



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:37 PM BST

PDB ID : 6N1G  
Title : Crystal structure of Aquaglyceroporin AQP7  
Authors : Vahedi-Faridi, A.; Lodowski, D.; Kowatz, T.  
Deposited on : 2018-11-08  
Resolution : 4.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

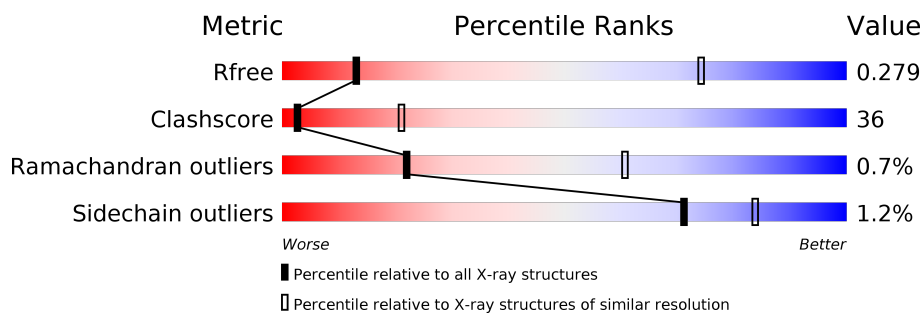
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	
1	C	376	
1	D	376	

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
2	GOL	D	403	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15472 atoms, of which 7776 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 Aquaporin-7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			
1	C	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			
1	B	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			
1	D	249	Total	C	H	N	O	S	0	0	0
			3826	1266	1920	308	319	13			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	GLY	-	expression tag	UNP O14520
A	344	GLY	-	expression tag	UNP O14520
A	345	SER	-	expression tag	UNP O14520
A	346	LEU	-	expression tag	UNP O14520
A	347	GLU	-	expression tag	UNP O14520
A	348	VAL	-	expression tag	UNP O14520
A	349	LEU	-	expression tag	UNP O14520
A	350	PHE	-	expression tag	UNP O14520
A	351	GLN	-	expression tag	UNP O14520
A	352	GLY	-	expression tag	UNP O14520
A	353	PRO	-	expression tag	UNP O14520
A	354	ALA	-	expression tag	UNP O14520
A	355	ALA	-	expression tag	UNP O14520
A	356	TYR	-	expression tag	UNP O14520
A	357	PRO	-	expression tag	UNP O14520
A	358	TYR	-	expression tag	UNP O14520
A	359	ASP	-	expression tag	UNP O14520
A	360	VAL	-	expression tag	UNP O14520
A	361	PRO	-	expression tag	UNP O14520
A	362	ASP	-	expression tag	UNP O14520
A	363	TYR	-	expression tag	UNP O14520

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Chain	Residue	Modelled	Actual	Comment	Reference
A	364	ALA	-	expression tag	UNP O14520
A	365	ALA	-	expression tag	UNP O14520
A	366	ALA	-	expression tag	UNP O14520
A	367	HIS	-	expression tag	UNP O14520
A	368	HIS	-	expression tag	UNP O14520
A	369	HIS	-	expression tag	UNP O14520
A	370	HIS	-	expression tag	UNP O14520
A	371	HIS	-	expression tag	UNP O14520
A	372	HIS	-	expression tag	UNP O14520
A	373	HIS	-	expression tag	UNP O14520
A	374	HIS	-	expression tag	UNP O14520
A	375	HIS	-	expression tag	UNP O14520
A	376	HIS	-	expression tag	UNP O14520
C	343	GLY	-	expression tag	UNP O14520
C	344	GLY	-	expression tag	UNP O14520
C	345	SER	-	expression tag	UNP O14520
C	346	LEU	-	expression tag	UNP O14520
C	347	GLU	-	expression tag	UNP O14520
C	348	VAL	-	expression tag	UNP O14520
C	349	LEU	-	expression tag	UNP O14520
C	350	PHE	-	expression tag	UNP O14520
C	351	GLN	-	expression tag	UNP O14520
C	352	GLY	-	expression tag	UNP O14520
C	353	PRO	-	expression tag	UNP O14520
C	354	ALA	-	expression tag	UNP O14520
C	355	ALA	-	expression tag	UNP O14520
C	356	TYR	-	expression tag	UNP O14520
C	357	PRO	-	expression tag	UNP O14520
C	358	TYR	-	expression tag	UNP O14520
C	359	ASP	-	expression tag	UNP O14520
C	360	VAL	-	expression tag	UNP O14520
C	361	PRO	-	expression tag	UNP O14520
C	362	ASP	-	expression tag	UNP O14520
C	363	TYR	-	expression tag	UNP O14520
C	364	ALA	-	expression tag	UNP O14520
C	365	ALA	-	expression tag	UNP O14520
C	366	ALA	-	expression tag	UNP O14520
C	367	HIS	-	expression tag	UNP O14520
C	368	HIS	-	expression tag	UNP O14520
C	369	HIS	-	expression tag	UNP O14520
C	370	HIS	-	expression tag	UNP O14520
C	371	HIS	-	expression tag	UNP O14520

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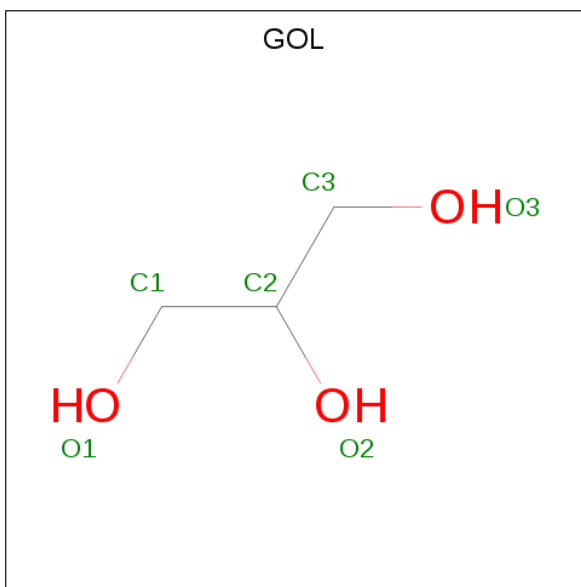
Chain	Residue	Modelled	Actual	Comment	Reference
C	372	HIS	-	expression tag	UNP O14520
C	373	HIS	-	expression tag	UNP O14520
C	374	HIS	-	expression tag	UNP O14520
C	375	HIS	-	expression tag	UNP O14520
C	376	HIS	-	expression tag	UNP O14520
B	343	GLY	-	expression tag	UNP O14520
B	344	GLY	-	expression tag	UNP O14520
B	345	SER	-	expression tag	UNP O14520
B	346	LEU	-	expression tag	UNP O14520
B	347	GLU	-	expression tag	UNP O14520
B	348	VAL	-	expression tag	UNP O14520
B	349	LEU	-	expression tag	UNP O14520
B	350	PHE	-	expression tag	UNP O14520
B	351	GLN	-	expression tag	UNP O14520
B	352	GLY	-	expression tag	UNP O14520
B	353	PRO	-	expression tag	UNP O14520
B	354	ALA	-	expression tag	UNP O14520
B	355	ALA	-	expression tag	UNP O14520
B	356	TYR	-	expression tag	UNP O14520
B	357	PRO	-	expression tag	UNP O14520
B	358	TYR	-	expression tag	UNP O14520
B	359	ASP	-	expression tag	UNP O14520
B	360	VAL	-	expression tag	UNP O14520
B	361	PRO	-	expression tag	UNP O14520
B	362	ASP	-	expression tag	UNP O14520
B	363	TYR	-	expression tag	UNP O14520
B	364	ALA	-	expression tag	UNP O14520
B	365	ALA	-	expression tag	UNP O14520
B	366	ALA	-	expression tag	UNP O14520
B	367	HIS	-	expression tag	UNP O14520
B	368	HIS	-	expression tag	UNP O14520
B	369	HIS	-	expression tag	UNP O14520
B	370	HIS	-	expression tag	UNP O14520
B	371	HIS	-	expression tag	UNP O14520
B	372	HIS	-	expression tag	UNP O14520
B	373	HIS	-	expression tag	UNP O14520
B	374	HIS	-	expression tag	UNP O14520
B	375	HIS	-	expression tag	UNP O14520
B	376	HIS	-	expression tag	UNP O14520
D	343	GLY	-	expression tag	UNP O14520
D	344	GLY	-	expression tag	UNP O14520
D	345	SER	-	expression tag	UNP O14520

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Chain	Residue	Modelled	Actual	Comment	Reference
D	346	LEU	-	expression tag	UNP O14520
D	347	GLU	-	expression tag	UNP O14520
D	348	VAL	-	expression tag	UNP O14520
D	349	LEU	-	expression tag	UNP O14520
D	350	PHE	-	expression tag	UNP O14520
D	351	GLN	-	expression tag	UNP O14520
D	352	GLY	-	expression tag	UNP O14520
D	353	PRO	-	expression tag	UNP O14520
D	354	ALA	-	expression tag	UNP O14520
D	355	ALA	-	expression tag	UNP O14520
D	356	TYR	-	expression tag	UNP O14520
D	357	PRO	-	expression tag	UNP O14520
D	358	TYR	-	expression tag	UNP O14520
D	359	ASP	-	expression tag	UNP O14520
D	360	VAL	-	expression tag	UNP O14520
D	361	PRO	-	expression tag	UNP O14520
D	362	ASP	-	expression tag	UNP O14520
D	363	TYR	-	expression tag	UNP O14520
D	364	ALA	-	expression tag	UNP O14520
D	365	ALA	-	expression tag	UNP O14520
D	366	ALA	-	expression tag	UNP O14520
D	367	HIS	-	expression tag	UNP O14520
D	368	HIS	-	expression tag	UNP O14520
D	369	HIS	-	expression tag	UNP O14520
D	370	HIS	-	expression tag	UNP O14520
D	371	HIS	-	expression tag	UNP O14520
D	372	HIS	-	expression tag	UNP O14520
D	373	HIS	-	expression tag	UNP O14520
D	374	HIS	-	expression tag	UNP O14520
D	375	HIS	-	expression tag	UNP O14520
D	376	HIS	-	expression tag	UNP O14520

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



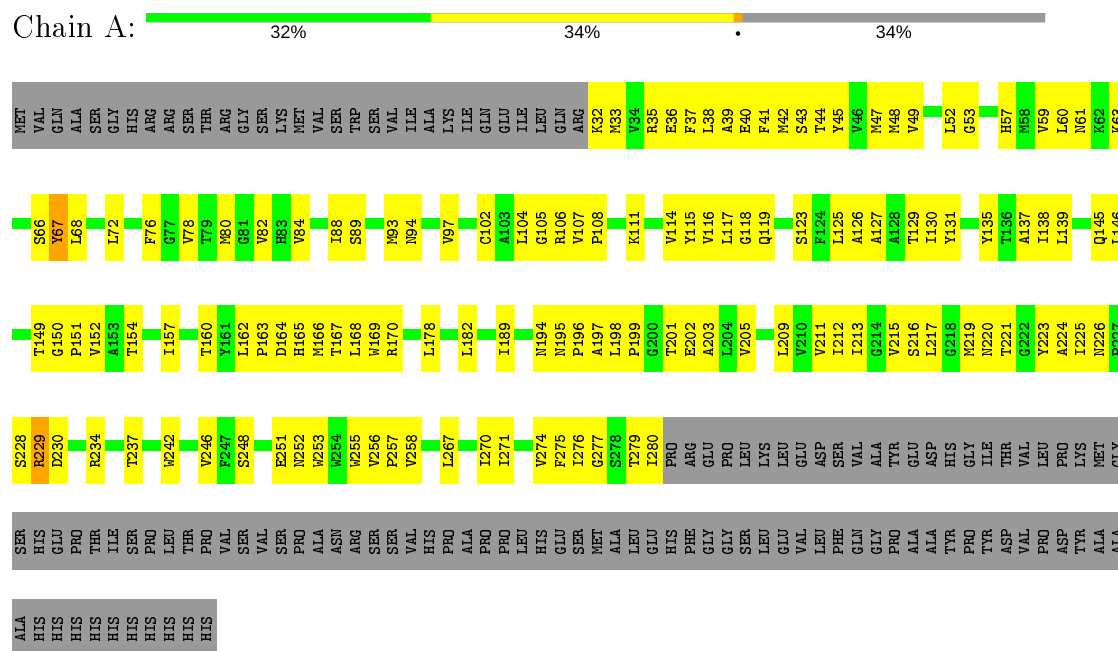
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	14	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		



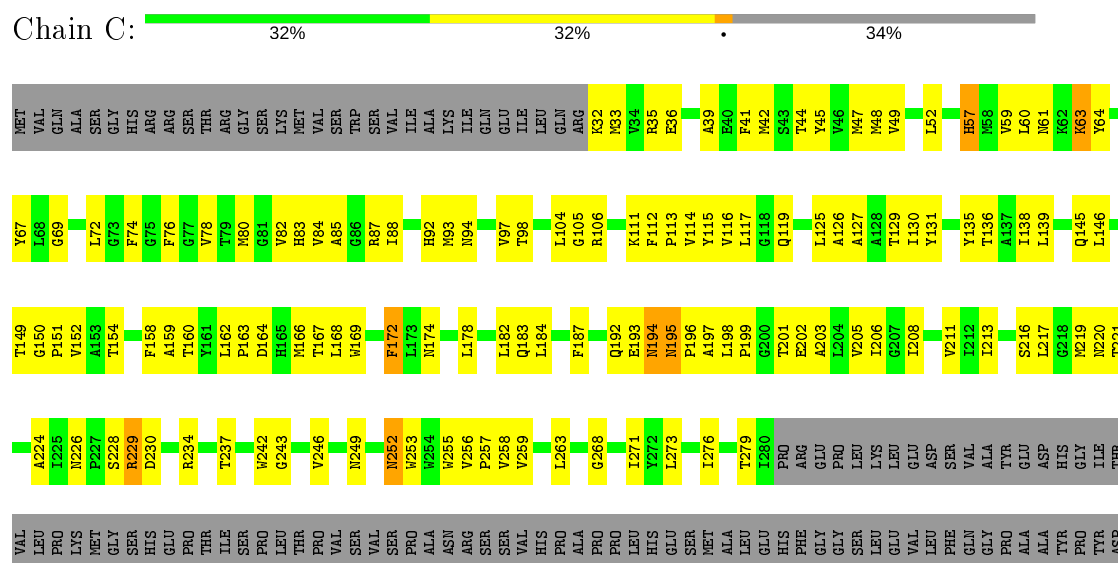
### 3 Residue-property plots

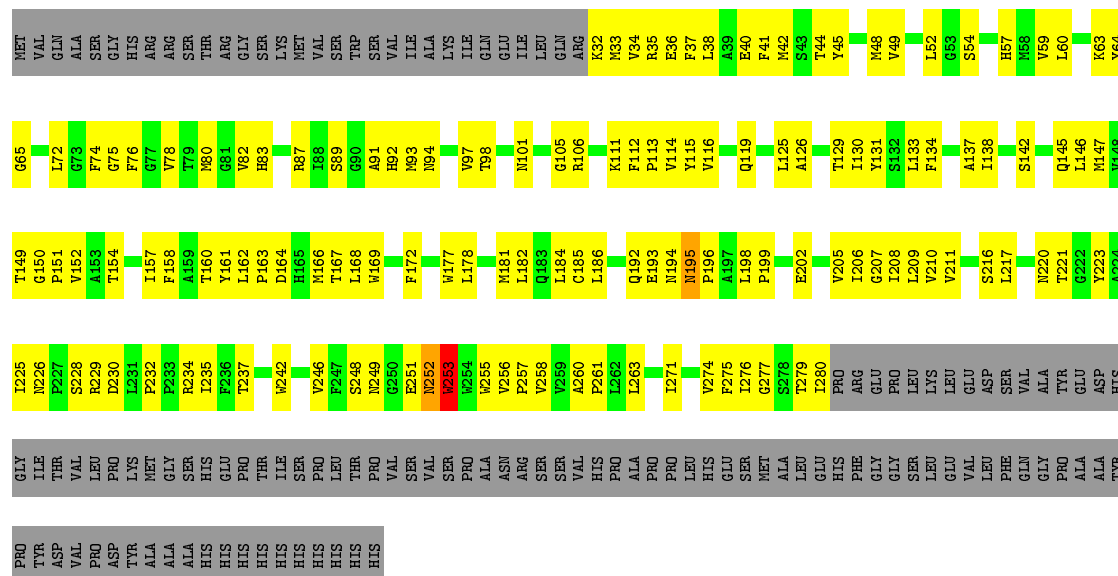
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

#### • Molecule 1: Aquaporin-7



#### • Molecule 1: Aquaporin-7





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	385.66Å 385.66Å 385.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.71 – 4.00 47.12 – 3.99	Depositor EDS
% Data completeness (in resolution range)	87.9 (32.71-4.00) 93.3 (47.12-3.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	50.00 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14 _3235: ???)	Depositor
R, $R_{free}$	0.232 , 0.277 0.233 , 0.279	Depositor DCC
$R_{free}$ test set	599 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	132.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.11 , -9.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7106e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/1963	0.58	0/2676
1	B	0.36	0/1963	0.58	0/2676
1	C	0.37	0/1963	0.56	0/2676
1	D	0.38	0/1963	0.59	1/2676 (0.0%)
All	All	0.37	0/7852	0.58	1/10704 (0.0%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	253	TRP	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	194	ASN	Peptide

## 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	1906	1920	1920	154	1
1	B	1906	1920	1920	155	1
1	C	1906	1920	1920	140	1
1	D	1906	1920	1920	166	1
2	A	12	16	16	0	0
2	B	18	24	24	0	0
2	C	18	24	24	3	0
2	D	24	32	32	7	0
All	All	7696	7776	7776	555	2

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 36.

All (555) 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:D:45:TYR:OH	1:D:129:THR:OG1	1.87	0.93
1:B:162:LEU:HD13	1:B:253:TRP:CH2	2.04	0.92
1:D:60:LEU:CD1	1:D:138:ILE:HD13	2.00	0.92
1:A:39:ALA:HB3	1:A:88:ILE:HD11	1.51	0.91
1:B:173:LEU:CD2	1:D:133:LEU:HD21	2.02	0.88
1:D:182:LEU:HD13	1:D:225:ILE:HG21	1.56	0.88
1:C:178:LEU:HD21	1:C:217:LEU:HD22	1.55	0.87
1:C:45:TYR:OH	1:C:129:THR:OG1	1.92	0.87
1:C:152:VAL:HG12	1:B:146:LEU:HD22	1.57	0.86
1:A:162:LEU:HD13	1:A:253:TRP:CH2	2.12	0.85
1:C:178:LEU:HD12	1:C:213:ILE:HG23	1.57	0.85
1:B:173:LEU:HD22	1:D:133:LEU:HD21	1.56	0.84
1:D:162:LEU:HD13	1:D:253:TRP:CH2	2.12	0.83
1:B:182:LEU:HD13	1:B:225:ILE:HG21	1.60	0.83
1:A:66:SER:OG	1:C:64:TYR:O	1.97	0.82
1:C:178:LEU:HD11	1:C:217:LEU:HD13	1.61	0.82
1:A:131:TYR:HE1	1:A:138:ILE:HD13	1.45	0.81
1:C:32:LYS:HG3	1:C:35:ARG:HG3	1.62	0.80
1:B:237:THR:HB	1:B:246:VAL:HG21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:VAL:HG13	1:D:60:LEU:HG	1.64	0.80
1:D:195:ASN:HB3	1:D:196:PRO:HD3	1.65	0.79
1:B:173:LEU:HD22	1:D:133:LEU:CD2	2.12	0.79
1:A:146:LEU:HB3	1:D:152:VAL:HG13	1.67	0.77
1:D:60:LEU:HD13	1:D:138:ILE:HD13	1.67	0.77
1:A:237:THR:HB	1:A:246:VAL:HG21	1.67	0.77
1:D:274:VAL:HG13	1:D:275:PHE:CD1	2.20	0.76
1:C:39:ALA:CB	1:C:88:ILE:HD11	2.16	0.76
1:A:170:ARG:HH12	1:C:136:THR:HG23	1.50	0.76
1:A:270:ILE:O	1:A:274:VAL:HG12	1.86	0.76
1:D:45:TYR:O	1:D:49:VAL:HG12	1.85	0.75
1:B:162:LEU:HD11	1:B:166:MET:SD	2.25	0.75
1:D:237:THR:HB	1:D:246:VAL:HG21	1.67	0.75
1:A:167:THR:HG21	1:A:169:TRP:CZ2	2.22	0.75
1:C:57:HIS:CE1	1:C:63:LYS:HB2	2.23	0.74
1:C:237:THR:HB	1:C:246:VAL:HG21	1.70	0.74
1:D:186:LEU:HD11	2:D:403:GOL:C3	2.18	0.74
1:D:54:SER:O	1:D:63:LYS:NZ	2.17	0.74
1:D:57:HIS:CE1	1:D:63:LYS:HB3	2.23	0.74
1:B:167:THR:HG21	1:B:169:TRP:CZ2	2.23	0.73
1:C:184:LEU:HD12	1:C:271:ILE:HG23	1.70	0.73
1:B:274:VAL:HG13	1:B:275:PHE:CD1	2.23	0.73
1:B:198:LEU:HD13	1:B:201:THR:HB	1.69	0.73
1:C:162:LEU:HD13	1:C:253:TRP:CH2	2.24	0.73
1:A:104:LEU:HD13	1:A:104:LEU:O	1.87	0.73
1:A:36:GLU:HA	1:A:88:ILE:HD13	1.71	0.72
1:C:59:VAL:HG23	1:C:60:LEU:HG	1.72	0.72
1:D:167:THR:HG21	1:D:169:TRP:CZ2	2.25	0.72
1:A:57:HIS:CE1	1:A:63:LYS:HB2	2.24	0.71
1:B:57:HIS:CE1	1:B:63:LYS:HB2	2.25	0.71
1:B:74:PHE:O	1:B:78:VAL:HG23	1.89	0.71
1:D:195:ASN:HB3	1:D:196:PRO:CD	2.20	0.71
1:B:45:TYR:CZ	1:B:126:ALA:HA	2.25	0.71
1:A:119:GLN:O	1:A:228:SER:OG	2.08	0.71
1:A:45:TYR:OH	1:A:129:THR:OG1	2.06	0.71
1:B:270:ILE:O	1:B:274:VAL:HG12	1.91	0.71
1:C:167:THR:HG21	1:C:169:TRP:CZ2	2.26	0.70
1:D:45:TYR:CZ	1:D:126:ALA:HA	2.27	0.70
1:B:189:ILE:HA	1:D:83:HIS:NE2	2.07	0.70
1:C:167:THR:HG21	1:C:169:TRP:CH2	2.28	0.68
1:C:195:ASN:HB3	1:C:196:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD22	1:C:130:ILE:HG21	1.75	0.67
1:C:45:TYR:O	1:C:49:VAL:HG12	1.94	0.67
1:A:67:TYR:CE2	1:A:215:VAL:HG22	2.28	0.67
1:B:198:LEU:HD13	1:B:201:THR:C	2.14	0.67
1:B:198:LEU:HD12	1:B:202:GLU:N	2.09	0.67
1:A:52:LEU:HD22	1:A:130:ILE:HG21	1.76	0.67
1:A:52:LEU:HD23	1:A:52:LEU:O	1.93	0.67
1:C:131:TYR:CE1	1:C:138:ILE:HD13	2.29	0.67
1:A:39:ALA:HB3	1:A:88:ILE:CD1	2.25	0.67
1:A:59:VAL:HG13	1:A:60:LEU:HG	1.77	0.67
1:A:162:LEU:HD11	1:A:166:MET:SD	2.36	0.66
1:B:45:TYR:OH	1:B:129:THR:OG1	2.11	0.66
1:A:47:MET:HG2	1:A:78:VAL:HG12	1.77	0.66
1:A:150:GLY:N	1:A:151:PRO:HD3	2.10	0.66
1:A:274:VAL:HG13	1:A:275:PHE:CD1	2.31	0.66
1:B:173:LEU:HD23	1:D:133:LEU:HD21	1.77	0.65
1:B:52:LEU:HD23	1:B:52:LEU:O	1.95	0.65
1:C:45:TYR:CZ	1:C:126:ALA:HA	2.31	0.65
1:A:45:TYR:CZ	1:A:126:ALA:HA	2.32	0.64
1:D:276:ILE:O	1:D:279:THR:OG1	2.10	0.64
1:A:138:ILE:HG13	1:A:139:LEU:N	2.11	0.64
1:B:44:THR:N	1:B:93:MET:SD	2.71	0.64
1:D:57:HIS:O	1:D:63:LYS:HG2	1.98	0.63
1:A:146:LEU:HB3	1:D:152:VAL:CG1	2.27	0.63
1:C:152:VAL:HA	1:B:146:LEU:HD13	1.79	0.63
1:B:198:LEU:CD1	1:B:201:THR:C	2.65	0.63
1:D:91:ALA:O	2:D:403:GOL:O3	2.03	0.63
1:C:152:VAL:CG1	1:B:146:LEU:HD22	2.27	0.63
1:C:150:GLY:N	1:C:151:PRO:HD3	2.14	0.62
1:B:198:LEU:CD1	1:B:202:GLU:N	2.63	0.62
1:B:198:LEU:HD11	1:B:202:GLU:HA	1.81	0.62
1:A:48:MET:O	1:A:52:LEU:N	2.20	0.62
1:A:88:ILE:HD12	1:A:89:SER:N	2.14	0.62
1:C:39:ALA:HB3	1:C:88:ILE:HD11	1.80	0.62
1:D:248:SER:O	1:D:251:GLU:O	2.18	0.62
1:D:52:LEU:HD21	1:D:158:PHE:CD1	2.35	0.61
1:D:44:THR:N	1:D:93:MET:SD	2.73	0.61
1:C:39:ALA:HB2	1:C:88:ILE:HD11	1.83	0.61
1:A:39:ALA:CB	1:A:88:ILE:HD11	2.28	0.60
1:C:52:LEU:O	1:C:52:LEU:HD23	2.01	0.60
1:D:82:VAL:HG22	2:D:403:GOL:H12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASN:O	1:B:254:TRP:N	2.31	0.60
1:A:256:VAL:HG13	1:A:257:PRO:HD3	1.82	0.60
1:C:32:LYS:CG	1:C:35:ARG:HG3	2.29	0.60
1:A:279:THR:HB	1:C:35:ARG:HD2	1.83	0.60
1:D:167:THR:HG21	1:D:169:TRP:CH2	2.36	0.60
1:D:48:MET:O	1:D:52:LEU:N	2.20	0.60
1:B:104:LEU:O	1:B:104:LEU:HG	2.01	0.60
1:B:32:LYS:HB3	1:B:35:ARG:NE	2.16	0.60
1:D:274:VAL:HG13	1:D:275:PHE:HD1	1.64	0.59
1:A:131:TYR:CE1	1:A:138:ILE:HD13	2.32	0.59
1:C:111:LYS:HD3	1:C:115:TYR:OH	2.02	0.59
1:D:60:LEU:HD11	1:D:138:ILE:HD13	1.82	0.59
1:B:60:LEU:HD23	1:B:137:ALA:O	2.02	0.58
1:A:33:MET:CE	1:A:111:LYS:HG2	2.34	0.58
1:A:194:ASN:OD1	1:C:87:ARG:HB2	2.03	0.58
1:B:45:TYR:O	1:B:49:VAL:HG12	2.04	0.58
1:A:94:ASN:HB3	1:A:97:VAL:HG22	1.86	0.58
1:D:198:LEU:O	1:D:202:GLU:HG3	2.04	0.58
1:A:146:LEU:O	1:D:152:VAL:HG21	2.04	0.58
1:B:178:LEU:HD21	1:B:217:LEU:HD22	1.85	0.58
1:A:219:MET:HB2	1:C:57:HIS:CE1	2.38	0.58
1:A:279:THR:HA	1:C:35:ARG:HD3	1.86	0.58
1:A:152:VAL:HG11	1:D:146:LEU:HB3	1.86	0.58
1:D:92:HIS:O	2:D:403:GOL:O2	2.21	0.58
1:B:67:TYR:CE1	1:D:63:LYS:HD2	2.39	0.57
1:B:256:VAL:CG1	1:B:257:PRO:HD3	2.35	0.57
1:C:195:ASN:HB3	1:C:196:PRO:CD	2.35	0.57
1:B:189:ILE:HG22	1:B:202:GLU:HG3	1.87	0.57
1:D:52:LEU:HG	1:D:130:ILE:HG21	1.87	0.57
1:A:198:LEU:O	1:A:202:GLU:HG3	2.04	0.57
1:C:52:LEU:HD22	1:C:130:ILE:CG2	2.34	0.57
1:A:88:ILE:HD12	1:A:89:SER:HB3	1.86	0.57
1:D:40:GLU:HA	1:D:93:MET:HE3	1.87	0.57
1:B:40:GLU:HA	1:B:93:MET:HE3	1.87	0.57
1:C:135:TYR:O	1:C:138:ILE:HG12	2.04	0.57
1:C:219:MET:HG3	1:C:219:MET:O	2.04	0.57
1:B:39:ALA:HB1	1:B:85:ALA:HB1	1.87	0.57
1:D:182:LEU:HD13	1:D:225:ILE:CG2	2.32	0.56
1:A:150:GLY:N	1:A:151:PRO:CD	2.68	0.56
1:B:98:THR:HG22	1:B:112:PHE:HD1	1.70	0.56
1:B:226:ASN:HB3	1:B:229:ARG:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:TYR:CE1	1:D:138:ILE:HG13	2.41	0.56
1:D:52:LEU:HD21	1:D:158:PHE:HD1	1.70	0.56
1:B:198:LEU:CD1	1:B:202:GLU:HA	2.36	0.56
1:C:113:PRO:O	1:C:116:VAL:HG12	2.05	0.56
1:C:168:LEU:HD22	1:C:252:ASN:HD21	1.71	0.56
1:A:152:VAL:CG1	1:D:146:LEU:HB3	2.36	0.56
1:C:72:LEU:HA	1:C:211:VAL:HG22	1.88	0.56
1:A:40:GLU:HA	1:A:93:MET:HE3	1.87	0.55
1:B:194:ASN:OD1	1:D:87:ARG:HB2	2.05	0.55
1:D:162:LEU:HD11	1:D:166:MET:SD	2.45	0.55
1:D:205:VAL:HA	1:D:208:ILE:HG12	1.87	0.55
1:A:44:THR:OG1	1:A:119:GLN:HB2	2.06	0.55
1:B:189:ILE:HD13	1:B:205:VAL:HG13	1.88	0.55
1:C:48:MET:HB3	1:C:126:ALA:HB1	1.87	0.55
1:B:32:LYS:HB3	1:B:35:ARG:CD	2.36	0.55
1:B:94:ASN:HB3	1:B:97:VAL:HB	1.88	0.55
1:C:146:LEU:HB2	1:B:152:VAL:CG1	2.36	0.55
1:A:44:THR:N	1:A:93:MET:SD	2.79	0.55
1:B:276:ILE:HD11	1:D:42:MET:SD	2.47	0.55
1:C:150:GLY:N	1:C:151:PRO:CD	2.70	0.55
1:C:205:VAL:HA	1:C:208:ILE:HG12	1.89	0.55
1:D:74:PHE:O	1:D:78:VAL:HG23	2.06	0.55
1:A:189:ILE:HD13	1:A:205:VAL:HG13	1.89	0.55
1:A:162:LEU:HD13	1:A:253:TRP:CZ2	2.42	0.54
1:A:57:HIS:HD1	1:A:61:ASN:HB3	1.73	0.54
1:B:198:LEU:HD12	1:B:198:LEU:O	2.07	0.54
1:A:57:HIS:ND1	1:A:63:LYS:HB2	2.21	0.54
1:B:44:THR:OG1	1:B:93:MET:SD	2.58	0.54
1:D:192:GLN:NE2	1:D:193:GLU:OE2	2.40	0.54
1:D:60:LEU:CD1	1:D:138:ILE:CD1	2.83	0.54
1:D:149:THR:O	1:D:149:THR:HG23	2.07	0.54
1:B:67:TYR:HE1	1:D:65:GLY:CA	2.21	0.54
1:B:178:LEU:HD11	1:B:217:LEU:CB	2.37	0.54
1:D:48:MET:HB3	1:D:126:ALA:HB1	1.89	0.54
1:B:212:ILE:HD11	1:D:76:PHE:HB3	1.89	0.54
1:D:105:GLY:O	1:D:106:ARG:HG2	2.08	0.54
1:C:174:ASN:O	1:C:178:LEU:HD23	2.08	0.54
1:C:47:MET:HG2	1:C:78:VAL:HG22	1.90	0.54
1:C:104:LEU:HG	1:C:104:LEU:O	2.08	0.53
1:C:184:LEU:HD12	1:C:271:ILE:CG2	2.38	0.53
1:A:195:ASN:OD1	1:A:196:PRO:HD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:MET:HB2	1:D:57:HIS:CE1	2.43	0.53
1:D:32:LYS:HG3	1:D:35:ARG:HG3	1.89	0.53
1:A:37:PHE:CZ	1:A:118:GLY:HA2	2.43	0.53
1:B:230:ASP:O	1:B:234:ARG:HG3	2.08	0.53
1:D:255:TRP:O	1:D:258:VAL:HG12	2.08	0.53
1:D:32:LYS:HG2	1:D:35:ARG:NE	2.22	0.53
1:D:40:GLU:HA	1:D:93:MET:CE	2.39	0.53
1:B:52:LEU:HD13	1:B:130:ILE:HG21	1.89	0.53
1:C:117:LEU:O	1:C:117:LEU:HD23	2.08	0.53
1:C:206:ILE:HG22	2:C:403:GOL:O2	2.09	0.53
1:D:178:LEU:HD21	1:D:217:LEU:HD13	1.89	0.53
1:A:48:MET:HB3	1:A:126:ALA:HB1	1.91	0.52
1:B:150:GLY:N	1:B:151:PRO:CD	2.72	0.52
1:D:195:ASN:CB	1:D:196:PRO:HD3	2.38	0.52
1:A:189:ILE:HA	1:C:83:HIS:NE2	2.24	0.52
1:B:279:THR:HG22	1:D:35:ARG:HG2	1.90	0.52
1:A:165:HIS:O	1:C:136:THR:OG1	2.11	0.52
1:A:230:ASP:O	1:A:234:ARG:HG3	2.09	0.52
1:B:142:SER:OG	1:B:147:MET:O	2.28	0.52
1:B:57:HIS:ND1	1:B:63:LYS:HB2	2.24	0.52
1:A:102:CYS:HA	1:A:107:VAL:HG12	1.92	0.52
1:B:195:ASN:CG	1:B:196:PRO:HD3	2.30	0.52
1:B:52:LEU:HD11	1:B:158:PHE:HD1	1.74	0.52
1:A:33:MET:HE1	1:A:111:LYS:HG2	1.92	0.52
1:D:98:THR:HG22	1:D:112:PHE:HD1	1.74	0.52
1:D:277:GLY:O	1:D:280:ILE:HG12	2.10	0.52
1:C:178:LEU:HD12	1:C:213:ILE:CG2	2.33	0.52
1:B:52:LEU:HD11	1:B:158:PHE:CD1	2.45	0.52
1:B:237:THR:HG23	1:B:242:TRP:CE3	2.44	0.52
1:D:36:GLU:HG2	1:D:89:SER:HA	1.92	0.52
1:B:67:TYR:CE2	1:B:215:VAL:HG22	2.45	0.52
1:C:198:LEU:O	1:C:202:GLU:HG3	2.10	0.52
1:D:249:ASN:O	1:D:249:ASN:ND2	2.43	0.52
1:A:93:MET:O	1:A:226:ASN:ND2	2.43	0.51
1:A:52:LEU:HD22	1:A:130:ILE:CG2	2.39	0.51
1:C:149:THR:O	1:C:149:THR:HG23	2.08	0.51
1:C:162:LEU:HD11	1:C:166:MET:SD	2.50	0.51
1:B:149:THR:HG23	1:B:149:THR:O	2.11	0.51
1:A:72:LEU:HA	1:A:211:VAL:HG22	1.93	0.51
1:B:198:LEU:CD1	1:B:202:GLU:CA	2.88	0.51
1:B:35:ARG:HG3	1:B:88:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:HA	1:D:211:VAL:HG22	1.93	0.51
1:B:40:GLU:HA	1:B:93:MET:CE	2.41	0.51
1:B:105:GLY:O	1:B:106:ARG:HG2	2.11	0.51
1:B:59:VAL:HB	1:B:60:LEU:HD12	1.93	0.51
1:C:154:THR:HG1	1:C:242:TRP:HZ2	1.58	0.51
1:D:150:GLY:N	1:D:151:PRO:CD	2.73	0.51
1:D:93:MET:O	1:D:226:ASN:ND2	2.44	0.51
1:B:149:THR:OG1	1:B:151:PRO:CD	2.58	0.51
1:C:119:GLN:O	1:C:228:SER:OG	2.28	0.51
1:C:255:TRP:O	1:C:258:VAL:HG12	2.10	0.51
1:A:68:LEU:HD22	1:C:69:GLY:HA2	1.93	0.51
1:B:182:LEU:HA	1:B:209:LEU:HD21	1.92	0.51
1:D:60:LEU:HD11	1:D:138:ILE:CD1	2.41	0.51
1:B:193:GLU:O	1:D:87:ARG:NH1	2.44	0.51
1:C:198:LEU:HD22	1:C:201:THR:OG1	2.11	0.51
1:A:32:LYS:HB3	1:A:35:ARG:NE	2.26	0.50
1:B:32:LYS:NZ	1:B:35:ARG:HB3	2.26	0.50
1:D:33:MET:SD	1:D:115:TYR:HE1	2.34	0.50
1:D:33:MET:HE1	1:D:114:VAL:HG13	1.94	0.50
1:D:186:LEU:HD11	2:D:403:GOL:H31	1.92	0.50
1:A:182:LEU:HA	1:A:209:LEU:HD21	1.93	0.50
1:A:255:TRP:O	1:A:258:VAL:HG12	2.12	0.50
1:C:48:MET:O	1:C:52:LEU:N	2.25	0.50
1:D:44:THR:OG1	1:D:93:MET:SD	2.58	0.50
1:A:149:THR:OG1	1:A:151:PRO:CD	2.60	0.50
1:D:57:HIS:CG	1:D:63:LYS:HD3	2.47	0.50
1:B:60:LEU:HB3	1:B:137:ALA:HB1	1.94	0.50
1:C:98:THR:HG22	1:C:112:PHE:HD1	1.76	0.50
1:D:149:THR:OG1	1:D:151:PRO:CD	2.60	0.50
1:D:161:TYR:CG	1:D:249:ASN:OD1	2.65	0.50
1:B:72:LEU:HA	1:B:211:VAL:HG22	1.93	0.50
1:B:216:SER:OG	1:B:217:LEU:HD12	2.11	0.50
1:C:33:MET:HE1	1:C:114:VAL:HG13	1.94	0.50
1:B:167:THR:HG21	1:B:169:TRP:CH2	2.45	0.50
1:D:111:LYS:HD3	1:D:115:TYR:OH	2.12	0.50
1:B:66:SER:HB3	1:D:64:TYR:O	2.12	0.50
1:C:111:LYS:HD3	1:C:115:TYR:CZ	2.47	0.50
1:C:249:ASN:O	1:C:249:ASN:ND2	2.45	0.49
1:C:192:GLN:NE2	1:C:193:GLU:OE2	2.46	0.49
1:B:178:LEU:HD21	1:B:217:LEU:HD13	1.95	0.49
1:B:253:TRP:CZ3	1:B:256:VAL:HG11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG21	1:D:146:LEU:O	2.12	0.49
1:A:178:LEU:HD21	1:A:217:LEU:HD22	1.93	0.49
1:C:160:THR:HG21	1:C:224:ALA:HB2	1.95	0.49
1:C:115:TYR:O	1:C:119:GLN:HG2	2.12	0.49
1:C:149:THR:OG1	1:C:151:PRO:HD2	2.12	0.49
1:D:154:THR:O	1:D:157:ILE:HG12	2.13	0.49
1:A:237:THR:HG23	1:A:242:TRP:CE3	2.48	0.49
1:C:131:TYR:HE1	1:C:138:ILE:HD13	1.78	0.49
1:C:256:VAL:CG1	1:C:257:PRO:HD3	2.42	0.49
1:A:279:THR:HB	1:C:35:ARG:CD	2.42	0.49
1:C:74:PHE:O	1:C:78:VAL:HG23	2.12	0.48
1:A:149:THR:HG23	1:A:149:THR:O	2.13	0.48
1:A:195:ASN:CG	1:A:196:PRO:CD	2.82	0.48
1:C:138:ILE:CG1	1:C:139:LEU:N	2.75	0.48
1:B:194:ASN:O	1:B:195:ASN:O	2.31	0.48
1:D:94:ASN:HB3	1:D:97:VAL:HG22	1.94	0.48
1:A:108:PRO:HG3	1:A:111:LYS:HE2	1.96	0.48
1:D:111:LYS:HB3	1:D:115:TYR:CE1	2.49	0.48
1:A:32:LYS:HG2	1:A:35:ARG:HB2	1.96	0.48
1:A:72:LEU:HD11	1:A:76:PHE:CZ	2.48	0.48
1:B:277:GLY:O	1:B:280:ILE:HG12	2.14	0.48
1:A:219:MET:CB	1:C:57:HIS:CE1	2.96	0.48
1:D:113:PRO:O	1:D:116:VAL:HG12	2.13	0.48
1:D:142:SER:OG	1:D:147:MET:O	2.32	0.48
1:D:178:LEU:HD11	1:D:217:LEU:CB	2.44	0.48
1:D:168:LEU:CD1	1:D:252:ASN:HD22	2.27	0.48
1:A:149:THR:OG1	1:A:151:PRO:HD2	2.14	0.48
1:A:197:ALA:O	1:A:199:PRO:HD3	2.14	0.48
1:D:52:LEU:CG	1:D:130:ILE:HG21	2.43	0.48
1:B:52:LEU:HD22	1:B:130:ILE:HG21	1.96	0.48
1:B:57:HIS:HD1	1:B:61:ASN:HB2	1.79	0.48
1:D:52:LEU:CD2	1:D:130:ILE:HG21	2.44	0.48
1:A:44:THR:OG1	1:A:93:MET:SD	2.59	0.47
1:B:183:GLN:NE2	1:B:187:PHE:CZ	2.82	0.47
1:C:111:LYS:HD3	1:C:115:TYR:CE1	2.49	0.47
1:C:192:GLN:N	1:C:192:GLN:OE1	2.31	0.47
1:C:194:ASN:O	1:C:195:ASN:C	2.51	0.47
1:A:160:THR:HB	1:A:221:THR:O	2.14	0.47
1:B:37:PHE:HD2	1:B:114:VAL:HG12	1.80	0.47
1:B:38:LEU:HD23	1:B:38:LEU:O	2.14	0.47
1:A:117:LEU:HD23	1:A:117:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LYS:O	1:C:115:TYR:CD1	2.67	0.47
1:B:67:TYR:HE1	1:D:65:GLY:HA2	1.80	0.47
1:B:198:LEU:HD12	1:B:202:GLU:CA	2.45	0.47
1:B:267:LEU:HD22	1:B:270:ILE:HD11	1.97	0.47
1:C:94:ASN:CG	1:C:226:ASN:OD1	2.53	0.47
1:B:67:TYR:CE1	1:D:65:GLY:CA	2.98	0.47
1:A:36:GLU:OE1	1:A:115:TYR:OH	2.33	0.47
1:C:138:ILE:HG13	1:C:139:LEU:N	2.30	0.47
1:D:237:THR:HG23	1:D:242:TRP:CE3	2.50	0.47
1:D:256:VAL:CG1	1:D:257:PRO:HD3	2.44	0.47
1:D:32:LYS:CG	1:D:35:ARG:HG3	2.45	0.47
1:D:149:THR:C	1:D:151:PRO:CD	2.83	0.47
1:A:256:VAL:CG1	1:A:257:PRO:HD3	2.45	0.47
1:D:32:LYS:N	1:D:35:ARG:HD2	2.29	0.47
1:C:162:LEU:HD13	1:C:253:TRP:CZ2	2.49	0.47
1:C:105:GLY:O	1:C:106:ARG:HG2	2.15	0.46
1:B:72:LEU:HD11	1:B:76:PHE:CZ	2.50	0.46
1:C:146:LEU:HB2	1:B:152:VAL:HG13	1.98	0.46
1:C:253:TRP:CH2	1:C:256:VAL:HG11	2.50	0.46
1:A:178:LEU:HD11	1:A:217:LEU:CB	2.45	0.46
1:A:40:GLU:HA	1:A:93:MET:CE	2.45	0.46
1:B:195:ASN:OD1	1:B:196:PRO:HD3	2.15	0.46
1:B:228:SER:O	1:B:232:PRO:HG2	2.15	0.46
1:D:115:TYR:O	1:D:119:GLN:HG3	2.16	0.46
1:D:271:ILE:O	1:D:275:PHE:HB2	2.16	0.46
1:B:256:VAL:HG12	1:B:257:PRO:HD3	1.97	0.46
1:C:146:LEU:HB2	1:B:152:VAL:HG11	1.97	0.46
1:C:160:THR:HB	1:C:221:THR:O	2.15	0.46
1:A:135:TYR:O	1:A:138:ILE:HG12	2.15	0.46
1:A:198:LEU:HB3	1:A:201:THR:OG1	2.15	0.46
1:B:36:GLU:OE2	1:B:40:GLU:HG3	2.15	0.46
1:A:102:CYS:CA	1:A:107:VAL:HG12	2.46	0.46
1:B:101:ASN:OD1	1:B:105:GLY:HA3	2.16	0.46
1:C:32:LYS:NZ	1:C:35:ARG:HG2	2.31	0.46
1:B:255:TRP:O	1:B:258:VAL:HG12	2.16	0.46
1:C:195:ASN:CB	1:C:196:PRO:HD3	2.45	0.46
1:A:219:MET:HG2	1:C:61:ASN:HB3	1.97	0.46
1:D:263:LEU:O	1:D:263:LEU:HD23	2.15	0.46
1:C:149:THR:OG1	1:C:151:PRO:CD	2.64	0.46
1:C:39:ALA:HA	1:C:42:MET:HG2	1.96	0.46
1:B:48:MET:O	1:B:52:LEU:N	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:HG2	1:A:111:LYS:HD2	1.98	0.45
1:A:178:LEU:HD21	1:A:217:LEU:HD13	1.99	0.45
1:D:192:GLN:N	1:D:192:GLN:OE1	2.30	0.45
1:D:253:TRP:CZ3	1:D:256:VAL:HG11	2.50	0.45
1:A:102:CYS:SG	1:A:107:VAL:CG1	3.04	0.45
1:B:206:ILE:O	1:B:210:VAL:HG23	2.17	0.45
1:C:172:PHE:CZ	1:C:259:VAL:HG13	2.51	0.45
1:D:198:LEU:O	1:D:199:PRO:C	2.55	0.45
1:A:170:ARG:NH1	1:C:136:THR:HG23	2.26	0.45
1:C:82:VAL:CG1	1:C:203:ALA:HB2	2.46	0.45
1:D:271:ILE:HA	1:D:274:VAL:HG12	1.97	0.45
1:A:45:TYR:O	1:A:49:VAL:HG22	2.17	0.45
1:B:173:LEU:HD22	1:D:133:LEU:HD23	1.98	0.45
1:D:130:ILE:HD11	1:D:134:PHE:CE1	2.52	0.45
1:A:146:LEU:HD23	1:D:152:VAL:HA	1.98	0.45
1:D:184:LEU:HD12	1:D:271:ILE:HG13	1.98	0.45
1:D:72:LEU:HD11	1:D:76:PHE:CZ	2.51	0.45
1:B:33:MET:CE	1:B:114:VAL:HB	2.45	0.45
1:D:216:SER:OG	1:D:217:LEU:HD12	2.16	0.45
1:D:228:SER:O	1:D:232:PRO:HG2	2.16	0.45
1:D:206:ILE:HD13	2:D:403:GOL:O1	2.15	0.45
1:A:212:ILE:HD11	1:C:76:PHE:HB3	1.99	0.45
1:B:198:LEU:HD13	1:B:201:THR:CB	2.45	0.45
1:A:88:ILE:HD12	1:A:89:SER:CB	2.46	0.45
1:A:277:GLY:O	1:A:280:ILE:HG12	2.16	0.45
1:B:178:LEU:HD11	1:B:217:LEU:HB3	1.98	0.45
1:D:82:VAL:HG22	2:D:403:GOL:C1	2.46	0.45
1:B:160:THR:HG21	1:B:224:ALA:HB2	1.99	0.45
1:B:164:ASP:OD1	1:B:164:ASP:N	2.47	0.45
1:B:274:VAL:HG13	1:B:275:PHE:HD1	1.80	0.45
1:C:276:ILE:HA	1:C:279:THR:HB	1.98	0.45
1:A:108:PRO:HG2	1:A:111:LYS:CD	2.46	0.44
1:B:36:GLU:OE1	1:B:115:TYR:CE1	2.70	0.44
1:C:183:GLN:NE2	1:C:187:PHE:CZ	2.86	0.44
1:D:182:LEU:CD1	1:D:225:ILE:HG21	2.38	0.44
1:D:32:LYS:HD2	1:D:34:VAL:HG12	2.00	0.44
1:A:182:LEU:HD22	1:A:225:ILE:HG21	1.99	0.44
1:A:36:GLU:HB3	1:A:115:TYR:OH	2.17	0.44
1:B:212:ILE:O	1:B:215:VAL:HG12	2.17	0.44
1:B:32:LYS:O	1:B:35:ARG:HG2	2.18	0.44
1:D:60:LEU:HB3	1:D:137:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:HZ	1:A:125:LEU:HD22	1.82	0.44
1:A:33:MET:HE3	1:A:111:LYS:HG2	1.99	0.44
1:A:33:MET:O	1:A:36:GLU:N	2.50	0.44
1:B:80:MET:O	1:B:84:VAL:HG12	2.17	0.44
1:A:223:TYR:O	1:A:223:TYR:CD2	2.71	0.44
1:A:39:ALA:O	1:A:42:MET:HG2	2.17	0.44
1:B:67:TYR:CZ	1:D:63:LYS:HD2	2.53	0.44
1:B:187:PHE:O	1:B:191:ASP:HB2	2.18	0.44
1:D:111:LYS:O	1:D:115:TYR:CD1	2.71	0.44
1:D:36:GLU:OE1	1:D:115:TYR:CE1	2.70	0.44
1:B:149:THR:C	1:B:151:PRO:CD	2.85	0.44
1:C:146:LEU:O	1:B:152:VAL:HG21	2.17	0.44
1:C:152:VAL:HB	1:B:146:LEU:HB3	1.98	0.44
1:C:230:ASP:O	1:C:234:ARG:HG3	2.18	0.44
1:C:268:GLY:O	1:C:271:ILE:HG22	2.17	0.44
1:D:160:THR:HB	1:D:221:THR:O	2.18	0.44
1:D:248:SER:HA	1:D:252:ASN:O	2.17	0.44
1:A:216:SER:OG	1:A:217:LEU:HD12	2.18	0.44
1:B:162:LEU:HD11	1:B:166:MET:HG3	2.00	0.44
1:B:41:PHE:HZ	1:B:125:LEU:HD22	1.83	0.44
1:C:67:TYR:HE2	1:C:219:MET:HB2	1.82	0.44
1:C:41:PHE:HZ	1:C:125:LEU:HD22	1.82	0.44
1:D:162:LEU:HD12	1:D:163:PRO:CD	2.47	0.44
1:A:194:ASN:OD1	1:C:87:ARG:CB	2.66	0.44
1:B:111:LYS:HD3	1:B:115:TYR:OH	2.17	0.44
1:B:253:TRP:O	1:B:253:TRP:CG	2.71	0.44
1:B:67:TYR:HE1	1:D:64:TYR:O	2.00	0.44
1:A:107:VAL:HG22	1:A:108:PRO:HD2	2.00	0.43
1:A:37:PHE:CZ	1:A:118:GLY:CA	3.01	0.43
1:A:168:LEU:HD13	1:A:252:ASN:O	2.19	0.43
1:A:160:THR:HG21	1:A:224:ALA:HB2	2.00	0.43
1:A:80:MET:O	1:A:84:VAL:HG12	2.18	0.43
1:C:237:THR:HG23	1:C:242:TRP:CE3	2.52	0.43
1:C:163:PRO:HG3	1:C:219:MET:O	2.18	0.43
1:C:78:VAL:HG11	2:C:403:GOL:C1	2.48	0.43
1:D:168:LEU:HD11	1:D:252:ASN:HD22	1.84	0.43
1:A:162:LEU:HD11	1:A:166:MET:HG3	2.00	0.43
1:B:163:PRO:CD	1:B:220:ASN:O	2.66	0.43
1:C:45:TYR:CE1	1:C:126:ALA:HA	2.52	0.43
1:C:178:LEU:CD1	1:C:213:ILE:HG23	2.40	0.43
1:A:116:VAL:HA	1:A:119:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:HA	1:A:130:ILE:HG22	2.01	0.43
1:A:166:MET:SD	1:A:220:ASN:O	2.76	0.43
1:B:163:PRO:HD3	1:B:220:ASN:O	2.18	0.43
1:B:67:TYR:CD1	1:D:63:LYS:HD2	2.53	0.43
1:C:72:LEU:HD11	1:C:76:PHE:CZ	2.53	0.43
1:D:150:GLY:N	1:D:151:PRO:HD3	2.34	0.43
1:A:160:THR:HG23	1:A:229:ARG:HH21	1.84	0.43
1:B:150:GLY:N	1:B:151:PRO:HD3	2.33	0.43
1:C:276:ILE:O	1:C:279:THR:HB	2.19	0.43
1:C:36:GLU:OE1	1:C:115:TYR:CE1	2.71	0.43
1:A:107:VAL:CG2	1:A:108:PRO:HD2	2.49	0.43
1:A:164:ASP:OD1	1:A:164:ASP:N	2.50	0.43
1:A:38:LEU:HD22	1:A:42:MET:CE	2.49	0.43
1:B:189:ILE:HG12	1:D:83:HIS:CE1	2.54	0.43
1:D:162:LEU:HD11	1:D:166:MET:HG3	2.00	0.43
1:A:111:LYS:HB3	1:A:115:TYR:CE2	2.53	0.43
1:B:256:VAL:HG13	1:B:257:PRO:HD3	2.01	0.43
1:C:164:ASP:N	1:C:164:ASP:OD1	2.51	0.43
1:D:37:PHE:CD2	1:D:114:VAL:O	2.72	0.43
1:D:52:LEU:HD23	1:D:130:ILE:HG21	2.01	0.43
1:A:152:VAL:HG11	1:D:146:LEU:CB	2.48	0.43
1:C:159:ALA:HA	1:C:229:ARG:HH12	1.84	0.43
1:B:232:PRO:HA	1:B:235:ILE:HG12	1.99	0.42
1:B:161:TYR:CE1	1:B:249:ASN:HB2	2.54	0.42
1:C:94:ASN:HB3	1:C:97:VAL:HG12	2.00	0.42
1:B:195:ASN:CG	1:B:196:PRO:CD	2.87	0.42
1:C:111:LYS:HB3	1:C:115:TYR:CE1	2.54	0.42
1:A:167:THR:HG21	1:A:169:TRP:CH2	2.54	0.42
1:A:267:LEU:O	1:A:267:LEU:HD23	2.19	0.42
1:C:197:ALA:O	1:C:199:PRO:HD3	2.20	0.42
1:C:80:MET:O	1:C:84:VAL:HG12	2.19	0.42
1:D:161:TYR:CE1	1:D:234:ARG:NH1	2.88	0.42
1:D:253:TRP:O	1:D:253:TRP:CG	2.71	0.42
1:A:115:TYR:O	1:A:119:GLN:OE1	2.38	0.42
1:C:182:LEU:HD11	2:C:403:GOL:H12	2.02	0.42
1:D:163:PRO:CD	1:D:220:ASN:O	2.67	0.42
1:D:194:ASN:O	1:D:195:ASN:C	2.57	0.42
1:D:237:THR:O	1:D:242:TRP:HB2	2.20	0.42
1:A:195:ASN:CG	1:A:196:PRO:HD2	2.40	0.42
1:B:148:VAL:HG13	1:B:149:THR:N	2.35	0.42
1:B:205:VAL:HG23	1:D:80:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ILE:O	1:B:275:PHE:HB2	2.19	0.42
1:A:146:LEU:HD23	1:D:152:VAL:HG22	2.01	0.42
1:D:41:PHE:HZ	1:D:125:LEU:HD22	1.85	0.42
1:A:60:LEU:HB3	1:A:137:ALA:HB1	2.01	0.42
1:A:271:ILE:O	1:A:275:PHE:HB2	2.19	0.42
1:D:256:VAL:O	1:D:260:ALA:HB3	2.19	0.42
1:A:145:GLN:O	1:A:145:GLN:HG2	2.19	0.42
1:A:162:LEU:CG	1:A:166:MET:HG3	2.50	0.42
1:A:48:MET:HB3	1:A:126:ALA:CB	2.50	0.42
1:B:154:THR:O	1:B:157:ILE:HG12	2.18	0.42
1:B:162:LEU:HD11	1:B:166:MET:CG	2.50	0.42
1:B:184:LEU:HD12	1:B:271:ILE:HG13	2.02	0.42
1:C:92:HIS:O	1:C:119:GLN:NE2	2.52	0.42
1:D:45:TYR:CE1	1:D:126:ALA:HA	2.54	0.42
1:A:38:LEU:HD23	1:A:38:LEU:O	2.19	0.42
1:D:230:ASP:O	1:D:234:ARG:HG3	2.20	0.42
1:D:232:PRO:HA	1:D:235:ILE:HG12	2.01	0.42
1:D:75:GLY:HA2	1:D:210:VAL:CG1	2.50	0.42
1:A:149:THR:C	1:A:151:PRO:CD	2.88	0.42
1:A:189:ILE:HG23	1:A:198:LEU:HD12	2.02	0.42
1:B:172:PHE:CZ	1:B:259:VAL:HG13	2.55	0.42
1:C:127:ALA:HA	1:C:130:ILE:HG22	2.01	0.42
1:C:145:GLN:O	1:C:145:GLN:HG2	2.20	0.41
1:C:52:LEU:HD22	1:C:130:ILE:HG12	2.02	0.41
1:B:279:THR:CG2	1:D:35:ARG:HG2	2.50	0.41
1:A:194:ASN:O	1:A:195:ASN:O	2.39	0.41
1:A:251:GLU:O	1:A:252:ASN:C	2.59	0.41
1:B:32:LYS:C	1:B:35:ARG:HG2	2.40	0.41
1:D:101:ASN:OD1	1:D:105:GLY:HA3	2.20	0.41
1:C:243:GLY:O	1:C:246:VAL:HG12	2.20	0.41
1:D:149:THR:C	1:D:151:PRO:HD2	2.41	0.41
1:D:185:CYS:CB	1:D:209:LEU:HD22	2.50	0.41
1:A:32:LYS:NZ	1:A:35:ARG:HB2	2.35	0.41
1:A:43:SER:HB3	1:A:93:MET:SD	2.61	0.41
1:D:260:ALA:HB3	1:D:261:PRO:HD3	2.02	0.41
1:A:105:GLY:O	1:A:106:ARG:HG2	2.20	0.41
1:A:37:PHE:CD2	1:A:114:VAL:O	2.74	0.41
1:B:149:THR:C	1:B:151:PRO:HD2	2.40	0.41
1:B:194:ASN:C	1:D:87:ARG:HD3	2.41	0.41
1:B:37:PHE:CD2	1:B:114:VAL:O	2.74	0.41
1:D:162:LEU:HD13	1:D:253:TRP:CZ3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LEU:HD21	1:D:83:HIS:HE1	1.85	0.41
1:A:178:LEU:HD11	1:A:217:LEU:HB3	2.03	0.41
1:B:194:ASN:OD1	1:D:87:ARG:CB	2.69	0.41
1:C:163:PRO:CG	1:C:219:MET:O	2.69	0.41
1:C:234:ARG:NH2	1:C:246:VAL:O	2.54	0.41
1:D:34:VAL:O	1:D:34:VAL:HG22	2.19	0.41
1:A:194:ASN:C	1:C:87:ARG:HD3	2.41	0.41
1:A:276:ILE:HD11	1:C:42:MET:SD	2.61	0.41
1:B:67:TYR:HE2	1:B:215:VAL:HG22	1.84	0.41
1:B:237:THR:O	1:B:242:TRP:HB2	2.21	0.41
1:C:263:LEU:O	1:C:263:LEU:HD23	2.20	0.41
1:D:164:ASP:OD1	1:D:164:ASP:N	2.54	0.41
1:A:154:THR:O	1:A:157:ILE:HG12	2.21	0.41
1:A:178:LEU:HD22	1:A:213:ILE:HG23	2.03	0.41
1:B:223:TYR:CD2	1:B:223:TYR:O	2.74	0.41
1:B:145:GLN:HG2	1:B:145:GLN:O	2.21	0.41
1:C:253:TRP:CZ3	1:C:256:VAL:HG11	2.56	0.41
1:D:145:GLN:HG2	1:D:145:GLN:O	2.21	0.41
1:D:177:TRP:O	1:D:181:MET:HG3	2.20	0.41
1:B:53:GLY:HA2	1:B:130:ILE:HD11	2.03	0.41
1:D:63:LYS:O	1:D:63:LYS:HG3	2.21	0.41
1:A:53:GLY:HA2	1:A:130:ILE:HD11	2.02	0.41
1:B:33:MET:O	1:B:36:GLU:N	2.54	0.41
1:C:59:VAL:HG23	1:C:60:LEU:CG	2.47	0.41
1:C:44:THR:N	1:C:93:MET:SD	2.94	0.41
1:D:223:TYR:CD2	1:D:223:TYR:O	2.74	0.41
1:B:166:MET:SD	1:B:220:ASN:O	2.79	0.40
1:C:39:ALA:HB1	1:C:85:ALA:HB1	2.03	0.40
1:A:189:ILE:HG22	1:A:202:GLU:HG2	2.04	0.40
1:C:216:SER:OG	1:C:217:LEU:HD12	2.21	0.40
1:C:52:LEU:HD11	1:C:158:PHE:CD2	2.56	0.40
1:A:163:PRO:HG3	1:A:219:MET:O	2.21	0.40
1:D:185:CYS:HB2	1:D:209:LEU:HD22	2.03	0.40
1:D:207:GLY:O	1:D:210:VAL:HG12	2.21	0.40
1:D:48:MET:HB3	1:D:126:ALA:CB	2.51	0.40
1:A:44:THR:HG22	1:A:123:SER:OG	2.22	0.40
1:A:248:SER:O	1:A:251:GLU:O	2.39	0.40
1:A:57:HIS:ND1	1:A:61:ASN:HB3	2.36	0.40
1:A:82:VAL:CG1	1:A:203:ALA:HB2	2.52	0.40
1:C:104:LEU:HD11	1:C:273:LEU:HD22	2.02	0.40
1:C:57:HIS:O	1:C:63:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ILE:O	1:B:261:PRO:HB3	2.21	0.40
1:C:166:MET:CE	1:C:220:ASN:HD22	2.34	0.40
1:D:38:LEU:HD23	1:D:38:LEU:O	2.22	0.40

All (2) 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:B:84:VAL:O	1:D:194:ASN:HD21[26_555]	1.51	0.09
1:A:84:VAL:O	1:C:194:ASN:HD21[26_555]	1.51	0.09

## 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	247/376 (66%)	226 (92%)	21 (8%)	0	100	100
1	B	247/376 (66%)	228 (92%)	17 (7%)	2 (1%)	19	58
1	C	247/376 (66%)	230 (93%)	15 (6%)	2 (1%)	19	58
1	D	247/376 (66%)	228 (92%)	16 (6%)	3 (1%)	13	49
All	All	988/1504 (66%)	912 (92%)	69 (7%)	7 (1%)	22	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	252	ASN
1	B	253	TRP
1	D	252	ASN
1	D	253	TRP
1	C	195	ASN
1	B	195	ASN

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Mol	Chain	Res	Type
1	D	195	ASN

### 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	195/304 (64%)	193 (99%)	2 (1%)	76	86
1	B	195/304 (64%)	194 (100%)	1 (0%)	88	93
1	C	195/304 (64%)	191 (98%)	4 (2%)	53	72
1	D	195/304 (64%)	193 (99%)	2 (1%)	76	86
All	All	780/1216 (64%)	771 (99%)	9 (1%)	71	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	TYR
1	A	229	ARG
1	C	57	HIS
1	C	63	LYS
1	C	172	PHE
1	C	229	ARG
1	B	229	ARG
1	D	172	PHE
1	D	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	ASN
1	D	61	ASN
1	D	252	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	C	402	-	5,5,5	0.86	0	5,5,5	0.99	0
2	GOL	D	404	-	5,5,5	0.84	0	5,5,5	0.96	0
2	GOL	B	403	-	5,5,5	0.96	0	5,5,5	1.00	0
2	GOL	D	403	-	5,5,5	0.87	0	5,5,5	1.02	0
2	GOL	C	403	-	5,5,5	0.97	0	5,5,5	0.80	0
2	GOL	B	402	-	5,5,5	0.86	0	5,5,5	0.94	0
2	GOL	D	402	-	5,5,5	0.86	0	5,5,5	1.01	0
2	GOL	B	401	-	5,5,5	1.33	2 (40%)	5,5,5	0.79	0
2	GOL	C	401	-	5,5,5	1.29	1 (20%)	5,5,5	0.84	0
2	GOL	A	401	-	5,5,5	1.11	0	5,5,5	0.97	0
2	GOL	D	401	-	5,5,5	1.25	1 (20%)	5,5,5	1.07	0
2	GOL	A	402	-	5,5,5	0.83	0	5,5,5	0.93	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
2	GOL	C	402	-	-	2/4/4/4	-
2	GOL	D	404	-	-	2/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	D	403	-	-	0/4/4/4	-
2	GOL	C	403	-	-	2/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	GOL	C1-C2	2.27	1.61	1.51
2	D	401	GOL	C1-C2	2.09	1.60	1.51
2	B	401	GOL	C1-C2	2.09	1.60	1.51
2	B	401	GOL	C3-C2	2.04	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	402	GOL	O1-C1-C2-C3
2	C	403	GOL	O1-C1-C2-O2
2	C	403	GOL	O1-C1-C2-C3
2	D	404	GOL	O1-C1-C2-O2
2	A	401	GOL	O2-C2-C3-O3
2	D	404	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	C	402	GOL	O1-C1-C2-O2
2	C	401	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	GOL	7	0
2	C	403	GOL	3	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.