLU:OE2	1.90	0.71
1:A:72:VAL:HG13	1:A:76:GLN:CB	2.19	0.71
1:A:86:ASP:OD2	1:A:87:MLY:HH13	1.91	0.71
1:A:618:THR:O	1:A:622:LEU:HD13	1.89	0.71
1:A:578:HIS:CB	1:A:592:ILE:HD12	2.21	0.71
1:A:56:GLU:CB	1:A:59:MLY:HB3	2.19	0.70
1:A:762:HIS:CD2	1:A:762:HIS:H	2.08	0.70
1:A:274:ARG:NH2	1:A:282:GLU:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:MET:HE1	1:A:254:PHE:HB2	1.73	0.70
1:A:754:ASP:HB3	1:A:757:GLN:HG2	1.72	0.70
1:A:123:CYS:HB2	1:A:158:ILE:HD11	1.73	0.69
1:A:810:ARG:HG2	1:A:810:ARG:HH11	1.57	0.69
1:A:578:HIS:HB2	1:A:592:ILE:HD12	1.74	0.69
1:A:782:MLY:C	1:A:783:LEU:HD12	2.22	0.69
1:A:802:GLU:HA	1:A:802:GLU:OE1	1.93	0.69
1:A:807:VAL:O	1:A:810:ARG:HB2	1.93	0.69
1:A:123:CYS:HB2	1:A:158:ILE:CD1	2.23	0.69
1:A:533:PHE:O	1:A:537:GLU:HG2	1.93	0.68
1:A:166:MET:HE1	1:A:254:PHE:HD2	1.56	0.68
1:A:815:CYS:O	1:A:819:ASN:HB2	1.93	0.68
1:A:62:VAL:HG12	1:A:63:MLY:O	1.94	0.68
1:A:787:ILE:HG22	1:A:788:THR:N	2.07	0.68
1:A:217:THR:O	1:A:221:GLN:HG2	1.94	0.68
1:A:652:LEU:O	1:A:655:GLU:N	2.27	0.68
1:A:61:THR:HG23	1:A:71:THR:OG1	1.94	0.67
1:A:480:ILE:HG22	1:A:481:ASN:ND2	2.09	0.67
1:A:550:PHE:HE2	1:A:592:ILE:HG23	1.59	0.67
1:A:52:ILE:N	1:A:52:ILE:HD13	2.09	0.67
1:A:184:GLY:N	4:A:5000:SO4:O1	2.28	0.67
1:A:648:THR:HG23	1:A:651:ALA:H	1.59	0.67
1:A:58:GLY:HA2	1:A:74:GLU:OE1	1.94	0.66
1:A:226:ASN:HB2	1:A:227:PRO:HD3	1.78	0.66
1:A:218:LEU:HA	1:A:221:GLN:HG3	1.75	0.66
1:A:78:PHE:HB3	1:A:98:HIS:CD2	2.30	0.66
1:A:131:TRP:O	1:A:132:LEU:HD12	1.95	0.66
1:A:161:ASN:O	1:A:165:PHE:HB2	1.96	0.66
1:A:322:VAL:HB	1:A:325:ILE:CD1	2.26	0.66
1:A:107:MLY:HB3	1:A:686:MET:CE	2.26	0.65
1:A:144:ARG:NH1	1:A:160:ASP:OD1	2.29	0.65
1:A:339:ASP:OD1	1:A:348:MLY:HH13	1.95	0.65
1:A:480:ILE:HG22	1:A:481:ASN:N	2.11	0.65
1:A:724:TYR:HD1	1:A:727:LEU:HD11	1.61	0.65
1:A:290:GLN:O	1:A:331:LEU:HD12	1.95	0.65
1:A:466:GLY:HA2	1:A:484:ASN:ND2	2.11	0.65
1:A:691:VAL:O	1:A:695:LEU:HD13	1.97	0.65
1:A:94:MET:HE1	1:A:101:ALA:HB1	1.79	0.65
1:A:296:MLY:HH11	1:A:348:MLY:HH21	1.78	0.65
1:A:546:THR:H	1:A:549:SER:HB3	1.59	0.65
1:A:579:PHE:HD2	1:A:592:ILE:HD11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:SER:O	1:A:825:ASN:HB2	1.97	0.65
1:A:174:SER:O	1:A:670:HIS:HB2	1.96	0.65
1:A:665:ARG:C	1:A:667:THR:H	2.05	0.65
1:A:278:GLN:CG	1:A:317:GLU:HB2	2.27	0.64
1:A:418:THR:HG22	1:A:419:VAL:N	2.11	0.64
1:A:374:GLN:HG3	1:A:375:ALA:H	1.60	0.64
1:A:783:LEU:HD12	1:A:783:LEU:N	2.13	0.64
1:A:49:MLY:HH23	1:A:80:MET:HE3	1.80	0.64
1:A:133:PRO:O	1:A:136:ASN:HB2	1.98	0.64
1:A:219:GLU:O	1:A:223:ILE:HG13	1.97	0.63
1:A:580:SER:HA	1:A:588:VAL:O	1.98	0.63
1:A:251:ARG:HB2	1:A:264:ASP:CB	2.29	0.63
1:A:771:LEU:O	1:A:774:LEU:N	2.32	0.63
1:A:406:VAL:HG12	1:A:407:GLY:N	2.13	0.63
1:A:161:ASN:HA	1:A:164:GLN:HE21	1.63	0.63
1:A:728:ASN:O	1:A:730:SER:N	2.32	0.63
1:A:466:GLY:HA2	1:A:484:ASN:HD21	1.61	0.63
1:A:479:CYS:HB3	1:A:653:PHE:CE2	2.33	0.63
1:A:127:ASN:HD22	1:A:128:PRO:CD	2.11	0.62
1:A:141:LEU:H	1:A:141:LEU:HD12	1.64	0.62
1:A:806:MET:O	1:A:809:ARG:HB2	1.98	0.62
1:A:98:HIS:HB3	1:A:100:PRO:CD	2.25	0.62
1:A:506:GLU:HG2	1:A:766:PHE:HE1	1.64	0.62
1:A:542:PHE:CZ	1:A:553:MLY:HH11	2.34	0.62
1:A:578:HIS:HB2	1:A:592:ILE:CD1	2.30	0.62
1:A:302:MET:HG2	1:A:303:LEU:CD1	2.30	0.62
1:A:520:ALA:O	1:A:524:GLU:HG2	2.00	0.62
1:A:173:GLN:C	1:A:667:THR:HG23	2.25	0.61
1:A:274:ARG:HB2	1:A:285:TYR:CE2	2.34	0.61
1:A:154:HIS:CE1	1:A:156:PHE:CD2	2.88	0.61
1:A:537:GLU:HB3	1:A:648:THR:HG21	1.83	0.61
1:A:724:TYR:HB3	1:A:727:LEU:HD12	1.81	0.61
1:A:40:VAL:HG22	1:A:41:VAL:N	2.16	0.60
1:A:81:ASN:OD1	1:A:96:HIS:HB2	2.00	0.60
1:A:755:HIS:HA	1:A:758:TYR:HE1	1.64	0.60
1:A:156:PHE:CD1	1:A:195:TYR:CD1	2.90	0.60
1:A:124:VAL:CG1	1:A:675:ILE:HD13	2.31	0.60
1:A:557:GLU:O	1:A:557:GLU:HG3	2.00	0.60
1:A:278:GLN:HG3	1:A:318:GLY:N	2.15	0.60
1:A:837:MLY:O	1:A:840:PRO:HD2	2.02	0.60
1:A:40:VAL:HG22	1:A:41:VAL:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLU:HG2	1:A:766:PHE:CE1	2.36	0.60
1:A:524:GLU:O	1:A:528:MLY:HB3	2.01	0.60
1:A:124:VAL:HG13	1:A:675:ILE:HD13	1.84	0.60
1:A:95:THR:HG23	1:A:96:HIS:ND1	2.17	0.60
1:A:686:MET:HG3	1:A:691:VAL:HG21	1.83	0.60
1:A:787:ILE:O	1:A:790:THR:N	2.35	0.60
1:A:648:THR:HG23	1:A:651:ALA:HB2	1.83	0.59
1:A:508:ILE:HD11	1:A:766:PHE:CG	2.37	0.59
1:A:49:MLY:HH13	1:A:108:GLU:OE2	2.02	0.59
1:A:536:LEU:HD13	1:A:550:PHE:CE1	2.37	0.59
1:A:550:PHE:CE2	1:A:592:ILE:HG23	2.37	0.59
1:A:166:MET:HE2	1:A:457:TYR:HB2	1.84	0.59
1:A:776:GLU:O	1:A:779:ARG:HB3	2.02	0.59
1:A:60:VAL:O	1:A:71:THR:HA	2.02	0.59
1:A:230:GLU:O	1:A:234:ASN:HB2	2.03	0.59
1:A:99:GLU:OE2	1:A:696:ARG:NH2	2.30	0.58
1:A:124:VAL:HG13	1:A:675:ILE:CD1	2.33	0.58
1:A:579:PHE:CE1	1:A:581:LEU:HD13	2.38	0.58
1:A:38:VAL:HB	1:A:52:ILE:HD11	1.84	0.58
1:A:601:ASP:N	1:A:602:PRO:HD3	2.18	0.58
1:A:107:MLY:CB	1:A:686:MET:HE2	2.32	0.58
1:A:546:THR:HG22	1:A:547:ASP:N	2.17	0.58
1:A:116:TYR:HB2	1:A:153:PRO:O	2.03	0.58
1:A:7:MET:HE3	1:A:14:ALA:HB1	1.85	0.58
1:A:464:ILE:HG22	1:A:465:ALA:N	2.18	0.58
1:A:135:TYR:N	1:A:135:TYR:CD1	2.70	0.58
1:A:141:LEU:O	1:A:144:ARG:HB3	2.03	0.58
1:A:254:PHE:CE2	1:A:459:ILE:HD12	2.39	0.58
1:A:538:GLU:O	1:A:541:MET:HB2	2.04	0.58
1:A:676:ILE:HG23	1:A:676:ILE:O	2.03	0.58
1:A:127:ASN:ND2	1:A:128:PRO:HD2	2.16	0.58
1:A:322:VAL:HG11	1:A:325:ILE:HD11	1.86	0.58
1:A:175:ILE:HA	1:A:670:HIS:O	2.03	0.58
1:A:279:LEU:HB3	1:A:280:PRO:HD2	1.86	0.58
1:A:715:VAL:HG11	1:A:720:PHE:HD1	1.68	0.58
1:A:48:VAL:HG22	1:A:49:MLY:N	2.18	0.57
1:A:813:ILE:O	1:A:816:ILE:N	2.37	0.57
1:A:481:ASN:N	1:A:481:ASN:ND2	2.51	0.57
1:A:64:THR:HG22	1:A:65:GLU:N	2.19	0.57
1:A:418:THR:HG22	1:A:419:VAL:H	1.69	0.57
1:A:677:PRO:HB2	1:A:678:ASN:ND2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:CYS:O	1:A:798:LEU:N	2.37	0.57
1:A:265:ILE:HG22	1:A:266:GLU:N	2.18	0.56
1:A:35:MLY:HH22	1:A:777:GLU:CD	2.30	0.56
1:A:203:GLY:HA3	1:A:217:THR:HG21	1.87	0.56
1:A:508:ILE:HD11	1:A:766:PHE:CE1	2.39	0.56
1:A:438:PHE:HA	1:A:441:MET:HE3	1.88	0.56
1:A:13:ALA:C	1:A:15:PRO:HD2	2.31	0.56
1:A:82:PRO:HD2	1:A:85:TYR:CD2	2.40	0.56
1:A:747:LEU:O	1:A:747:LEU:HD23	2.05	0.56
1:A:116:TYR:CE2	1:A:154:HIS:CD2	2.94	0.56
1:A:435:GLU:O	1:A:438:PHE:HB3	2.06	0.56
1:A:604:ASN:OD1	1:A:607:VAL:HG23	2.06	0.56
1:A:290:GLN:HG2	1:A:331:LEU:HA	1.87	0.56
1:A:406:VAL:HG12	1:A:407:GLY:H	1.71	0.56
1:A:549:SER:OG	1:A:550:PHE:N	2.36	0.56
1:A:22:LYS:O	1:A:26:GLU:HG3	2.06	0.55
1:A:559:LEU:C	1:A:559:LEU:HD23	2.31	0.55
1:A:7:MET:HE3	1:A:14:ALA:CB	2.36	0.55
1:A:345:ALA:O	1:A:349:THR:N	2.40	0.55
1:A:32:PHE:CG	1:A:83:PRO:HD3	2.41	0.55
1:A:338:ILE:HG21	1:A:348:MLY:HB3	1.87	0.55
1:A:578:HIS:CD2	1:A:591:ASN:HA	2.37	0.55
1:A:22:LYS:HA	1:A:25:ILE:HB	1.87	0.55
1:A:305:ILE:HG22	1:A:312:TYR:CE2	2.42	0.55
1:A:546:THR:HB	1:A:549:SER:H	1.71	0.55
1:A:723:ARG:HH11	1:A:723:ARG:CG	2.20	0.55
1:A:78:PHE:HB3	1:A:98:HIS:NE2	2.22	0.55
1:A:135:TYR:N	1:A:135:TYR:HD1	2.04	0.55
1:A:470:PHE:O	1:A:473:ASN:ND2	2.40	0.54
1:A:546:THR:HG21	1:A:548:THR:HB	1.88	0.54
1:A:738:MET:HG3	1:A:739:ASP:H	1.71	0.54
1:A:290:GLN:NE2	1:A:334:THR:OG1	2.40	0.54
1:A:813:ILE:O	1:A:817:GLN:N	2.30	0.54
1:A:295:MLY:CG	1:A:332:MET:HE2	2.36	0.54
1:A:791:GLN:O	1:A:794:CYS:HB2	2.08	0.54
1:A:126:VAL:HG13	1:A:675:ILE:HG22	1.90	0.54
1:A:51:THR:C	1:A:62:VAL:HG13	2.32	0.54
1:A:305:ILE:HG22	1:A:312:TYR:CZ	2.42	0.54
1:A:10:PHE:O	1:A:12:GLU:N	2.40	0.54
1:A:103:LEU:C	1:A:103:LEU:HD12	2.33	0.54
1:A:38:VAL:CB	1:A:52:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:C	1:A:136:ASN:H	2.16	0.54
1:A:135:TYR:HD2	1:A:191:ARG:HG2	1.72	0.54
1:A:404:PRO:CG	1:A:417:GLU:HG3	2.38	0.54
1:A:295:MLY:CD	1:A:332:MET:HE2	2.37	0.53
1:A:302:MET:HG2	1:A:303:LEU:HD13	1.87	0.53
1:A:82:PRO:HD2	1:A:85:TYR:HD2	1.72	0.53
1:A:584:TYR:CD1	1:A:585:ALA:N	2.77	0.53
1:A:742:LYS:O	1:A:745:GLU:HB2	2.08	0.53
1:A:135:TYR:HD2	1:A:191:ARG:HD3	1.73	0.53
1:A:154:HIS:CE1	1:A:156:PHE:HD2	2.27	0.53
1:A:277:PHE:CG	1:A:278:GLN:N	2.76	0.53
1:A:251:ARG:HB2	1:A:264:ASP:HB2	1.91	0.53
1:A:491:PHE:HD1	1:A:671:PHE:CE2	2.27	0.53
1:A:727:LEU:HD21	1:A:778:MET:HB2	1.90	0.53
1:A:765:VAL:HG12	1:A:766:PHE:N	2.22	0.53
1:A:404:PRO:HG3	1:A:417:GLU:HG3	1.91	0.53
1:A:661:MET:O	1:A:665:ARG:HG3	2.09	0.53
1:A:838:ILE:C	1:A:840:PRO:HD2	2.34	0.53
1:A:32:PHE:CD1	1:A:83:PRO:HD3	2.44	0.53
1:A:156:PHE:HD1	1:A:195:TYR:CD1	2.27	0.53
1:A:221:GLN:HB2	1:A:449:LEU:HD11	1.91	0.53
1:A:42:HIS:HB3	1:A:45:GLN:O	2.09	0.52
1:A:232:PHE:CE1	1:A:287:ILE:HD13	2.45	0.52
1:A:493:HIS:ND1	1:A:514:ASP:OD2	2.41	0.52
1:A:135:TYR:CD2	1:A:191:ARG:HG2	2.44	0.52
1:A:40:VAL:HG13	1:A:41:VAL:O	2.10	0.52
1:A:579:PHE:HE1	1:A:581:LEU:HD13	1.74	0.52
1:A:63:MLY:HG3	1:A:64:THR:H	1.75	0.52
1:A:648:THR:HG23	1:A:651:ALA:N	2.25	0.52
1:A:400:ALA:HB1	1:A:606:THR:HG22	1.92	0.52
1:A:546:THR:CG2	1:A:548:THR:HB	2.41	0.51
1:A:128:PRO:O	1:A:129:TYR:HB2	2.09	0.51
1:A:41:VAL:HG13	1:A:42:HIS:N	2.25	0.51
1:A:355:THR:OG1	1:A:437:MET:HE1	2.09	0.51
1:A:41:VAL:HG21	1:A:76:GLN:HG3	1.92	0.51
1:A:494:HIS:O	1:A:498:LEU:HB2	2.09	0.51
1:A:135:TYR:HD2	1:A:191:ARG:CD	2.23	0.51
1:A:278:GLN:HG3	1:A:318:GLY:H	1.75	0.51
1:A:448:GLN:C	1:A:450:ASP:H	2.19	0.51
1:A:38:VAL:CG1	1:A:39:PHE:N	2.74	0.51
1:A:195:TYR:O	1:A:199:ILE:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:O	1:A:691:VAL:HG23	2.11	0.51
1:A:724:TYR:HE1	1:A:775:LEU:HB3	1.68	0.51
1:A:217:THR:HG21	1:A:219:GLU:OE1	2.11	0.51
1:A:592:ILE:O	1:A:592:ILE:HG22	2.10	0.51
1:A:783:LEU:O	1:A:787:ILE:N	2.28	0.51
1:A:248:MLY:N	1:A:463:ASP:O	2.44	0.51
1:A:291:ILE:HA	1:A:331:LEU:CD1	2.39	0.51
1:A:109:ARG:HD3	1:A:117:THR:HB	1.92	0.51
1:A:267:THR:HG21	1:A:438:PHE:HE2	1.76	0.51
1:A:311:ASP:HB2	1:A:312:TYR:CE1	2.46	0.50
1:A:418:THR:O	1:A:422:VAL:HG23	2.11	0.50
1:A:418:THR:CB	1:A:421:GLU:HG3	2.37	0.50
1:A:89:GLU:CD	1:A:153:PRO:HD2	2.36	0.50
1:A:237:THR:O	1:A:240:ASN:O	2.29	0.50
1:A:109:ARG:O	1:A:114:MET:N	2.37	0.50
1:A:168:THR:HG22	1:A:169:ASP:OD1	2.12	0.50
1:A:429:LEU:O	1:A:433:VAL:HG23	2.11	0.50
1:A:486:MLY:HH22	1:A:527:GLU:CD	2.37	0.50
1:A:128:PRO:O	1:A:683:PRO:HB3	2.12	0.49
1:A:839:MLY:N	1:A:840:PRO:CD	2.75	0.49
1:A:715:VAL:O	1:A:764:MLY:HB3	2.12	0.49
1:A:64:THR:CG2	1:A:65:GLU:N	2.75	0.49
1:A:292:MET:HE2	1:A:309:PRO:HD3	1.93	0.49
1:A:154:HIS:CD2	1:A:155:ILE:H	2.30	0.49
1:A:251:ARG:O	1:A:263:ALA:HA	2.12	0.49
1:A:192:VAL:O	1:A:195:TYR:HB3	2.13	0.49
1:A:547:ASP:O	1:A:550:PHE:HB3	2.12	0.49
1:A:839:MLY:HB2	1:A:840:PRO:HD3	1.94	0.49
1:A:601:ASP:N	1:A:602:PRO:CD	2.75	0.49
1:A:762:HIS:CD2	1:A:762:HIS:N	2.78	0.49
1:A:220:ASP:O	1:A:224:SER:N	2.30	0.48
1:A:346:ASP:O	1:A:349:THR:HB	2.11	0.48
1:A:756:THR:O	1:A:758:TYR:N	2.45	0.48
1:A:817:GLN:HE22	2:B:125:GLY:CA	2.26	0.48
1:A:290:GLN:HG2	1:A:331:LEU:CA	2.43	0.48
1:A:312:TYR:N	1:A:312:TYR:CD1	2.81	0.48
1:A:648:THR:HG23	1:A:651:ALA:CB	2.44	0.48
1:A:715:VAL:HG12	1:A:716:LEU:O	2.12	0.48
1:A:97:LEU:HD13	1:A:97:LEU:N	2.28	0.48
1:A:173:GLN:OE1	1:A:668:HIS:HB3	2.13	0.48
1:A:310:TYR:CE2	1:A:320:ILE:CD1	2.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PRO:HD2	1:A:415:MLY:O	2.13	0.48
1:A:717:TYR:HB3	1:A:740:SER:O	2.14	0.48
1:A:499:GLU:HA	1:A:499:GLU:OE1	2.13	0.48
1:A:154:HIS:CE1	1:A:156:PHE:CE2	3.02	0.48
1:A:22:LYS:O	1:A:26:GLU:N	2.29	0.48
1:A:237:THR:HG22	1:A:238:VAL:N	2.28	0.48
1:A:251:ARG:HB2	1:A:264:ASP:HB3	1.95	0.48
1:A:617:MLY:O	1:A:620:ALA:HB3	2.14	0.48
1:A:713:SER:HB2	1:A:772:LEU:HD22	1.96	0.48
1:A:747:LEU:C	1:A:749:GLY:H	2.20	0.48
1:A:765:VAL:CG1	1:A:766:PHE:N	2.77	0.48
1:A:579:PHE:CD2	1:A:592:ILE:HD11	2.43	0.48
1:A:20:SER:HB3	1:A:23:GLU:OE1	2.13	0.48
1:A:314:TYR:CZ	1:A:362:GLY:HA2	2.48	0.48
1:A:405:ARG:HB2	1:A:414:THR:OG1	2.13	0.48
1:A:675:ILE:CG2	1:A:676:ILE:N	2.74	0.48
1:A:169:ASP:OD1	1:A:169:ASP:N	2.44	0.48
1:A:289:TYR:OH	1:A:315:VAL:O	2.27	0.48
1:A:720:PHE:CD2	1:A:744:SER:HB3	2.48	0.48
1:A:175:ILE:C	1:A:176:LEU:HD12	2.38	0.47
1:A:295:MLY:HE2	1:A:332:MET:HE1	1.95	0.47
1:A:689:GLU:O	1:A:689:GLU:HG2	2.14	0.47
1:A:309:PRO:C	1:A:311:ASP:H	2.22	0.47
1:A:602:PRO:O	1:A:603:LEU:HD12	2.14	0.47
1:A:166:MET:HE3	1:A:459:ILE:HG13	1.96	0.47
1:A:248:MLY:HE2	1:A:250:ILE:HD11	1.95	0.47
1:A:402:CYS:C	1:A:404:PRO:HD3	2.40	0.47
1:A:550:PHE:CE2	1:A:592:ILE:CG2	2.97	0.47
1:A:332:MET:O	1:A:336:SER:OG	2.27	0.47
1:A:564:ASN:HD22	1:A:582:VAL:HB	1.79	0.47
1:A:106:LEU:HD12	1:A:117:THR:HG21	1.96	0.47
1:A:496:PHE:CE2	1:A:514:ASP:HA	2.50	0.47
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.78	0.47
1:A:759:ALA:O	1:A:766:PHE:N	2.32	0.47
1:A:695:LEU:HB3	1:A:701:LEU:HD22	1.97	0.47
1:A:10:PHE:CD2	1:A:17:LEU:HD23	2.49	0.47
1:A:122:PHE:CE2	1:A:700:VAL:HA	2.50	0.47
1:A:311:ASP:CB	1:A:312:TYR:CE1	2.98	0.47
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.56	0.47
1:A:708:ARG:HA	1:A:712:PRO:HG3	1.96	0.47
1:A:476:GLU:H	1:A:476:GLU:CD	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:TRP:CD1	1:A:595:TRP:N	2.80	0.47
1:A:181:SER:O	4:A:5000:SO4:O3	2.33	0.46
1:A:188:ASN:ND2	1:A:674:CYS:SG	2.88	0.46
1:A:400:ALA:HB1	1:A:606:THR:CG2	2.45	0.46
1:A:136:ASN:HA	1:A:137:PRO:HD3	1.49	0.46
1:A:265:ILE:CG2	1:A:266:GLU:N	2.78	0.46
1:A:546:THR:CG2	1:A:547:ASP:N	2.77	0.46
1:A:714:ARG:HD3	1:A:766:PHE:CE2	2.50	0.46
1:A:715:VAL:CG1	1:A:720:PHE:HB2	2.45	0.46
1:A:361:TYR:O	1:A:364:LEU:HB2	2.16	0.46
1:A:221:GLN:HG2	1:A:221:GLN:H	1.49	0.46
1:A:335:ASP:OD1	1:A:348:MLY:NZ	2.49	0.46
1:A:374:GLN:NE2	1:A:403:TYR:CE1	2.84	0.46
1:A:406:VAL:CG1	1:A:407:GLY:N	2.77	0.46
1:A:418:THR:CG2	1:A:419:VAL:N	2.79	0.46
1:A:701:LEU:HA	1:A:701:LEU:HD12	1.55	0.46
1:A:747:LEU:C	1:A:749:GLY:N	2.71	0.46
1:A:322:VAL:HB	1:A:325:ILE:HG13	1.98	0.46
1:A:449:LEU:HA	1:A:449:LEU:HD12	1.60	0.46
1:A:30:MLY:HB3	1:A:31:PRO:HD2	1.97	0.46
1:A:724:TYR:HB3	1:A:727:LEU:CD1	2.46	0.46
1:A:739:ASP:O	1:A:743:ALA:HB2	2.15	0.46
1:A:42:HIS:O	1:A:45:GLN:O	2.33	0.46
1:A:82:PRO:HG2	1:A:85:TYR:CE2	2.50	0.46
1:A:524:GLU:HB3	1:A:528:MLY:HG2	1.96	0.46
1:A:559:LEU:HD23	1:A:560:GLY:N	2.30	0.46
1:A:667:THR:O	1:A:669:PRO:HD3	2.16	0.46
1:A:103:LEU:HD22	1:A:692:LEU:HG	1.98	0.46
1:A:326:ASP:O	1:A:330:GLU:HG2	2.16	0.46
1:A:406:VAL:CG1	1:A:407:GLY:H	2.28	0.46
1:A:783:LEU:HA	1:A:786:ILE:HB	1.96	0.46
1:A:835:PHE:O	1:A:839:MLY:N	2.49	0.46
1:A:794:CYS:O	1:A:797:PHE:HB3	2.17	0.45
1:A:488:GLN:O	1:A:491:PHE:HB3	2.17	0.45
1:A:578:HIS:O	1:A:579:PHE:HB3	2.15	0.45
1:A:139:VAL:HG12	1:A:143:TYR:HD2	1.81	0.45
1:A:664:LEU:HA	1:A:664:LEU:HD12	1.52	0.45
1:A:673:ARG:HD2	1:A:673:ARG:HA	1.79	0.45
1:A:88:ILE:HG22	1:A:90:ASP:C	2.42	0.45
1:A:186:THR:O	1:A:190:MLY:HG2	2.17	0.45
1:A:195:TYR:CE2	1:A:199:ILE:CD1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASP:O	1:A:350:ALA:N	2.46	0.45
1:A:476:GLU:OE2	1:A:598:MLY:HH13	2.16	0.45
1:A:783:LEU:N	1:A:783:LEU:CD1	2.78	0.45
1:A:464:ILE:CG2	1:A:465:ALA:N	2.79	0.45
1:A:767:PHE:CD1	1:A:771:LEU:CD2	2.99	0.45
1:A:37:SER:O	1:A:38:VAL:HG23	2.17	0.45
1:A:41:VAL:CG1	1:A:42:HIS:N	2.75	0.45
1:A:179:GLY:O	1:A:185:LYS:HE2	2.17	0.45
1:A:330:GLU:O	1:A:333:ALA:HB3	2.16	0.45
1:A:322:VAL:CG1	1:A:325:ILE:HD11	2.47	0.45
1:A:612:GLN:HG3	1:A:623:PHE:O	2.17	0.45
1:A:55:MLY:HH23	1:A:60:VAL:HG22	1.99	0.44
1:A:64:THR:HB	1:A:68:GLU:N	2.33	0.44
1:A:99:GLU:N	1:A:100:PRO:CD	2.80	0.44
1:A:568:PRO:HG2	1:A:577:ALA:O	2.16	0.44
1:A:597:GLU:O	1:A:600:MLY:N	2.50	0.44
1:A:163:TYR:O	1:A:166:MET:HB3	2.17	0.44
1:A:173:GLN:HG3	1:A:670:HIS:HD2	1.82	0.44
1:A:224:SER:O	1:A:227:PRO:HD2	2.17	0.44
1:A:508:ILE:CD1	1:A:766:PHE:CG	3.00	0.44
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.79	0.44
1:A:724:TYR:O	1:A:727:LEU:HD12	2.17	0.44
1:A:226:ASN:N	1:A:227:PRO:HD2	2.32	0.44
1:A:767:PHE:CD1	1:A:771:LEU:HD23	2.52	0.44
1:A:155:ILE:HG22	1:A:156:PHE:N	2.33	0.44
1:A:485:GLU:OE1	1:A:583:HIS:ND1	2.49	0.44
1:A:493:HIS:O	1:A:496:PHE:HB3	2.18	0.44
1:A:715:VAL:HG12	1:A:720:PHE:HB2	2.00	0.44
1:A:767:PHE:CE1	1:A:771:LEU:HD23	2.52	0.44
1:A:123:CYS:CB	1:A:158:ILE:HD13	2.48	0.44
1:A:665:ARG:C	1:A:667:THR:N	2.74	0.44
1:A:675:ILE:HG23	1:A:676:ILE:N	2.32	0.44
1:A:711:PHE:HB3	1:A:766:PHE:HB3	1.99	0.44
1:A:14:ALA:HB3	1:A:15:PRO:CD	2.46	0.44
1:A:14:ALA:N	1:A:15:PRO:HD2	2.32	0.44
1:A:174:SER:OG	1:A:669:PRO:HA	2.18	0.44
1:A:266:GLU:OE1	1:A:659:MLY:NZ	2.51	0.44
1:A:787:ILE:HG21	1:A:787:ILE:HD13	1.67	0.44
1:A:296:MLY:HH11	1:A:348:MLY:CH2	2.48	0.44
1:A:194:GLN:HE21	1:A:194:GLN:HB3	1.43	0.44
1:A:226:ASN:HB2	1:A:227:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:GLU:HA	1:A:692:LEU:HB2	2.00	0.44
1:A:728:ASN:C	1:A:730:SER:H	2.26	0.44
1:A:14:ALA:N	1:A:15:PRO:CD	2.81	0.43
1:A:48:VAL:HA	1:A:104:TYR:OH	2.17	0.43
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.67	0.43
1:A:391:GLY:HA3	1:A:616:VAL:HG23	2.00	0.43
1:A:519:LEU:N	1:A:519:LEU:CD1	2.77	0.43
1:A:568:PRO:HD3	1:A:579:PHE:HA	1.99	0.43
1:A:584:TYR:CD1	1:A:584:TYR:C	2.96	0.43
1:A:246:PHE:HB3	1:A:270:LEU:HD12	2.01	0.43
1:A:296:MLY:O	1:A:299:LEU:HB2	2.17	0.43
1:A:322:VAL:CG1	1:A:325:ILE:HG13	2.49	0.43
1:A:400:ALA:CB	1:A:606:THR:HG22	2.48	0.43
1:A:754:ASP:C	1:A:756:THR:H	2.26	0.43
1:A:829:TRP:O	1:A:832:MET:N	2.50	0.43
1:A:40:VAL:HG23	1:A:76:GLN:O	2.19	0.43
1:A:136:ASN:O	1:A:139:VAL:N	2.47	0.43
1:A:320:ILE:O	1:A:320:ILE:HG22	2.18	0.43
1:A:443:ILE:HG22	1:A:444:ARG:N	2.29	0.43
1:A:516:GLY:O	1:A:518:ASP:N	2.51	0.43
1:A:810:ARG:HG2	1:A:810:ARG:NH1	2.29	0.43
1:A:500:GLN:HB2	1:A:512:PHE:CZ	2.54	0.43
1:A:110:TYR:O	1:A:113:TRP:N	2.42	0.43
1:A:442:VAL:O	1:A:445:ILE:HB	2.19	0.43
1:A:496:PHE:HB2	1:A:515:PHE:CD2	2.53	0.43
1:A:692:LEU:O	1:A:696:ARG:HG3	2.18	0.43
1:A:56:GLU:HB2	1:A:59:MLY:CB	2.30	0.43
1:A:109:ARG:CD	1:A:117:THR:HB	2.48	0.43
1:A:193:ILE:HD11	1:A:250:ILE:CD1	2.48	0.43
1:A:747:LEU:HD23	1:A:747:LEU:C	2.43	0.43
1:A:64:THR:CG2	1:A:65:GLU:H	2.32	0.43
1:A:294:ASN:OD1	1:A:307:THR:HG21	2.19	0.43
1:A:485:GLU:HA	1:A:584:TYR:HE2	1.83	0.43
1:A:715:VAL:HG11	1:A:720:PHE:CD1	2.50	0.43
1:A:751:GLY:C	1:A:753:VAL:HG22	2.43	0.43
1:A:60:VAL:O	1:A:72:VAL:N	2.51	0.42
1:A:62:VAL:O	1:A:69:THR:HA	2.19	0.42
1:A:86:ASP:OD2	1:A:87:MLY:HH22	2.19	0.42
1:A:439:LEU:N	1:A:439:LEU:CD1	2.81	0.42
1:A:445:ILE:HG22	1:A:449:LEU:HD22	2.01	0.42
1:A:798:LEU:HA	1:A:798:LEU:HD12	1.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ASN:C	1:A:730:SER:N	2.77	0.42
1:A:787:ILE:HG23	1:A:791:GLN:HG3	2.00	0.42
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.79	0.42
1:A:123:CYS:HB2	1:A:158:ILE:HD13	2.00	0.42
1:A:169:ASP:O	1:A:170:ARG:HB2	2.19	0.42
1:A:406:VAL:O	1:A:412:ALA:HA	2.19	0.42
1:A:141:LEU:HD12	1:A:141:LEU:N	2.32	0.42
1:A:462:LEU:HD11	1:A:464:ILE:CD1	2.50	0.42
1:A:826:VAL:O	1:A:828:HIS:N	2.53	0.42
1:A:842:LEU:N	1:A:842:LEU:CD1	2.82	0.42
1:A:195:TYR:CE2	1:A:199:ILE:HD13	2.54	0.42
1:A:295:MLY:CE	1:A:332:MET:CE	2.97	0.42
1:A:135:TYR:HD2	1:A:191:ARG:CG	2.33	0.42
1:A:218:LEU:O	1:A:222:ILE:HG12	2.20	0.42
1:A:747:LEU:O	1:A:749:GLY:N	2.52	0.42
1:A:42:HIS:C	1:A:42:HIS:ND1	2.77	0.42
1:A:174:SER:HA	1:A:460:GLY:O	2.20	0.42
1:A:449:LEU:N	1:A:449:LEU:CD1	2.81	0.42
1:A:62:VAL:HG12	1:A:63:MLY:N	2.35	0.42
1:A:132:LEU:C	1:A:134:VAL:H	2.28	0.42
1:A:218:LEU:HD23	1:A:222:ILE:HG12	2.01	0.42
1:A:144:ARG:HH11	1:A:160:ASP:CG	2.28	0.42
1:A:151:ALA:HB1	1:A:152:PRO:HD2	2.01	0.42
1:A:839:MLY:N	1:A:840:PRO:HD2	2.35	0.42
1:A:136:ASN:C	1:A:138:MLY:N	2.75	0.41
1:A:274:ARG:HH22	1:A:282:GLU:CD	2.27	0.41
1:A:322:VAL:HA	1:A:323:PRO:HD3	1.87	0.41
1:A:797:PHE:CD2	1:A:798:LEU:HD12	2.55	0.41
1:A:38:VAL:HG13	1:A:39:PHE:N	2.35	0.41
1:A:136:ASN:O	1:A:138:MLY:N	2.54	0.41
1:A:502:GLU:C	1:A:504:MLY:N	2.77	0.41
1:A:361:TYR:C	1:A:363:ASN:N	2.79	0.41
1:A:724:TYR:HD1	1:A:727:LEU:CD1	2.29	0.41
1:A:81:ASN:CG	1:A:96:HIS:HB2	2.45	0.41
1:A:110:TYR:C	1:A:112:ALA:N	2.79	0.41
1:A:223:ILE:C	1:A:225:ALA:N	2.76	0.41
1:A:744:SER:O	1:A:748:LEU:HD12	2.20	0.41
1:A:11:GLY:O	1:A:14:ALA:HB3	2.20	0.41
1:A:25:ILE:HG23	1:A:29:ASN:HD22	1.85	0.41
1:A:661:MET:HE3	1:A:661:MET:HB3	1.74	0.41
1:A:193:ILE:HD11	1:A:250:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:325:ILE:HG13	2.03	0.41
1:A:330:GLU:OE1	1:A:330:GLU:HA	2.20	0.41
1:A:539:GLU:OE2	1:A:553:MLY:HD3	2.20	0.41
1:A:771:LEU:C	1:A:773:GLY:N	2.75	0.41
1:A:166:MET:HE1	1:A:254:PHE:CB	2.46	0.41
1:A:528:MLY:HB2	1:A:529:PRO:HD2	2.03	0.41
1:A:555:TYR:C	1:A:557:GLU:N	2.77	0.41
1:A:607:VAL:C	1:A:609:GLY:N	2.77	0.41
1:A:690:LEU:O	1:A:694:GLN:HG3	2.20	0.41
1:A:717:TYR:OH	1:A:760:PHE:HB3	2.21	0.41
1:A:840:PRO:C	1:A:842:LEU:N	2.79	0.41
1:A:271:GLU:OE1	1:A:274:ARG:NH1	2.53	0.41
1:A:89:GLU:HB3	1:A:153:PRO:HG3	2.03	0.40
1:A:173:GLN:HG3	1:A:670:HIS:CD2	2.55	0.40
1:A:305:ILE:HG22	1:A:312:TYR:OH	2.22	0.40
1:A:335:ASP:O	1:A:338:ILE:HB	2.20	0.40
1:A:384:ASP:HA	1:A:394:SER:OG	2.21	0.40
1:A:610:LEU:N	1:A:610:LEU:CD1	2.84	0.40
1:A:193:ILE:CD1	1:A:250:ILE:HD13	2.51	0.40
1:A:195:TYR:CD2	1:A:199:ILE:HD13	2.57	0.40
1:A:278:GLN:HE21	1:A:278:GLN:HB3	1.42	0.40
1:A:309:PRO:C	1:A:311:ASP:N	2.79	0.40
1:A:485:GLU:OE1	1:A:583:HIS:HB3	2.21	0.40
1:A:578:HIS:CD2	1:A:578:HIS:N	2.89	0.40
1:A:659:MLY:HH22	1:A:659:MLY:HD2	1.42	0.40
1:A:772:LEU:HD12	1:A:772:LEU:HA	1.83	0.40
1:A:303:LEU:O	1:A:304:LEU:HB2	2.21	0.40
1:A:400:ALA:CB	1:A:606:THR:CG2	3.00	0.40
1:A:322:VAL:HB	1:A:325:ILE:CG1	2.52	0.40
1:A:407:GLY:HA2	1:A:411:GLU:O	2.21	0.40
1:A:519:LEU:HD12	1:A:519:LEU:H	1.83	0.40
1:A:657:LEU:HD12	1:A:657:LEU:O	2.21	0.40
1:A:668:HIS:CD2	1:A:668:HIS:C	2.99	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LYS:NZ	1:A:561:LYS:NZ[4_566]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	745/843 (88%)	619 (83%)	106 (14%)	20 (3%)	4	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	712	PRO
1	A	729	ALA
1	A	757	GLN
1	A	762	HIS
1	A	11	GLY
1	A	21	GLU
1	A	517	MET
1	A	532	ILE
1	A	58	GLY
1	A	294	ASN
1	A	435	GLU
1	A	817	GLN
1	A	8	ALA
1	A	219	GLU
1	A	269	LEU
1	A	79	SER
1	A	556	ASP
1	A	840	PRO
1	A	287	ILE

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	645/674 (96%)	463 (72%)	182 (28%)	0 1

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	12	GLU
1	A	17	LEU
1	A	20	SER
1	A	22	LYS
1	A	23	GLU
1	A	25	ILE
1	A	36	SER
1	A	37	SER
1	A	38	VAL
1	A	40	VAL
1	A	41	VAL
1	A	46	SER
1	A	52	ILE
1	A	61	THR
1	A	65	GLU
1	A	69	THR
1	A	70	LEU
1	A	72	VAL
1	A	73	LYS
1	A	75	ASP
1	A	76	GLN
1	A	88	ILE
1	A	97	LEU
1	A	106	LEU
1	A	109	ARG
1	A	114	MET
1	A	117	THR
1	A	121	LEU
1	A	125	THR
1	A	126	VAL
1	A	127	ASN
1	A	136	ASN
1	A	146	LYS
1	A	149	GLN
1	A	155	ILE

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Mol	Chain	Res	Type
1	A	157	SER
1	A	158	ILE
1	A	159	SER
1	A	166	MET
1	A	167	LEU
1	A	169	ASP
1	A	170	ARG
1	A	173	GLN
1	A	175	ILE
1	A	178	THR
1	A	180	GLU
1	A	185	LYS
1	A	186	THR
1	A	187	VAL
1	A	189	THR
1	A	191	ARG
1	A	193	ILE
1	A	194	GLN
1	A	198	THR
1	A	199	ILE
1	A	202	SER
1	A	217	THR
1	A	218	LEU
1	A	221	GLN
1	A	223	ILE
1	A	229	LEU
1	A	244	SER
1	A	245	ARG
1	A	251	ARG
1	A	273	SER
1	A	274	ARG
1	A	278	GLN
1	A	282	GLU
1	A	287	ILE
1	A	290	GLN
1	A	291	ILE
1	A	294	ASN
1	A	298	GLU
1	A	300	ILE
1	A	302	MET
1	A	303	LEU
1	A	305	ILE

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Mol	Chain	Res	Type
1	A	315	VAL
1	A	325	ILE
1	A	331	LEU
1	A	332	MET
1	A	336	SER
1	A	351	ILE
1	A	354	LEU
1	A	359	MET
1	A	364	LEU
1	A	365	LYS
1	A	372	GLU
1	A	376	GLU
1	A	381	GLU
1	A	389	LEU
1	A	392	LEU
1	A	394	SER
1	A	399	LYS
1	A	401	LEU
1	A	405	ARG
1	A	410	ASN
1	A	411	GLU
1	A	439	LEU
1	A	448	GLN
1	A	449	LEU
1	A	452	LYS
1	A	453	GLN
1	A	455	ARG
1	A	456	GLN
1	A	457	TYR
1	A	462	LEU
1	A	471	ASP
1	A	480	ILE
1	A	487	LEU
1	A	495	MET
1	A	498	LEU
1	A	499	GLU
1	A	506	GLU
1	A	513	ILE
1	A	524	GLU
1	A	530	MET
1	A	532	ILE
1	A	534	SER

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Mol	Chain	Res	Type
1	A	537	GLU
1	A	549	SER
1	A	561	LYS
1	A	562	SER
1	A	580	SER
1	A	593	SER
1	A	596	LEU
1	A	597	GLU
1	A	604	ASN
1	A	608	ILE
1	A	610	LEU
1	A	615	SER
1	A	621	LEU
1	A	625	THR
1	A	664	LEU
1	A	666	SER
1	A	673	ARG
1	A	675	ILE
1	A	676	ILE
1	A	686	MET
1	A	689	GLU
1	A	690	LEU
1	A	693	HIS
1	A	698	ASN
1	A	700	VAL
1	A	701	LEU
1	A	702	GLU
1	A	704	ILE
1	A	705	ARG
1	A	707	CYS
1	A	708	ARG
1	A	713	SER
1	A	714	ARG
1	A	716	LEU
1	A	722	GLN
1	A	723	ARG
1	A	727	LEU
1	A	728	ASN
1	A	744	SER
1	A	745	GLU
1	A	748	LEU
1	A	752	ASP

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Mol	Chain	Res	Type
1	A	753	VAL
1	A	754	ASP
1	A	762	HIS
1	A	772	LEU
1	A	774	LEU
1	A	785	GLU
1	A	787	ILE
1	A	793	ARG
1	A	798	LEU
1	A	799	MET
1	A	802	GLU
1	A	810	ARG
1	A	816	ILE
1	A	819	ASN
1	A	822	SER
1	A	832	MET
1	A	834	LEU
1	A	838	ILE
1	A	842	LEU
1	A	843	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	76	GLN
1	A	127	ASN
1	A	149	GLN
1	A	164	GLN
1	A	188	ASN
1	A	194	GLN
1	A	234	ASN
1	A	253	HIS
1	A	290	GLN
1	A	360	HIS
1	A	368	GLN
1	A	424	ASN
1	A	447	GLN
1	A	453	GLN
1	A	481	ASN
1	A	484	ASN
1	A	488	GLN

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Mol	Chain	Res	Type
1	A	563	ASN
1	A	564	ASN
1	A	578	HIS
1	A	591	ASN
1	A	656	ASN
1	A	670	HIS
1	A	698	ASN
1	A	762	HIS
1	A	825	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	107	1	9,10,11	0.49	0	6,11,13	0.32	0
1	MLY	A	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	A	617	1	9,10,11	0.89	0	6,11,13	0.35	0
1	MLY	A	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.59	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	A	553	1	9,10,11	0.63	0	6,11,13	0.54	0
1	MLY	A	598	1	9,10,11	0.81	0	6,11,13	0.42	0
1	MLY	A	782	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	A	827	1	9,10,11	0.67	0	6,11,13	0.47	0
1	MLY	A	272	1	9,10,11	0.90	1 (11%)	6,11,13	0.56	0
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	A	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	A	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	768	1	9,10,11	0.78	0	6,11,13	0.41	0
1	MLY	A	348	1	9,10,11	0.78	0	6,11,13	0.47	0
1	MLY	A	248	1	9,10,11	0.80	0	6,11,13	0.64	0
1	MLY	A	833	1	9,10,11	1.13	2 (22%)	6,11,13	0.30	0
1	MLY	A	839	1	9,10,11	0.67	0	6,11,13	0.79	0
1	MLY	A	385	1	9,10,11	0.91	1 (11%)	6,11,13	0.45	0
1	MLY	A	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.42	0
1	MLY	A	837	1	9,10,11	0.59	0	6,11,13	0.55	0
1	MLY	A	681	1	9,10,11	0.58	0	6,11,13	0.45	0
1	MLY	A	130	1	9,10,11	0.77	0	6,11,13	0.72	0
1	MLY	A	84	1	9,10,11	0.51	0	6,11,13	0.81	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	A	35	1	9,10,11	0.75	0	6,11,13	0.38	0
1	MLY	A	63	1	9,10,11	0.88	0	6,11,13	0.44	0
1	MLY	A	505	1	9,10,11	0.82	0	6,11,13	0.35	0
1	MLY	A	295	1	9,10,11	0.77	0	6,11,13	0.36	0
1	MLY	A	431	1	9,10,11	0.51	0	6,11,13	0.46	0
1	MLY	A	764	1	9,10,11	0.83	0	6,11,13	0.36	0
1	MLY	A	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	A	504	1	9,10,11	0.86	0	6,11,13	0.23	0
1	MLY	A	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.74	0
1	MLY	A	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.82	0
1	MLY	A	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	A	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	A	19	1	9,10,11	1.08	1 (11%)	6,11,13	0.58	0
1	MLY	A	367	1	9,10,11	0.59	0	6,11,13	0.37	0
1	MLY	A	486	1	9,10,11	0.66	0	6,11,13	0.40	0
1	MLY	A	415	1	9,10,11	0.74	0	6,11,13	0.19	0
1	MLY	A	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.49	0
1	MLY	A	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	A	553	1	-	4/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	MLY	CB-CA	-3.19	1.48	1.53
1	A	19	MLY	CB-CA	-2.81	1.49	1.53
1	A	87	MLY	CB-CA	-2.75	1.49	1.53
1	A	436	MLY	CB-CA	-2.59	1.49	1.53
1	A	49	MLY	CB-CA	-2.51	1.49	1.53
1	A	272	MLY	CB-CA	-2.40	1.49	1.53
1	A	236	MLY	CA-N	-2.27	1.41	1.48
1	A	190	MLY	CB-CA	-2.20	1.50	1.53
1	A	385	MLY	CB-CA	-2.10	1.50	1.53
1	A	833	MLY	CA-N	-2.09	1.42	1.48
1	A	190	MLY	CA-N	-2.07	1.42	1.48
1	A	659	MLY	CA-N	-2.04	1.42	1.48
1	A	833	MLY	CB-CA	-2.02	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	MLY	C-CA-CB-CG
1	A	49	MLY	N-CA-CB-CG
1	A	49	MLY	C-CA-CB-CG
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG
1	A	84	MLY	C-CA-CB-CG
1	A	130	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	248	MLY	N-CA-CB-CG
1	A	248	MLY	C-CA-CB-CG
1	A	348	MLY	N-CA-CB-CG
1	A	348	MLY	C-CA-CB-CG
1	A	436	MLY	C-CA-CB-CG
1	A	486	MLY	C-CA-CB-CG
1	A	505	MLY	N-CA-CB-CG
1	A	505	MLY	C-CA-CB-CG
1	A	528	MLY	C-CA-CB-CG
1	A	551	MLY	C-CA-CB-CG
1	A	553	MLY	C-CA-CB-CG
1	A	598	MLY	N-CA-CB-CG
1	A	598	MLY	C-CA-CB-CG
1	A	613	MLY	N-CA-CB-CG
1	A	613	MLY	C-CA-CB-CG
1	A	681	MLY	C-CA-CB-CG
1	A	782	MLY	C-CA-CB-CG
1	A	782	MLY	O-C-CA-CB
1	A	84	MLY	CD-CE-NZ-CH1
1	A	248	MLY	CD-CE-NZ-CH1
1	A	296	MLY	CD-CE-NZ-CH1
1	A	296	MLY	CD-CE-NZ-CH2
1	A	367	MLY	CD-CE-NZ-CH2
1	A	431	MLY	CD-CE-NZ-CH2
1	A	600	MLY	CD-CE-NZ-CH2
1	A	764	MLY	CD-CE-NZ-CH1
1	A	764	MLY	CD-CE-NZ-CH2
1	A	782	MLY	CD-CE-NZ-CH2
1	A	833	MLY	CD-CE-NZ-CH1
1	A	833	MLY	CD-CE-NZ-CH2
1	A	837	MLY	CD-CE-NZ-CH2
1	A	295	MLY	CG-CD-CE-NZ
1	A	659	MLY	CG-CD-CE-NZ
1	A	35	MLY	CG-CD-CE-NZ
1	A	55	MLY	CD-CE-NZ-CH2
1	A	59	MLY	CD-CE-NZ-CH1
1	A	59	MLY	CD-CE-NZ-CH2
1	A	63	MLY	CD-CE-NZ-CH1
1	A	84	MLY	CD-CE-NZ-CH2
1	A	130	MLY	CD-CE-NZ-CH1
1	A	130	MLY	CD-CE-NZ-CH2
1	A	138	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	A	138	MLY	CD-CE-NZ-CH2
1	A	190	MLY	CD-CE-NZ-CH1
1	A	190	MLY	CD-CE-NZ-CH2
1	A	248	MLY	CD-CE-NZ-CH2
1	A	272	MLY	CD-CE-NZ-CH1
1	A	348	MLY	CD-CE-NZ-CH1
1	A	348	MLY	CD-CE-NZ-CH2
1	A	353	MLY	CD-CE-NZ-CH1
1	A	353	MLY	CD-CE-NZ-CH2
1	A	367	MLY	CD-CE-NZ-CH1
1	A	385	MLY	CD-CE-NZ-CH1
1	A	385	MLY	CD-CE-NZ-CH2
1	A	431	MLY	CD-CE-NZ-CH1
1	A	505	MLY	CD-CE-NZ-CH1
1	A	505	MLY	CD-CE-NZ-CH2
1	A	528	MLY	CD-CE-NZ-CH1
1	A	528	MLY	CD-CE-NZ-CH2
1	A	553	MLY	CD-CE-NZ-CH2
1	A	600	MLY	CD-CE-NZ-CH1
1	A	659	MLY	CD-CE-NZ-CH2
1	A	768	MLY	CD-CE-NZ-CH1
1	A	782	MLY	CD-CE-NZ-CH1
1	A	837	MLY	CD-CE-NZ-CH1
1	A	839	MLY	CD-CE-NZ-CH2
1	A	87	MLY	CG-CD-CE-NZ
1	A	782	MLY	CG-CD-CE-NZ
1	A	138	MLY	CG-CD-CE-NZ
1	A	130	MLY	CG-CD-CE-NZ
1	A	272	MLY	CD-CE-NZ-CH2
1	A	369	MLY	CD-CE-NZ-CH2
1	A	504	MLY	CD-CE-NZ-CH1
1	A	504	MLY	CD-CE-NZ-CH2
1	A	768	MLY	CD-CE-NZ-CH2
1	A	84	MLY	CG-CD-CE-NZ
1	A	504	MLY	CG-CD-CE-NZ
1	A	681	MLY	CG-CD-CE-NZ
1	A	598	MLY	CG-CD-CE-NZ
1	A	63	MLY	CD-CE-NZ-CH2
1	A	87	MLY	CD-CE-NZ-CH1
1	A	55	MLY	CD-CE-NZ-CH1
1	A	415	MLY	CD-CE-NZ-CH1
1	A	415	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	A	553	MLY	CD-CE-NZ-CH1
1	A	295	MLY	CA-CB-CG-CD
1	A	551	MLY	CG-CD-CE-NZ
1	A	19	MLY	CD-CE-NZ-CH2
1	A	504	MLY	CA-CB-CG-CD
1	A	768	MLY	CA-CB-CG-CD
1	A	49	MLY	CE-CD-CG-CB
1	A	505	MLY	CE-CD-CG-CB
1	A	272	MLY	CE-CD-CG-CB
1	A	30	MLY	CE-CD-CG-CB
1	A	296	MLY	CE-CD-CG-CB
1	A	107	MLY	CD-CE-NZ-CH1
1	A	190	MLY	CE-CD-CG-CB
1	A	353	MLY	CE-CD-CG-CB
1	A	681	MLY	CE-CD-CG-CB
1	A	190	MLY	CG-CD-CE-NZ
1	A	768	MLY	CE-CD-CG-CB
1	A	369	MLY	CE-CD-CG-CB
1	A	839	MLY	CD-CE-NZ-CH1
1	A	782	MLY	CE-CD-CG-CB
1	A	415	MLY	CA-CB-CG-CD
1	A	107	MLY	CD-CE-NZ-CH2
1	A	236	MLY	CD-CE-NZ-CH1
1	A	659	MLY	CD-CE-NZ-CH1
1	A	55	MLY	CG-CD-CE-NZ
1	A	833	MLY	CE-CD-CG-CB
1	A	436	MLY	CA-CB-CG-CD
1	A	617	MLY	CE-CD-CG-CB
1	A	551	MLY	CE-CD-CG-CB
1	A	59	MLY	CE-CD-CG-CB
1	A	553	MLY	CE-CD-CG-CB
1	A	55	MLY	CE-CD-CG-CB
1	A	528	MLY	CG-CD-CE-NZ
1	A	248	MLY	CG-CD-CE-NZ
1	A	431	MLY	CE-CD-CG-CB
1	A	248	MLY	CE-CD-CG-CB
1	A	35	MLY	CE-CD-CG-CB
1	A	431	MLY	CA-CB-CG-CD
1	A	837	MLY	CA-CB-CG-CD
1	A	436	MLY	CE-CD-CG-CB
1	A	598	MLY	CE-CD-CG-CB
1	A	600	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	A	486	MLY	CE-CD-CG-CB
1	A	236	MLY	CA-CB-CG-CD
1	A	833	MLY	CA-CB-CG-CD
1	A	839	MLY	CE-CD-CG-CB
1	A	138	MLY	CA-CB-CG-CD
1	A	296	MLY	CA-CB-CG-CD
1	A	63	MLY	C-CA-CB-CG
1	A	353	MLY	C-CA-CB-CG
1	A	827	MLY	C-CA-CB-CG
1	A	833	MLY	C-CA-CB-CG
1	A	35	MLY	N-CA-CB-CG
1	A	63	MLY	N-CA-CB-CG
1	A	130	MLY	N-CA-CB-CG
1	A	436	MLY	N-CA-CB-CG
1	A	681	MLY	N-CA-CB-CG
1	A	833	MLY	N-CA-CB-CG
1	A	837	MLY	N-CA-CB-CG
1	A	19	MLY	CA-CB-CG-CD
1	A	837	MLY	CE-CD-CG-CB
1	A	19	MLY	CE-CD-CG-CB
1	A	613	MLY	CE-CD-CG-CB
1	A	236	MLY	CD-CE-NZ-CH2
1	A	598	MLY	CD-CE-NZ-CH2
1	A	30	MLY	C-CA-CB-CG
1	A	617	MLY	C-CA-CB-CG
1	A	837	MLY	C-CA-CB-CG
1	A	348	MLY	CE-CD-CG-CB
1	A	30	MLY	CA-CB-CG-CD

There are no ring outliers.

28 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	3	0
1	A	617	MLY	1	0
1	A	659	MLY	2	0
1	A	553	MLY	2	0
1	A	598	MLY	1	0
1	A	782	MLY	1	0
1	A	600	MLY	1	0
1	A	272	MLY	1	0
1	A	296	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	30	MLY	1	0
1	A	190	MLY	2	0
1	A	348	MLY	5	0
1	A	248	MLY	2	0
1	A	839	MLY	4	0
1	A	87	MLY	2	0
1	A	837	MLY	1	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	35	MLY	1	0
1	A	63	MLY	3	0
1	A	295	MLY	6	0
1	A	764	MLY	1	0
1	A	504	MLY	1	0
1	A	49	MLY	3	0
1	A	138	MLY	2	0
1	A	59	MLY	3	0
1	A	486	MLY	3	0
1	A	415	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	SO4	A	5000	-	4,4,4	0.35	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5000	SO4	2	0

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

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.