



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 AM GMT

PDB ID : 2MYS  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

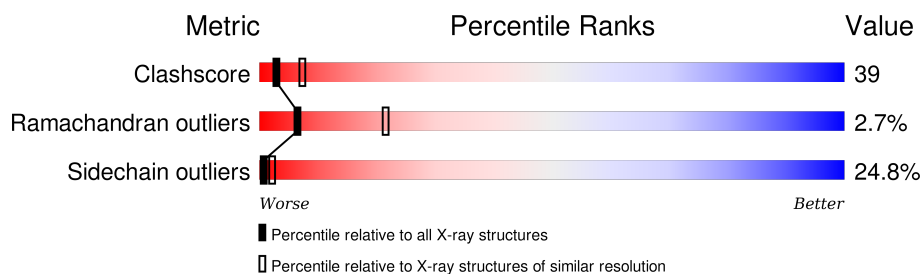
# 1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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
5	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



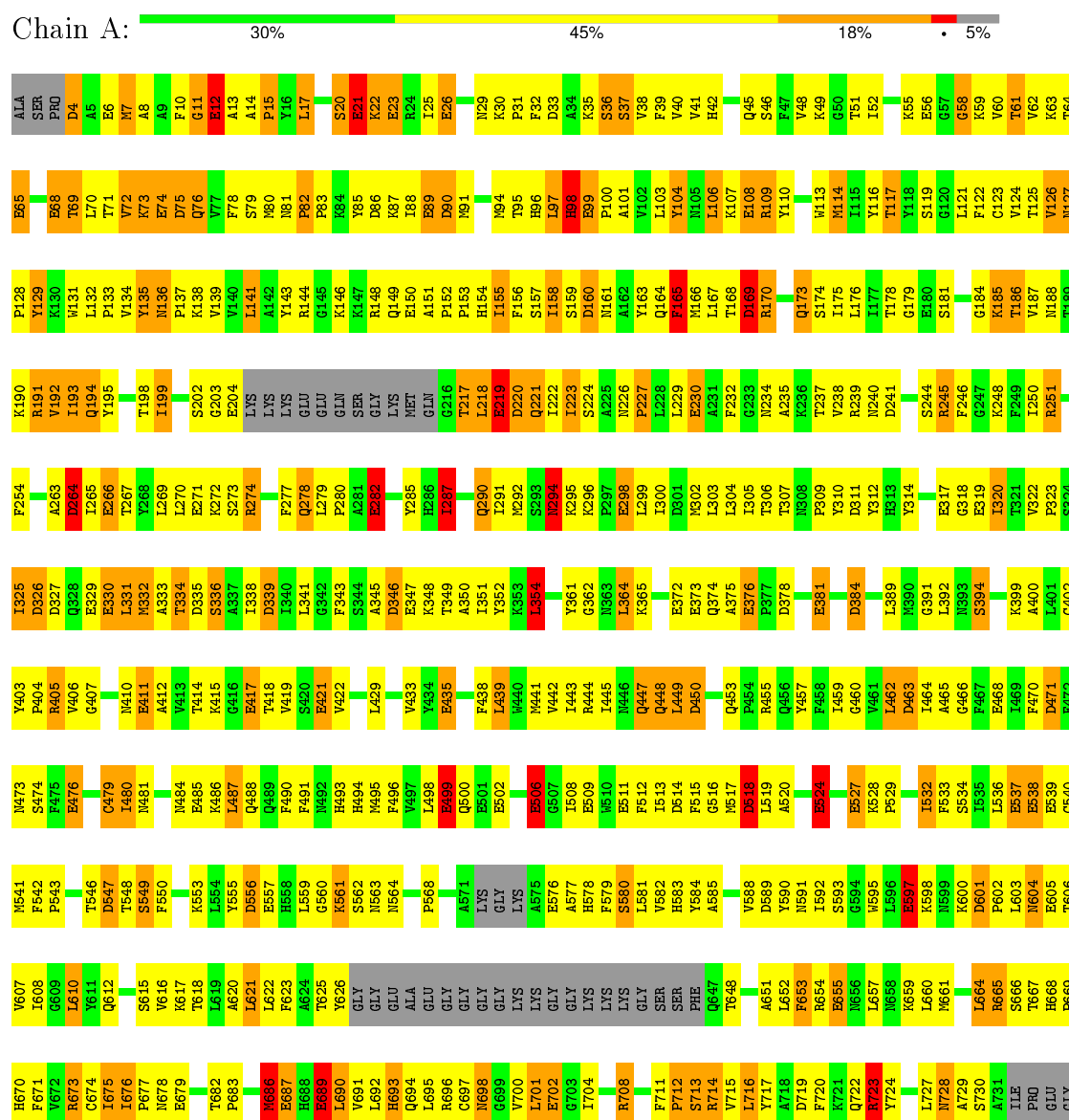
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

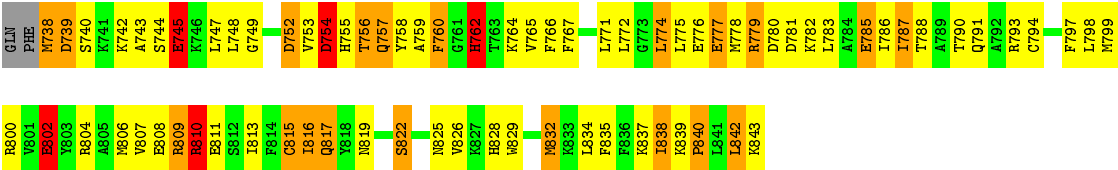
### 3 Residue-property plots [i](#)

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

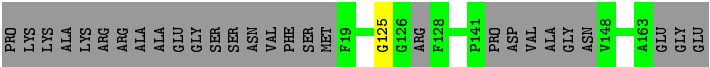
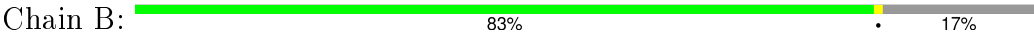
Note EDS was not executed.

#### • Molecule 1: MYOSIN

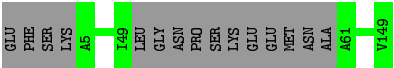




• Molecule 2: MYOSIN



• Molecule 3: MYOSIN





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.40 Å   124.20 Å   274.90 Å 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 <sup>2</sup> )	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: MG, MLY, SO4

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	1.25	58/6156 (0.9%)	1.51	91/8350 (1.1%)

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 (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	GLU	CD-OE1	8.78	1.35	1.25
1	A	576	GLU	CD-OE1	8.71	1.35	1.25
1	A	204	GLU	CD-OE2	8.33	1.34	1.25
1	A	745	GLU	CD-OE2	8.26	1.34	1.25
1	A	411	GLU	CD-OE1	8.20	1.34	1.25
1	A	381	GLU	CD-OE1	7.93	1.34	1.25
1	A	108	GLU	CD-OE1	7.88	1.34	1.25
1	A	689	GLU	CD-OE2	7.43	1.33	1.25
1	A	347	GLU	CD-OE1	7.18	1.33	1.25
1	A	23	GLU	CD-OE1	7.15	1.33	1.25
1	A	511	GLU	CD-OE1	7.00	1.33	1.25
1	A	524	GLU	CD-OE1	7.00	1.33	1.25
1	A	26	GLU	CD-OE1	6.98	1.33	1.25
1	A	68	GLU	CD-OE2	6.92	1.33	1.25
1	A	376	GLU	CD-OE1	6.92	1.33	1.25
1	A	330	GLU	CD-OE1	6.88	1.33	1.25
1	A	811	GLU	CD-OE1	6.75	1.33	1.25
1	A	538	GLU	CD-OE1	6.64	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	655	GLU	CD-OE1	6.63	1.32	1.25
1	A	319	GLU	CD-OE1	6.56	1.32	1.25
1	A	538	GLU	CD-OE2	-6.52	1.18	1.25
1	A	266	GLU	CD-OE2	6.51	1.32	1.25
1	A	89	GLU	CD-OE1	6.45	1.32	1.25
1	A	808	GLU	CD-OE1	6.33	1.32	1.25
1	A	99	GLU	CD-OE2	6.31	1.32	1.25
1	A	502	GLU	CD-OE2	6.30	1.32	1.25
1	A	6	GLU	CD-OE1	6.26	1.32	1.25
1	A	605	GLU	CD-OE1	6.21	1.32	1.25
1	A	802	GLU	CD-OE1	6.20	1.32	1.25
1	A	509	GLU	CD-OE1	6.07	1.32	1.25
1	A	329	GLU	CD-OE1	5.94	1.32	1.25
1	A	417	GLU	CD-OE1	5.86	1.32	1.25
1	A	540	CYS	CB-SG	-5.82	1.72	1.81
1	A	476	GLU	CD-OE2	-5.81	1.19	1.25
1	A	230	GLU	CD-OE2	5.75	1.31	1.25
1	A	468	GLU	CD-OE1	5.68	1.31	1.25
1	A	785	GLU	CD-OE2	5.67	1.31	1.25
1	A	527	GLU	CD-OE1	5.67	1.31	1.25
1	A	597	GLU	CD-OE1	5.66	1.31	1.25
1	A	74	GLU	CD-OE2	5.62	1.31	1.25
1	A	499	GLU	CD-OE2	5.61	1.31	1.25
1	A	219	GLU	CD-OE1	5.59	1.31	1.25
1	A	687	GLU	CD-OE1	5.58	1.31	1.25
1	A	777	GLU	CD-OE2	5.54	1.31	1.25
1	A	421	GLU	CD-OE2	5.49	1.31	1.25
1	A	373	GLU	CD-OE1	5.49	1.31	1.25
1	A	479	CYS	CB-SG	-5.47	1.73	1.81
1	A	298	GLU	CD-OE2	5.39	1.31	1.25
1	A	65	GLU	CD-OE1	5.30	1.31	1.25
1	A	506	GLU	CD-OE2	5.28	1.31	1.25
1	A	679	GLU	CD-OE2	5.19	1.31	1.25
1	A	21	GLU	CD-OE2	5.13	1.31	1.25
1	A	527	GLU	CD-OE2	-5.11	1.20	1.25
1	A	702	GLU	CD-OE2	5.11	1.31	1.25
1	A	12	GLU	CD-OE2	5.09	1.31	1.25
1	A	282	GLU	CD-OE1	5.08	1.31	1.25
1	A	150	GLU	CD-OE1	5.04	1.31	1.25
1	A	697	CYS	CB-SG	5.03	1.90	1.82

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	A	98	HIS	CB-CA-C	-11.56	87.28	110.40
1	A	327	ASP	CB-CG-OD1	-9.97	109.33	118.30
1	A	241	ASP	CB-CG-OD1	-9.78	109.50	118.30
1	A	264	ASP	CB-CG-OD2	-9.48	109.77	118.30
1	A	378	ASP	CB-CG-OD2	8.99	126.39	118.30
1	A	352	TYR	CB-CG-CD1	8.94	126.36	121.00
1	A	601	ASP	CB-CG-OD1	-8.51	110.64	118.30
1	A	352	TYR	CB-CG-CD2	-8.26	116.04	121.00
1	A	33	ASP	CB-CG-OD1	-8.23	110.89	118.30
1	A	339	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	A	654	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	653	PHE	CB-CG-CD1	-7.55	115.52	120.80
1	A	518	ASP	CB-CG-OD1	-7.36	111.67	118.30
1	A	346	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	104	TYR	CB-CG-CD2	7.15	125.29	121.00
1	A	148	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	264	ASP	N-CA-CB	-6.97	98.06	110.60
1	A	75	ASP	N-CA-CB	6.85	122.93	110.60
1	A	450	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	781	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	A	555	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	756	THR	N-CA-CB	-6.63	97.70	110.30
1	A	739	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	A	343	PHE	CB-CG-CD1	6.54	125.38	120.80
1	A	75	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	332	MET	CG-SD-CE	-6.52	89.77	100.20
1	A	334	THR	CA-CB-CG2	-6.50	103.30	112.40
1	A	141	LEU	CB-CA-C	-6.48	97.88	110.20
1	A	169	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	A	589	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	A	341	LEU	CB-CA-C	6.31	122.18	110.20
1	A	129	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	A	327	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	760	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	590	TYR	CB-CG-CD2	6.16	124.70	121.00
1	A	698	ASN	CB-CA-C	-6.14	98.12	110.40
1	A	463	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	682	THR	CA-CB-CG2	-6.09	103.88	112.40
1	A	104	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	754	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	810	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	447	GLN	N-CA-CB	6.03	121.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	378	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	450	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	192	VAL	CA-CB-CG1	-5.98	101.93	110.90
1	A	780	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	339	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	346	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	752	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	556	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	779	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	471	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	809	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	815	CYS	CA-CB-SG	-5.78	103.60	114.00
1	A	780	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	A	165	PHE	N-CA-CB	-5.75	100.25	110.60
1	A	4	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	781	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	352	TYR	N-CA-CB	5.64	120.76	110.60
1	A	686	MET	N-CA-CB	-5.57	100.57	110.60
1	A	693	HIS	CA-CB-CG	-5.57	104.13	113.60
1	A	752	ASP	CB-CA-C	5.52	121.44	110.40
1	A	306	THR	CA-CB-CG2	-5.50	104.70	112.40
1	A	320	ILE	CB-CA-C	-5.48	100.63	111.60
1	A	220	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	220	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	723	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	326	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	33	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	241	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	547	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	686	MET	CG-SD-CE	-5.35	91.64	100.20
1	A	800	ARG	NH1-CZ-NH2	5.33	125.26	119.40
1	A	384	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	601	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	660	LEU	CB-CG-CD2	5.30	120.01	111.00
1	A	125	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	343	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	A	354	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	760	PHE	CB-CG-CD1	5.22	124.45	120.80
1	A	4	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	170	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	346	ASP	N-CA-CB	-5.17	101.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	555	TYR	CB-CG-CD1	5.12	124.08	121.00
1	A	160	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	90	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	621	LEU	CA-CB-CG	-5.07	103.63	115.30
1	A	82	PRO	N-CA-CB	5.03	109.33	103.30
1	A	235	ALA	N-CA-CB	-5.00	103.09	110.10

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	6500	524	1
2	B	138	0	0	1	0
3	C	134	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	2	0
All	All	6788	0	6500	524	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 39.

All (524) 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:546:THR:HG22	1:A:548:THR:H	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:107:MLY:HB3	1:A:686:MET:HE2	1.59	0.85
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
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:174:SER:CB	1:A:667:THR:HG21	2.13	0.78
1:A:51:THR:O	1:A:62:VAL:HG13	1.84	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: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:310:TYR:CE2	1:A:320:ILE:HD11	2.22	0.74
1:A:481:ASN:N	1:A:481:ASN:HD22	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:487:LEU:O	1:A:490:PHE:HB3	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:21:GLU:O	1:A:25:ILE:HG13	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:290:GLN:C	1:A:331:LEU:HD12	2.09	0.73
1:A:536:LEU:HD13	1:A:550:PHE:CZ	2.24	0.72
1:A:295:MLY:HG3	1:A:332:MET:CE	2.19	0.72
1:A:131:TRP:C	1:A:132:LEU:HD12	2.09	0.72
1:A:519:LEU:HD12	1:A:519:LEU:N	2.04	0.72
1:A:190:MLY:HE3	1:A:230:GLU:OE2	1.89	0.72
1:A:546:THR:HG22	1:A:548:THR:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD12	1:A:176:LEU:N	2.05	0.72
1:A:36:SER:O	1:A:52:ILE:HG12	1.90	0.72
1:A:166:MET:HE1	1:A:254:PHE:HB2	1.71	0.71
1:A:245:ARG:HD3	1:A:271:GLU:OE1	1.90	0.71
1:A:486:MLY:HH22	1:A:527:GLU:OE2	1.90	0.71
1:A:14:ALA:HB3	1:A:15:PRO:HD3	1.72	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
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:HH11	1:A:810:ARG:HG2	1.57	0.69
1:A:578:HIS:HB2	1:A:592:ILE:HD12	1.74	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:782:MLY:C	1:A:783:LEU:HD12	2.22	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: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:550:PHE:HE2	1:A:592:ILE:HG23	1.59	0.67
1:A:480:ILE:HG22	1:A:481:ASN:ND2	2.09	0.67
1:A:52:ILE:N	1:A:52:ILE:HD13	2.09	0.67
1:A:184:GLY:N	5:A:5000:SO4:O1	2.28	0.67
1:A:648:THR:HG23	1:A:651:ALA:H	1.59	0.67
1:A:290:GLN:O	1:A:331:LEU:HD12	1.95	0.67
1:A:166:MET:HE3	1:A:254:PHE:CD2	2.30	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:322:VAL:HB	1:A:325:ILE:CD1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:O	1:A:165:PHE:HB2	1.96	0.66
1:A:724:TYR:HD1	1:A:727:LEU:HD11	1.61	0.65
1:A:107:MLY:HB3	1:A:686:MET:CE	2.26	0.65
1:A:480:ILE:HG22	1:A:481:ASN:N	2.11	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: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: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
1:A:296:MLY:HH11	1:A:348:MLY:HH21	1.78	0.65
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:94:MET:HE1	1:A:101:ALA:HB1	1.79	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:166:MET:HE3	1:A:254:PHE:HD2	1.62	0.64
1:A:374:GLN:HG3	1:A:375:ALA:H	1.60	0.64
1:A:783:LEU:N	1:A:783:LEU:HD12	2.13	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:771:LEU:O	1:A:774:LEU:N	2.32	0.63
1:A:251:ARG:HB2	1:A:264:ASP:CB	2.29	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:91:MET:HE3	1:A:119:SER:HB2	1.81	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:806:MET:O	1:A:809:ARG:HB2	1.98	0.62
1:A:141:LEU:HD12	1:A:141:LEU:H	1.64	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:274:ARG:HB2	1:A:285:TYR:CE2	2.34	0.61
1:A:292:MET:HE3	1:A:309:PRO:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:755:HIS:HA	1:A:758:TYR:HE1	1.64	0.60
1:A:81:ASN:OD1	1:A:96:HIS:HB2	2.00	0.60
1:A:156:PHE:CD1	1:A:195:TYR:CD1	2.90	0.60
1:A:557:GLU:O	1:A:557:GLU:HG3	2.00	0.60
1:A:124:VAL:CG1	1:A:675:ILE:HD13	2.31	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
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:665:ARG:C	1:A:667:THR:H	2.05	0.60
1:A:124:VAL:HG13	1:A:675:ILE:HD13	1.84	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:95:THR:HG23	1:A:96:HIS:ND1	2.17	0.60
1:A:648:THR:HG23	1:A:651:ALA:HB2	1.83	0.59
1:A:7:MET:HE3	1:A:14:ALA:HB1	1.84	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: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:579:PHE:CE1	1:A:581:LEU:HD13	2.38	0.58
1:A:124:VAL:HG13	1:A:675:ILE:CD1	2.33	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: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:464:ILE:HG22	1:A:465:ALA:N	2.18	0.58
1:A:254:PHE:CE2	1:A:459:ILE:HD12	2.39	0.58
1:A:141:LEU:O	1:A:144:ARG:HB3	2.03	0.58
1:A:538:GLU:O	1:A:541:MET:HB2	2.04	0.58
1:A:135:TYR:CD1	1:A:135:TYR:N	2.70	0.58
1:A:676:ILE:O	1:A:676:ILE:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:GLN:C	1:A:667:THR:HG23	2.25	0.57
1:A:418:THR:HG22	1:A:419:VAL:H	1.69	0.57
1:A:794:CYS:O	1:A:798:LEU:N	2.37	0.57
1:A:677:PRO:HB2	1:A:678:ASN:ND2	2.20	0.57
1:A:265:ILE:HG22	1:A:266:GLU:N	2.18	0.56
1:A:508:ILE:HD11	1:A:766:PHE:CE1	2.39	0.56
1:A:203:GLY:HA3	1:A:217:THR:HG21	1.87	0.56
1:A:747:LEU:HD23	1:A:747:LEU:O	2.05	0.56
1:A:82:PRO:HD2	1:A:85:TYR:CD2	2.40	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:549:SER:OG	1:A:550:PHE:N	2.36	0.56
1:A:406:VAL:HG12	1:A:407:GLY:H	1.71	0.56
1:A:22:LYS:O	1:A:26:GLU:HG3	2.06	0.55
1:A:295:MLY:HG3	1:A:332:MET:HE1	1.88	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:546:THR:HB	1:A:549:SER:H	1.71	0.55
1:A:22:LYS:HA	1:A:25:ILE:HB	1.87	0.55
1:A:7:MET:HE3	1:A:14:ALA:CB	2.36	0.55
1:A:305:ILE:HG22	1:A:312:TYR:CE2	2.42	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:546:THR:HG21	1:A:548:THR:HB	1.88	0.54
1:A:470:PHE:O	1:A:473:ASN:ND2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:ILE:O	1:A:817:GLN:N	2.30	0.54
1:A:292:MET:HE1	1:A:309:PRO:CD	2.37	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: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:38:VAL:CB	1:A:52:ILE:HD11	2.38	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: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:277:PHE:CG	1:A:278:GLN:N	2.76	0.53
1:A:154:HIS:CE1	1:A:156:PHE:HD2	2.27	0.53
1:A:135:TYR:HD2	1:A:191:ARG:HD3	1.73	0.53
1:A:727:LEU:HD21	1:A:778:MET:HB2	1.90	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:765:VAL:HG12	1:A:766:PHE:N	2.22	0.53
1:A:661:MET:O	1:A:665:ARG:HG3	2.09	0.53
1:A:404:PRO:HG3	1:A:417:GLU:HG3	1.91	0.53
1:A:292:MET:CE	1:A:309:PRO:HA	2.39	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:32:PHE:CD1	1:A:83:PRO:HD3	2.44	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:295:MLY:HE2	1:A:332:MET:HE1	1.91	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:128:PRO:O	1:A:129:TYR:HB2	2.09	0.52
1:A:35:MLY:HH22	1:A:777:GLU:CD	2.30	0.52
1:A:648:THR:HG23	1:A:651:ALA:N	2.25	0.52
1:A:63:MLY:HG3	1:A:64:THR:H	1.75	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:13:ALA:C	1:A:15:PRO:HD2	2.31	0.51
1:A:41:VAL:HG13	1:A:42:HIS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:GLN:HG3	1:A:318:GLY:H	1.75	0.51
1:A:135:TYR:HD2	1:A:191:ARG:CD	2.23	0.51
1:A:724:TYR:HE1	1:A:775:LEU:HB3	1.68	0.51
1:A:687:GLU:O	1:A:691:VAL:HG23	2.11	0.51
1:A:195:TYR:O	1:A:199:ILE:HG23	2.11	0.51
1:A:38:VAL:CG1	1:A:39:PHE:N	2.74	0.51
1:A:592:ILE:O	1:A:592:ILE:HG22	2.10	0.51
1:A:217:THR:HG21	1:A:219:GLU:OE1	2.11	0.51
1:A:295:MLY:HG3	1:A:332:MET:HE2	1.92	0.51
1:A:783:LEU:O	1:A:787:ILE:N	2.28	0.51
1:A:291:ILE:HA	1:A:331:LEU:CD1	2.39	0.51
1:A:248:MLY:N	1:A:463:ASP:O	2.44	0.51
1:A:559:LEU:C	1:A:559:LEU:HD23	2.31	0.51
1:A:267:THR:HG21	1:A:438:PHE:HE2	1.76	0.51
1:A:675:ILE:CG2	1:A:676:ILE:N	2.74	0.51
1:A:109:ARG:HD3	1:A:117:THR:HB	1.92	0.51
1:A:311:ASP:HB2	1:A:312:TYR:CE1	2.46	0.50
1:A:418:THR:CB	1:A:421:GLU:HG3	2.37	0.50
1:A:418:THR:O	1:A:422:VAL:HG23	2.11	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: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:51:THR:C	1:A:62:VAL:HG13	2.32	0.49
1:A:64:THR:CG2	1:A:65:GLU:N	2.75	0.49
1:A:41:VAL:CG1	1:A:42:HIS:N	2.75	0.49
1:A:103:LEU:C	1:A:103:LEU:HD12	2.33	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:547:ASP:O	1:A:550:PHE:HB3	2.12	0.49
1:A:192:VAL:O	1:A:195:TYR:HB3	2.13	0.49
1:A:839:MLY:HB2	1:A:840:PRO:HD3	1.94	0.49
1:A:237:THR:HG22	1:A:238:VAL:N	2.28	0.49
1:A:762:HIS:N	1:A:762:HIS:CD2	2.78	0.49
1:A:601:ASP:N	1:A:602:PRO:CD	2.75	0.49
1:A:756:THR:O	1:A:758:TYR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASP:O	1:A:349:THR:HB	2.11	0.48
1:A:220:ASP:O	1:A:224:SER:N	2.30	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:648:THR:HG23	1:A:651:ALA:CB	2.44	0.48
1:A:312:TYR:CD1	1:A:312:TYR:N	2.81	0.48
1:A:715:VAL:HG12	1:A:716:LEU:O	2.12	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
1:A:404:PRO:HD2	1:A:415:MLY:O	2.13	0.48
1:A:97:LEU:HD13	1:A:97:LEU:N	2.28	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:765:VAL:CG1	1:A:766:PHE:N	2.77	0.48
1:A:22:LYS:O	1:A:26:GLU:N	2.29	0.48
1:A:251:ARG:HB2	1:A:264:ASP:HB3	1.95	0.48
1:A:838:ILE:C	1:A:840:PRO:HD2	2.34	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:579:PHE:CD2	1:A:592:ILE:HD11	2.43	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:20:SER:HB3	1:A:23:GLU:OE1	2.13	0.48
1:A:720:PHE:CD2	1:A:744:SER:HB3	2.48	0.48
1:A:169:ASP:OD1	1:A:169:ASP:N	2.44	0.48
1:A:689:GLU:O	1:A:689:GLU:HG2	2.14	0.47
1:A:602:PRO:O	1:A:603:LEU:HD12	2.14	0.47
1:A:550:PHE:CE2	1:A:592:ILE:CG2	2.97	0.47
1:A:248:MLY:HE2	1:A:250:ILE:HD11	1.95	0.47
1:A:564:ASN:HD22	1:A:582:VAL:HB	1.79	0.47
1:A:759:ALA:O	1:A:766:PHE:N	2.32	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:106:LEU:HD12	1:A:117:THR:HG21	1.96	0.47
1:A:695:LEU:HB3	1:A:701:LEU:HD22	1.97	0.47
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.56	0.47
1:A:311:ASP:CB	1:A:312:TYR:CE1	2.98	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:708:ARG:HA	1:A:712:PRO:HG3	1.96	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	5:A:5000:SO4:O3	2.33	0.46
1:A:400:ALA:HB1	1:A:606:THR:CG2	2.45	0.46
1:A:188:ASN:ND2	1:A:674:CYS:SG	2.88	0.46
1:A:546:THR:CG2	1:A:547:ASP:N	2.77	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: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:448:GLN:C	1:A:450:ASP:H	2.19	0.46
1:A:361:TYR:O	1:A:364:LEU:HB2	2.16	0.46
1:A:701:LEU:HD12	1:A:701:LEU:HA	1.55	0.46
1:A:418:THR:CG2	1:A:419:VAL:N	2.79	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: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:449:LEU:HA	1:A:449:LEU:HD12	1.60	0.46
1:A:322:VAL:HB	1:A:325:ILE:HG13	1.98	0.46
1:A:724:TYR:HB3	1:A:727:LEU:CD1	2.46	0.46
1:A:292:MET:HE1	1:A:309:PRO:CG	2.45	0.46
1:A:739:ASP:O	1:A:743:ALA:HB2	2.15	0.46
1:A:30:MLY:HB3	1:A:31:PRO:HD2	1.97	0.46
1:A:42:HIS:O	1:A:45:GLN:O	2.33	0.46
1:A:667:THR:O	1:A:669:PRO:HD3	2.16	0.46
1:A:524:GLU:HB3	1:A:528:MLY:HG2	1.96	0.46
1:A:82:PRO:HG2	1:A:85:TYR:CE2	2.50	0.46
1:A:559:LEU:HD23	1:A:560:GLY:N	2.30	0.46
1:A:103:LEU:HD22	1:A:692:LEU:HG	1.98	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:326:ASP:O	1:A:330:GLU:HG2	2.16	0.46
1:A:89:GLU:CD	1:A:153:PRO:HD2	2.36	0.45
1:A:794:CYS:O	1:A:797:PHE:HB3	2.17	0.45
1:A:578:HIS:O	1:A:579:PHE:HB3	2.15	0.45
1:A:488:GLN:O	1:A:491:PHE:HB3	2.17	0.45
1:A:664:LEU:HA	1:A:664:LEU:HD12	1.52	0.45
1:A:139:VAL:HG12	1:A:143:TYR:HD2	1.81	0.45
1:A:673:ARG:HA	1:A:673:ARG:HD2	1.79	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:486:MLY:HH22	1:A:527:GLU:CD	2.37	0.45
1:A:346:ASP:O	1:A:350:ALA:N	2.46	0.45
1:A:186:THR:O	1:A:190:MLY:HG2	2.17	0.45
1:A:783:LEU:N	1:A:783:LEU:CD1	2.78	0.45
1:A:476:GLU:OE2	1:A:598:MLY:HH13	2.16	0.45
1:A:767:PHE:CD1	1:A:771:LEU:CD2	2.99	0.45
1:A:292:MET:HE1	1:A:309:PRO:HD3	1.99	0.45
1:A:464:ILE:CG2	1:A:465:ALA:N	2.79	0.45
1:A:37:SER:O	1:A:38:VAL:HG23	2.17	0.45
1:A:330:GLU:O	1:A:333:ALA:HB3	2.16	0.45
1:A:179:GLY:O	1:A:185:LYS:HE2	2.17	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: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:64:THR:HB	1:A:68:GLU:N	2.33	0.44
1:A:597:GLU:O	1:A:600:MLY:N	2.50	0.44
1:A:173:GLN:HG3	1:A:670:HIS:HD2	1.82	0.44
1:A:508:ILE:CD1	1:A:766:PHE:CG	3.00	0.44
1:A:724:TYR:O	1:A:727:LEU:HD12	2.17	0.44
1:A:163:TYR:O	1:A:166:MET:HB3	2.17	0.44
1:A:224:SER:O	1:A:227:PRO:HD2	2.17	0.44
1:A:723:ARG:NH1	1:A:723:ARG:CG	2.79	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:767:PHE:CE1	1:A:771:LEU:HD23	2.52	0.44
1:A:715:VAL:HG12	1:A:720:PHE:HB2	2.00	0.44
1:A:711:PHE:HB3	1:A:766:PHE:HB3	1.99	0.44
1:A:123:CYS:CB	1:A:158:ILE:HD13	2.48	0.44
1:A:675:ILE:HG23	1:A:676:ILE:N	2.32	0.44
1:A:174:SER:OG	1:A:669:PRO:HA	2.18	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:787:ILE:HG21	1:A:787:ILE:HD13	1.67	0.44
1:A:266:GLU:OE1	1:A:659:MLY:NZ	2.51	0.44
1:A:296:MLY:HH11	1:A:348:MLY:CH2	2.48	0.44
1:A:747:LEU:C	1:A:749:GLY:N	2.71	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:226:ASN:HB2	1:A:227:PRO:CD	2.47	0.44
1:A:194:GLN:HE21	1:A:194:GLN:HB3	1.43	0.44
1:A:568:PRO:HD3	1:A:579:PHE:HA	1.99	0.43
1:A:519:LEU:CD1	1:A:519:LEU:N	2.77	0.43
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:107:MLY:CB	1:A:686:MET:HE2	2.39	0.43
1:A:246:PHE:HB3	1:A:270:LEU:HD12	2.01	0.43
1:A:322:VAL:CG1	1:A:325:ILE:HG13	2.49	0.43
1:A:296:MLY:O	1:A:299:LEU:HB2	2.17	0.43
1:A:134:VAL:C	1:A:136:ASN:H	2.16	0.43
1:A:292:MET:CE	1:A:309:PRO:CA	2.97	0.43
1:A:747:LEU:C	1:A:749:GLY:H	2.20	0.43
1:A:400:ALA:CB	1:A:606:THR:HG22	2.48	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:320:ILE:O	1:A:320:ILE:HG22	2.18	0.43
1:A:810:ARG:NH1	1:A:810:ARG:HG2	2.29	0.43
1:A:136:ASN:O	1:A:139:VAL:N	2.47	0.43
1:A:516:GLY:O	1:A:518:ASP:N	2.51	0.43
1:A:443:ILE:HG22	1:A:444:ARG:N	2.29	0.43
1:A:500:GLN:HB2	1:A:512:PHE:CZ	2.54	0.43
1:A:692:LEU:O	1:A:696:ARG:HG3	2.18	0.43
1:A:496:PHE:HB2	1:A:515:PHE:CD2	2.53	0.43
1:A:442:VAL:O	1:A:445:ILE:HB	2.19	0.43
1:A:110:TYR:O	1:A:113:TRP:N	2.42	0.43
1:A:56:GLU:HB2	1:A:59:MLY:CB	2.30	0.43
1:A:193:ILE:HD11	1:A:250:ILE:CD1	2.48	0.43
1:A:109:ARG:CD	1:A:117:THR:HB	2.48	0.43
1:A:175:ILE:C	1:A:176:LEU:HD12	2.38	0.43
1:A:64:THR:CG2	1:A:65:GLU:H	2.32	0.43
1:A:715:VAL:HG11	1:A:720:PHE:CD1	2.50	0.43
1:A:485:GLU:HA	1:A:584:TYR:HE2	1.83	0.43
1:A:294:ASN:OD1	1:A:307:THR:HG21	2.19	0.43
1:A:309:PRO:C	1:A:311:ASP:H	2.22	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:445:ILE:HG22	1:A:449:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:OD2	1:A:87:MLY:HH22	2.19	0.42
1:A:798:LEU:HD12	1:A:798:LEU:HA	1.36	0.42
1:A:439:LEU:N	1:A:439:LEU:CD1	2.81	0.42
1:A:62:VAL:HG12	1:A:63:MLY:N	2.35	0.42
1:A:787:ILE:HG23	1:A:791:GLN:HG3	2.00	0.42
1:A:402:CYS:C	1:A:404:PRO:HD3	2.40	0.42
1:A:406:VAL:O	1:A:412:ALA:HA	2.19	0.42
1:A:332:MET:O	1:A:336:SER:OG	2.27	0.42
1:A:123:CYS:HB2	1:A:158:ILE:HD13	2.00	0.42
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.79	0.42
1:A:169:ASP:O	1:A:170:ARG:HB2	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:842:LEU:N	1:A:842:LEU:CD1	2.82	0.42
1:A:826:VAL:O	1:A:828:HIS:N	2.53	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:218:LEU:O	1:A:222:ILE:HG12	2.20	0.42
1:A:135:TYR:HD2	1:A:191:ARG:CG	2.33	0.42
1:A:747:LEU:O	1:A:749:GLY:N	2.52	0.42
1:A:174:SER:HA	1:A:460:GLY:O	2.20	0.42
1:A:449:LEU:CD1	1:A:449:LEU:N	2.81	0.42
1:A:218:LEU:HD23	1:A:222:ILE:HG12	2.01	0.42
1:A:839:MLY:N	1:A:840:PRO:HD2	2.35	0.42
1:A:151:ALA:HB1	1:A:152:PRO:HD2	2.01	0.42
1:A:797:PHE:CD2	1:A:798:LEU:HD12	2.55	0.41
1:A:322:VAL:HA	1:A:323:PRO:HD3	1.87	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:91:MET:CE	1:A:119:SER:HB2	2.48	0.41
1:A:476:GLU:H	1:A:476:GLU:CD	2.21	0.41
1:A:724:TYR:HD1	1:A:727:LEU:CD1	2.29	0.41
1:A:744:SER:O	1:A:748:LEU:HD12	2.20	0.41
1:A:25:ILE:HG23	1:A:29:ASN:HD22	1.85	0.41
1:A:166:MET:CE	1:A:254:PHE:CD2	3.01	0.41
1:A:11:GLY:O	1:A:14:ALA:HB3	2.20	0.41
1:A:295:MLY:CD	1:A:332:MET:HE2	2.50	0.41
1:A:322:VAL:HG12	1:A:325:ILE:HG13	2.03	0.41
1:A:539:GLU:OE2	1:A:553:MLY:HD3	2.20	0.41
1:A:193:ILE:HD11	1:A:250:ILE:HD12	2.03	0.41
1:A:330:GLU:HA	1:A:330:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:MLY:HB2	1:A:529:PRO:HD2	2.03	0.41
1:A:717:TYR:OH	1:A:760:PHE:HB3	2.21	0.41
1:A:690:LEU:O	1:A:694:GLN:HG3	2.20	0.41
1:A:271:GLU:OE1	1:A:274:ARG:NH1	2.53	0.41
1:A:173:GLN:HG3	1:A:670:HIS:CD2	2.55	0.40
1:A:89:GLU:HB3	1:A:153:PRO:HG3	2.03	0.40
1:A:335:ASP:O	1:A:338:ILE:HB	2.20	0.40
1:A:305:ILE:HG22	1:A:312:TYR:OH	2.22	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:578:HIS:CD2	1:A:578:HIS:N	2.89	0.40
1:A:278:GLN:HB3	1:A:278:GLN:HE21	1.42	0.40
1:A:195:TYR:CD2	1:A:199:ILE:HD13	2.57	0.40
1:A:49:MLY:HH23	1:A:80:MET:CE	2.51	0.40
1:A:659:MLY:HD2	1:A:659:MLY:HH22	1.42	0.40
1:A:485:GLU:OE1	1:A:583:HIS:HB3	2.21	0.40
1:A:193:ILE:CD1	1:A:250:ILE:HD13	2.51	0.40
1:A:772:LEU:HD12	1:A:772:LEU:HA	1.83	0.40
1:A:88:ILE:HG22	1:A:90:ASP:C	2.42	0.40
1:A:166:MET:CE	1:A:254:PHE:HB2	2.46	0.40
1:A:303:LEU:O	1:A:304:LEU:HB2	2.21	0.40
1:A:49:MLY:HH23	1:A:80:MET:HE1	2.03	0.40
1:A:400:ALA:CB	1:A:606:THR:CG2	3.00	0.40
1:A:407:GLY:HA2	1:A:411:GLU:O	2.21	0.40
1:A:519:LEU:H	1:A:519:LEU:HD12	1.83	0.40
1:A:322:VAL:HB	1:A:325:ILE:CG1	2.52	0.40
1:A:657:LEU:HD12	1:A:657:LEU:O	2.21	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

### 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	745/843 (88%)	619 (83%)	106 (14%)	20 (3%)	6	21

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 ⓘ

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%)	485 (75%)	160 (25%)	1	2

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	7	MET
1	A	12	GLU
1	A	15	PRO
1	A	17	LEU
1	A	20	SER
1	A	22	LYS
1	A	36	SER
1	A	37	SER
1	A	46	SER
1	A	61	THR
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	97	LEU
1	A	106	LEU
1	A	109	ARG
1	A	114	MET
1	A	117	THR
1	A	121	LEU
1	A	126	VAL
1	A	127	ASN
1	A	135	TYR
1	A	136	ASN
1	A	146	LYS
1	A	149	GLN
1	A	155	ILE
1	A	157	SER
1	A	158	ILE
1	A	159	SER
1	A	165	PHE
1	A	167	LEU
1	A	169	ASP
1	A	173	GLN
1	A	178	THR
1	A	185	LYS
1	A	186	THR
1	A	187	VAL
1	A	191	ARG
1	A	193	ILE

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Mol	Chain	Res	Type
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	227	PRO
1	A	229	LEU
1	A	244	SER
1	A	245	ARG
1	A	251	ARG
1	A	264	ASP
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	294	ASN
1	A	298	GLU
1	A	300	ILE
1	A	325	ILE
1	A	331	LEU
1	A	336	SER
1	A	351	ILE
1	A	354	LEU
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	405	ARG
1	A	410	ASN
1	A	439	LEU
1	A	447	GLN
1	A	448	GLN

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Mol	Chain	Res	Type
1	A	449	LEU
1	A	453	GLN
1	A	455	ARG
1	A	457	TYR
1	A	462	LEU
1	A	471	ASP
1	A	474	SER
1	A	480	ILE
1	A	487	LEU
1	A	495	MET
1	A	499	GLU
1	A	506	GLU
1	A	513	ILE
1	A	518	ASP
1	A	524	GLU
1	A	532	ILE
1	A	534	SER
1	A	537	GLU
1	A	543	PRO
1	A	549	SER
1	A	561	LYS
1	A	562	SER
1	A	563	ASN
1	A	580	SER
1	A	593	SER
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	626	TYR
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

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Mol	Chain	Res	Type
1	A	698	ASN
1	A	701	LEU
1	A	702	GLU
1	A	704	ILE
1	A	708	ARG
1	A	713	SER
1	A	714	ARG
1	A	716	LEU
1	A	719	ASP
1	A	722	GLN
1	A	723	ARG
1	A	728	ASN
1	A	738	MET
1	A	745	GLU
1	A	752	ASP
1	A	753	VAL
1	A	754	ASP
1	A	762	HIS
1	A	774	LEU
1	A	785	GLU
1	A	787	ILE
1	A	793	ARG
1	A	799	MET
1	A	802	GLU
1	A	804	ARG
1	A	810	ARG
1	A	816	ILE
1	A	822	SER
1	A	832	MET
1	A	834	LEU
1	A	838	ILE
1	A	842	LEU
1	A	843	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	127	ASN
1	A	149	GLN
1	A	164	GLN
1	A	188	ASN

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Mol	Chain	Res	Type
1	A	194	GLN
1	A	253	HIS
1	A	290	GLN
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	563	ASN
1	A	564	ASN
1	A	578	HIS
1	A	656	ASN
1	A	670	HIS
1	A	698	ASN
1	A	757	GLN
1	A	762	HIS

### 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	0.44	0	9,11,13	0.66	0
1	MLY	A	130	1	9,10,11	0.91	1 (11%)	9,11,13	1.05	1 (11%)
1	MLY	A	138	1	9,10,11	1.80	1 (11%)	9,11,13	0.81	0
1	MLY	A	19	1	9,10,11	1.61	1 (11%)	9,11,13	0.68	0
1	MLY	A	190	1	9,10,11	1.48	1 (11%)	9,11,13	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	236	1	9,10,11	0.72	0	9,11,13	1.32	1 (11%)
1	MLY	A	248	1	9,10,11	0.96	1 (11%)	9,11,13	0.90	1 (11%)
1	MLY	A	272	1	9,10,11	1.37	1 (11%)	9,11,13	0.55	0
1	MLY	A	295	1	9,10,11	0.97	1 (11%)	9,11,13	0.47	0
1	MLY	A	296	1	9,10,11	0.78	0	9,11,13	0.76	0
1	MLY	A	30	1	9,10,11	0.86	0	9,11,13	0.82	0
1	MLY	A	348	1	9,10,11	1.07	1 (11%)	9,11,13	0.81	0
1	MLY	A	35	1	9,10,11	0.71	0	9,11,13	0.67	0
1	MLY	A	353	1	9,10,11	0.89	0	9,11,13	0.78	0
1	MLY	A	367	1	9,10,11	0.78	0	9,11,13	0.59	0
1	MLY	A	369	1	9,10,11	0.69	0	9,11,13	0.91	1 (11%)
1	MLY	A	385	1	9,10,11	1.27	1 (11%)	9,11,13	0.54	0
1	MLY	A	415	1	9,10,11	0.91	1 (11%)	9,11,13	0.42	0
1	MLY	A	431	1	9,10,11	0.61	0	9,11,13	0.76	0
1	MLY	A	436	1	9,10,11	1.47	1 (11%)	9,11,13	0.56	0
1	MLY	A	486	1	9,10,11	0.57	0	9,11,13	0.58	0
1	MLY	A	49	1	9,10,11	1.46	1 (11%)	9,11,13	0.98	0
1	MLY	A	504	1	9,10,11	0.94	0	9,11,13	0.47	0
1	MLY	A	505	1	9,10,11	1.17	1 (11%)	9,11,13	0.39	0
1	MLY	A	528	1	9,10,11	0.88	0	9,11,13	1.17	1 (11%)
1	MLY	A	55	1	9,10,11	0.68	0	9,11,13	0.96	0
1	MLY	A	551	1	9,10,11	0.48	0	9,11,13	0.64	0
1	MLY	A	553	1	9,10,11	0.77	0	9,11,13	0.57	0
1	MLY	A	59	1	9,10,11	0.98	1 (11%)	9,11,13	0.75	0
1	MLY	A	598	1	9,10,11	1.16	1 (11%)	9,11,13	0.71	0
1	MLY	A	600	1	9,10,11	0.55	0	9,11,13	0.45	0
1	MLY	A	613	1	9,10,11	0.52	0	9,11,13	0.91	0
1	MLY	A	617	1	9,10,11	1.20	1 (11%)	9,11,13	0.44	0
1	MLY	A	63	1	9,10,11	1.15	1 (11%)	9,11,13	0.94	0
1	MLY	A	659	1	9,10,11	0.82	0	9,11,13	0.93	0
1	MLY	A	681	1	9,10,11	0.75	0	9,11,13	0.62	0
1	MLY	A	764	1	9,10,11	1.04	1 (11%)	9,11,13	0.56	0
1	MLY	A	768	1	9,10,11	0.77	0	9,11,13	0.85	0
1	MLY	A	782	1	9,10,11	0.73	0	9,11,13	0.92	1 (11%)
1	MLY	A	827	1	9,10,11	0.82	0	9,11,13	0.94	1 (11%)
1	MLY	A	833	1	9,10,11	1.37	1 (11%)	9,11,13	0.56	0
1	MLY	A	837	1	9,10,11	0.67	0	9,11,13	0.56	0
1	MLY	A	839	1	9,10,11	0.91	1 (11%)	9,11,13	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	84	1	9,10,11	0.52	0	9,11,13	0.79	0
1	MLY	A	87	1	9,10,11	1.60	1 (11%)	9,11,13	0.66	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	-	0/7/9/11	0/0/0/0
1	MLY	A	130	1	-	0/7/9/11	0/0/0/0
1	MLY	A	138	1	-	0/7/9/11	0/0/0/0
1	MLY	A	19	1	-	0/7/9/11	0/0/0/0
1	MLY	A	190	1	-	0/7/9/11	0/0/0/0
1	MLY	A	236	1	-	0/7/9/11	0/0/0/0
1	MLY	A	248	1	-	0/7/9/11	0/0/0/0
1	MLY	A	272	1	-	0/7/9/11	0/0/0/0
1	MLY	A	295	1	-	0/7/9/11	0/0/0/0
1	MLY	A	296	1	-	0/7/9/11	0/0/0/0
1	MLY	A	30	1	-	0/7/9/11	0/0/0/0
1	MLY	A	348	1	-	0/7/9/11	0/0/0/0
1	MLY	A	35	1	-	0/7/9/11	0/0/0/0
1	MLY	A	353	1	-	0/7/9/11	0/0/0/0
1	MLY	A	367	1	-	0/7/9/11	0/0/0/0
1	MLY	A	369	1	-	0/7/9/11	0/0/0/0
1	MLY	A	385	1	-	0/7/9/11	0/0/0/0
1	MLY	A	415	1	-	0/7/9/11	0/0/0/0
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLY	A	436	1	-	0/7/9/11	0/0/0/0
1	MLY	A	486	1	-	0/7/9/11	0/0/0/0
1	MLY	A	49	1	-	0/7/9/11	0/0/0/0
1	MLY	A	504	1	-	0/7/9/11	0/0/0/0
1	MLY	A	505	1	-	0/7/9/11	0/0/0/0
1	MLY	A	528	1	-	0/7/9/11	0/0/0/0
1	MLY	A	55	1	-	0/7/9/11	0/0/0/0
1	MLY	A	551	1	-	0/7/9/11	0/0/0/0
1	MLY	A	553	1	-	0/7/9/11	0/0/0/0
1	MLY	A	59	1	-	0/7/9/11	0/0/0/0
1	MLY	A	598	1	-	0/7/9/11	0/0/0/0
1	MLY	A	600	1	-	0/7/9/11	0/0/0/0
1	MLY	A	613	1	-	0/7/9/11	0/0/0/0
1	MLY	A	617	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0
1	MLY	A	659	1	-	0/7/9/11	0/0/0/0
1	MLY	A	681	1	-	0/7/9/11	0/0/0/0
1	MLY	A	764	1	-	0/7/9/11	0/0/0/0
1	MLY	A	768	1	-	0/7/9/11	0/0/0/0
1	MLY	A	782	1	-	0/7/9/11	0/0/0/0
1	MLY	A	827	1	-	0/7/9/11	0/0/0/0
1	MLY	A	833	1	-	0/7/9/11	0/0/0/0
1	MLY	A	837	1	-	0/7/9/11	0/0/0/0
1	MLY	A	839	1	-	0/7/9/11	0/0/0/0
1	MLY	A	84	1	-	0/7/9/11	0/0/0/0
1	MLY	A	87	1	-	0/7/9/11	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	MLY	CB-CA	-5.20	1.48	1.53
1	A	19	MLY	CB-CA	-4.59	1.49	1.53
1	A	87	MLY	CB-CA	-4.49	1.49	1.53
1	A	436	MLY	CB-CA	-4.25	1.49	1.53
1	A	49	MLY	CB-CA	-4.12	1.49	1.53
1	A	272	MLY	CB-CA	-3.95	1.49	1.53
1	A	190	MLY	CB-CA	-3.64	1.50	1.53
1	A	385	MLY	CB-CA	-3.48	1.50	1.53
1	A	833	MLY	CB-CA	-3.35	1.50	1.53
1	A	505	MLY	CB-CA	-3.22	1.50	1.53
1	A	617	MLY	CB-CA	-3.20	1.50	1.53
1	A	598	MLY	CB-CA	-3.20	1.50	1.53
1	A	63	MLY	CB-CA	-2.96	1.50	1.53
1	A	348	MLY	CB-CA	-2.85	1.51	1.53
1	A	764	MLY	CB-CA	-2.62	1.51	1.53
1	A	295	MLY	CB-CA	-2.46	1.51	1.53
1	A	839	MLY	CB-CA	-2.38	1.51	1.53
1	A	248	MLY	CB-CA	-2.24	1.51	1.53
1	A	130	MLY	CB-CA	-2.21	1.51	1.53
1	A	415	MLY	CB-CA	-2.18	1.51	1.53
1	A	59	MLY	CB-CA	-2.16	1.51	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	MLY	O-C-CA	-3.20	117.14	125.49

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	MLY	O-C-CA	-3.08	117.47	125.49
1	A	827	MLY	O-C-CA	-2.52	118.93	125.49
1	A	130	MLY	O-C-CA	-2.46	119.09	125.49
1	A	369	MLY	O-C-CA	-2.16	119.87	125.49
1	A	248	MLY	O-C-CA	-2.15	119.88	125.49
1	A	782	MLY	CB-CA-N	2.06	116.39	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107	MLY	3	0
1	A	138	MLY	1	0
1	A	190	MLY	2	0
1	A	248	MLY	2	0
1	A	272	MLY	1	0
1	A	295	MLY	6	0
1	A	296	MLY	3	0
1	A	30	MLY	1	0
1	A	348	MLY	5	0
1	A	35	MLY	1	0
1	A	415	MLY	1	0
1	A	486	MLY	3	0
1	A	49	MLY	4	0
1	A	528	MLY	3	0
1	A	55	MLY	1	0
1	A	553	MLY	2	0
1	A	59	MLY	3	0
1	A	598	MLY	1	0
1	A	600	MLY	1	0
1	A	617	MLY	1	0
1	A	63	MLY	3	0
1	A	659	MLY	2	0
1	A	764	MLY	1	0
1	A	782	MLY	1	0
1	A	837	MLY	1	0
1	A	839	MLY	4	0
1	A	87	MLY	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
5	SO4	A	5000	-	4,4,4	0.82	0	6,6,6	0.19	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
5	SO4	A	5000	-	-	0/0/0/0	0/0/0/0

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
5	A	5000	SO4	2	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.