



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:53 pm BST

PDB ID : 5ZEA  
Title : Crystal structure of the nucleotide-free mutant A3B3  
Authors : Maruyama, S.; Suzuki, K.; Mizutani, K.; Saito, Y.; Imai, F.L.; Ishizuka-Katsura, Y.; Shirouzu, M.; Ichiro, Y.; Murata, T.  
Deposited on : 2018-02-27  
Resolution : 3.38 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 : 2.11  
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) : 2.11

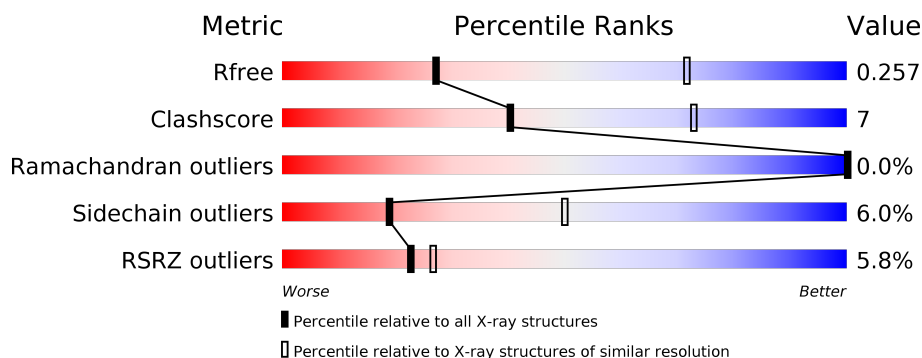
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>17%</span> <span>..</span> </div> </div>
1	B	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 19%, green 78%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>78%</span> <span>19%</span> <span>..</span> </div> </div>
1	C	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 18%, green 79%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>79%</span> <span>18%</span> <span>..</span> </div> </div>
1	G	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 13%, green 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>85%</span> <span>13%</span> <span>..</span> </div> </div>
1	H	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 1%, yellow 17%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>80%</span> <span>17%</span> <span>..</span> </div> </div>
1	I	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 12%, orange 1%, yellow 20%, green 76%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>12%</span> <span>76%</span> <span>20%</span> <span>..</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	462	
2	E	462	
2	F	462	
2	J	462	
2	K	462	
2	L	462	

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
3	GOL	A	601	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47987 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4571	2871	767	907	26			
1	B	586	Total	C	N	O	S	0	0	0
			4471	2800	756	891	24			
1	C	584	Total	C	N	O	S	0	0	0
			4486	2820	751	889	26			
1	G	587	Total	C	N	O	S	0	0	0
			4519	2840	759	894	26			
1	H	586	Total	C	N	O	S	0	0	0
			4489	2815	757	893	24			
1	I	584	Total	C	N	O	S	0	0	0
			4406	2770	736	876	24			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636
G	-6	GLY	-	expression tag	UNP Q08636
G	-5	SER	-	expression tag	UNP Q08636
G	-4	SER	-	expression tag	UNP Q08636
G	-3	GLY	-	expression tag	UNP Q08636
G	-2	SER	-	expression tag	UNP Q08636
G	-1	SER	-	expression tag	UNP Q08636
G	0	GLY	-	expression tag	UNP Q08636
H	-6	GLY	-	expression tag	UNP Q08636
H	-5	SER	-	expression tag	UNP Q08636
H	-4	SER	-	expression tag	UNP Q08636
H	-3	GLY	-	expression tag	UNP Q08636
H	-2	SER	-	expression tag	UNP Q08636
H	-1	SER	-	expression tag	UNP Q08636
H	0	GLY	-	expression tag	UNP Q08636
I	-6	GLY	-	expression tag	UNP Q08636
I	-5	SER	-	expression tag	UNP Q08636
I	-4	SER	-	expression tag	UNP Q08636
I	-3	GLY	-	expression tag	UNP Q08636
I	-2	SER	-	expression tag	UNP Q08636
I	-1	SER	-	expression tag	UNP Q08636
I	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	454	Total	C	N	O	S	0	0	0
			3528	2236	605	673	14			
2	E	452	Total	C	N	O	S	0	0	0
			3449	2184	595	656	14			
2	F	451	Total	C	N	O	S	0	0	0
			3412	2156	589	654	13			
2	J	455	Total	C	N	O	S	0	0	0
			3517	2230	601	672	14			
2	K	454	Total	C	N	O	S	0	0	0
			3502	2220	600	668	14			
2	L	455	Total	C	N	O	S	0	0	0
			3435	2167	589	667	12			

There are 48 discrepancies between the modelled and reference sequences:

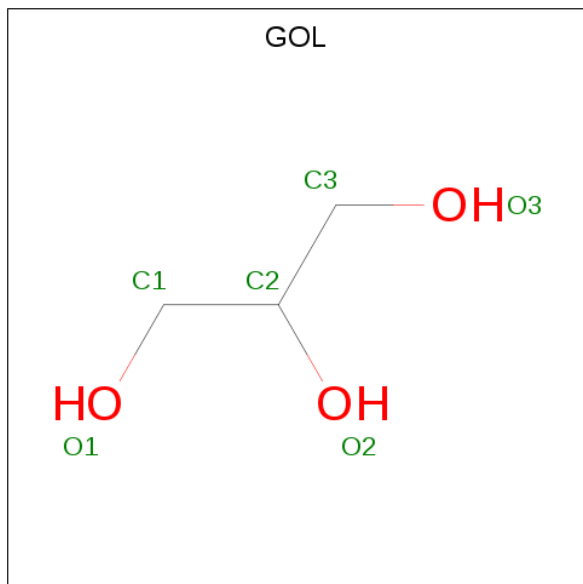
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
D	65	TYR	LEU	engineered mutation	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
E	65	TYR	LEU	engineered mutation	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637
F	65	TYR	LEU	engineered mutation	UNP Q08637
J	-6	GLY	-	expression tag	UNP Q08637
J	-5	SER	-	expression tag	UNP Q08637
J	-4	SER	-	expression tag	UNP Q08637
J	-3	GLY	-	expression tag	UNP Q08637
J	-2	SER	-	expression tag	UNP Q08637
J	-1	SER	-	expression tag	UNP Q08637
J	0	GLY	-	expression tag	UNP Q08637
J	65	TYR	LEU	engineered mutation	UNP Q08637
K	-6	GLY	-	expression tag	UNP Q08637
K	-5	SER	-	expression tag	UNP Q08637
K	-4	SER	-	expression tag	UNP Q08637
K	-3	GLY	-	expression tag	UNP Q08637
K	-2	SER	-	expression tag	UNP Q08637
K	-1	SER	-	expression tag	UNP Q08637
K	0	GLY	-	expression tag	UNP Q08637
K	65	TYR	LEU	engineered mutation	UNP Q08637
L	-6	GLY	-	expression tag	UNP Q08637
L	-5	SER	-	expression tag	UNP Q08637
L	-4	SER	-	expression tag	UNP Q08637

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q08637
L	-2	SER	-	expression tag	UNP Q08637
L	-1	SER	-	expression tag	UNP Q08637
L	0	GLY	-	expression tag	UNP Q08637
L	65	TYR	LEU	engineered mutation	UNP Q08637

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	K	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

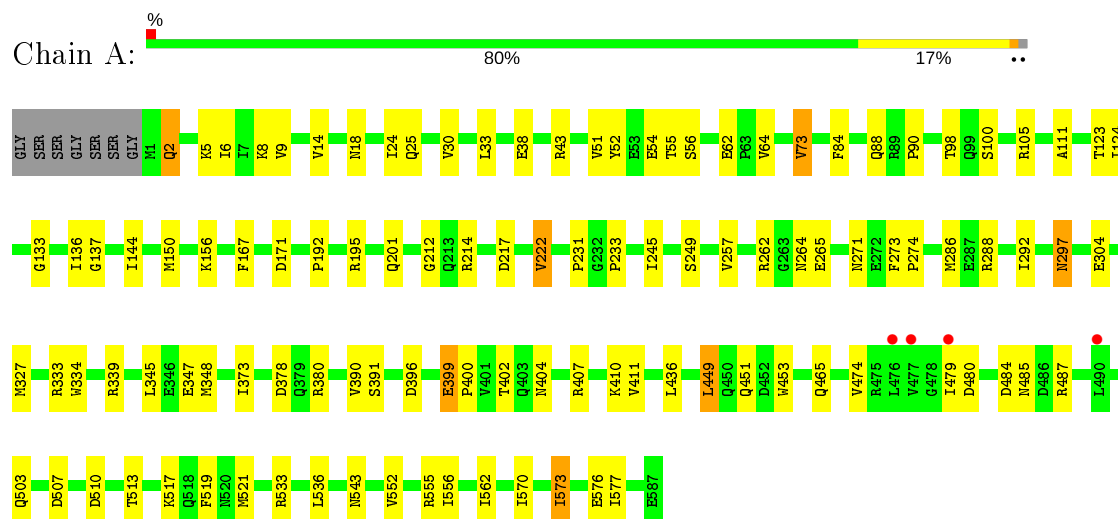
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	3	Total 3	O 3	0	0
4	C	8	Total 8	O 8	0	0
4	D	9	Total 9	O 9	0	0
4	E	9	Total 9	O 9	0	0
4	F	3	Total 3	O 3	0	0
4	G	5	Total 5	O 5	0	0
4	H	10	Total 10	O 10	0	0
4	I	8	Total 8	O 8	0	0
4	J	9	Total 9	O 9	0	0
4	K	6	Total 6	O 6	0	0



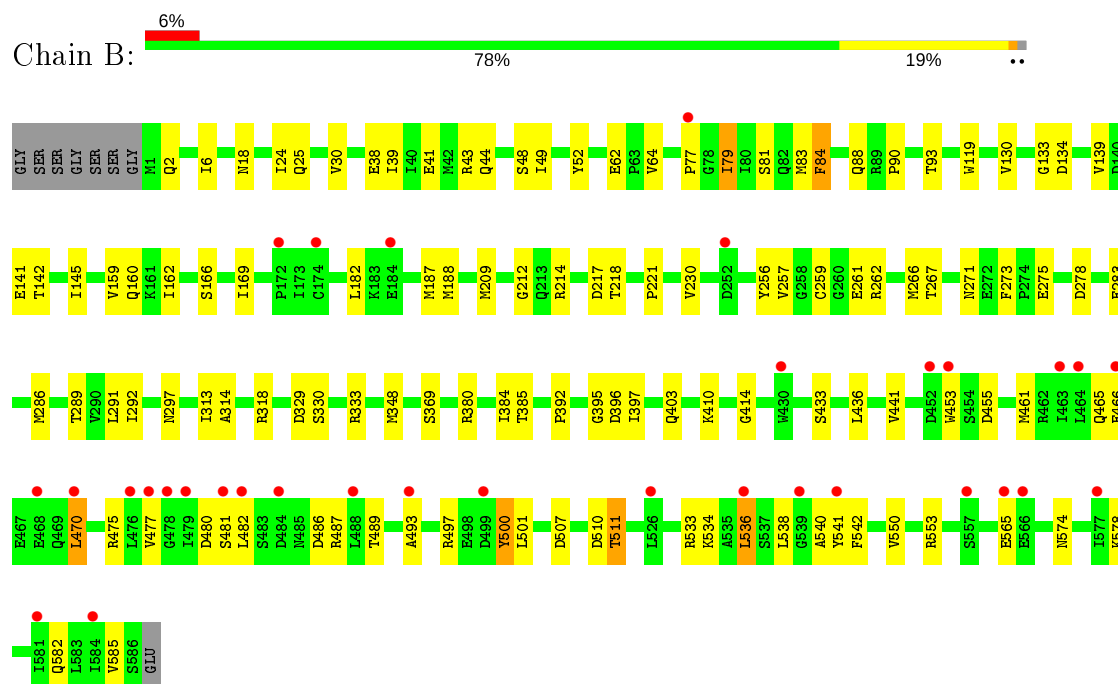
### 3 Residue-property plots

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

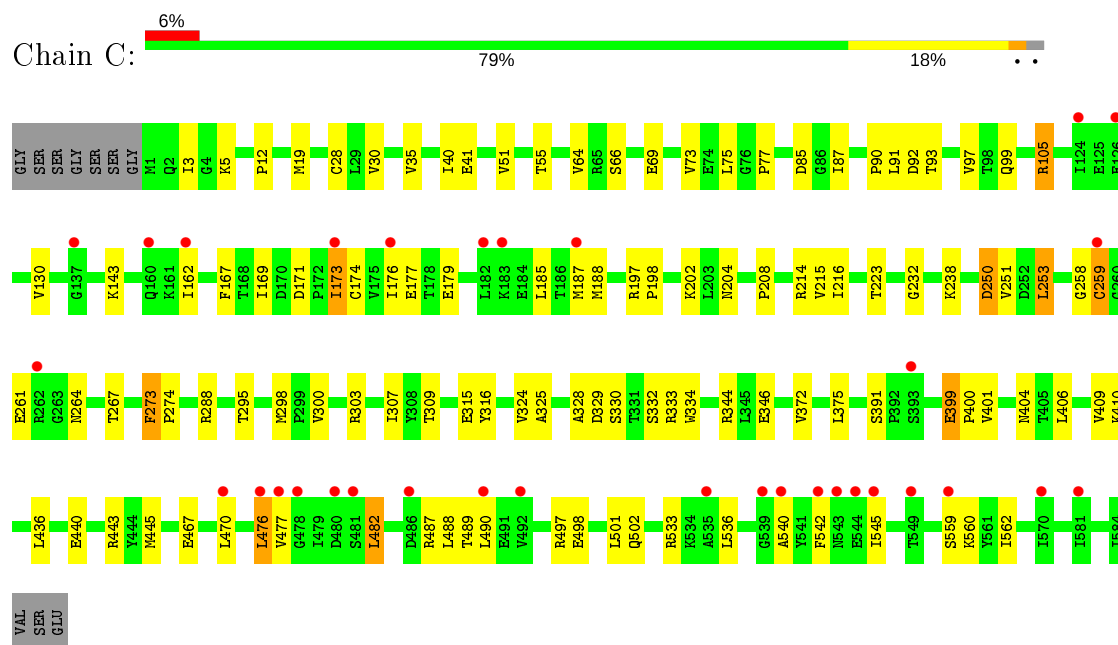
- Molecule 1: V-type sodium ATPase catalytic subunit A



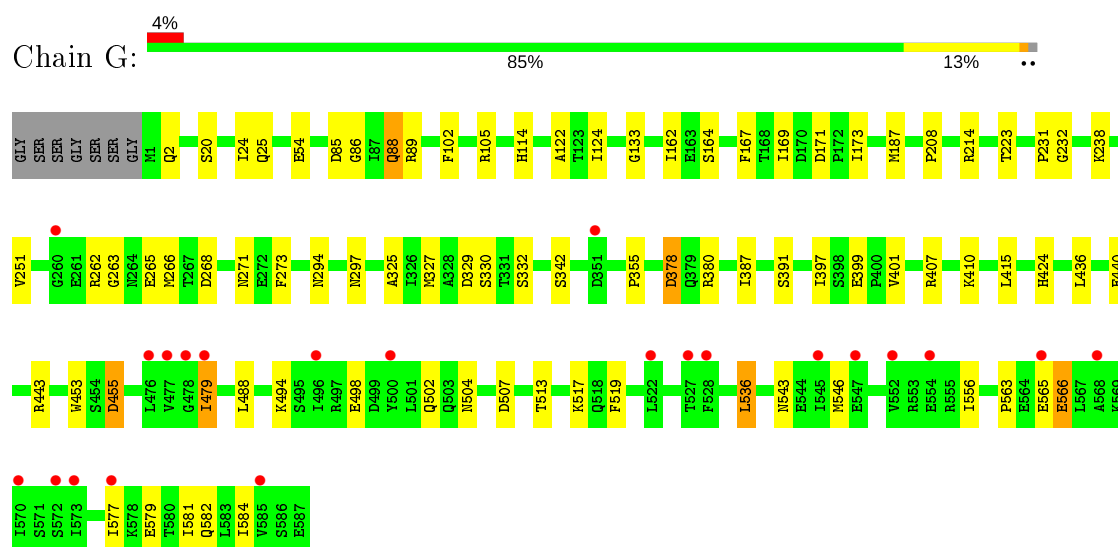
- Molecule 1: V-type sodium ATPase catalytic subunit A



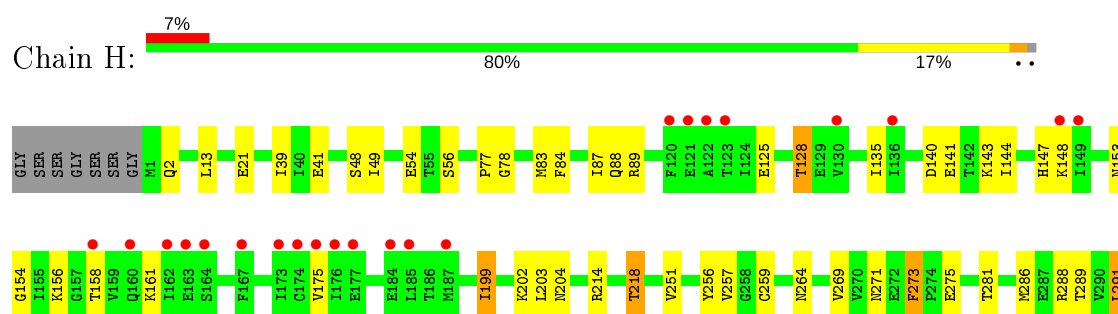
- Molecule 1: V-type sodium ATPase catalytic subunit A

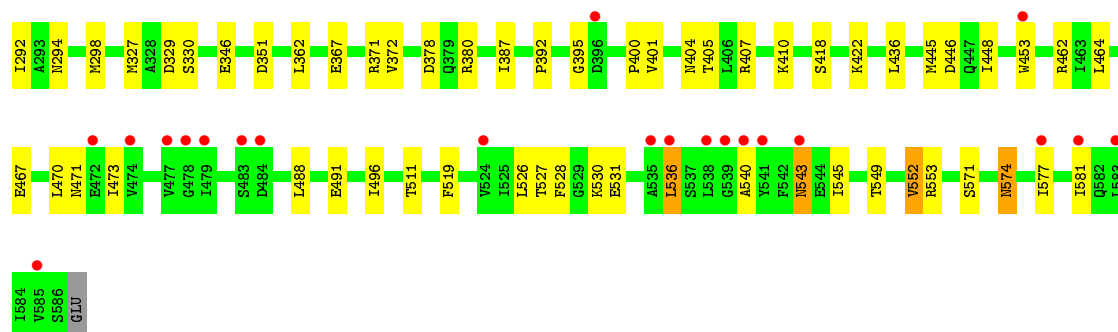


- Molecule 1: V-type sodium ATPase catalytic subunit A

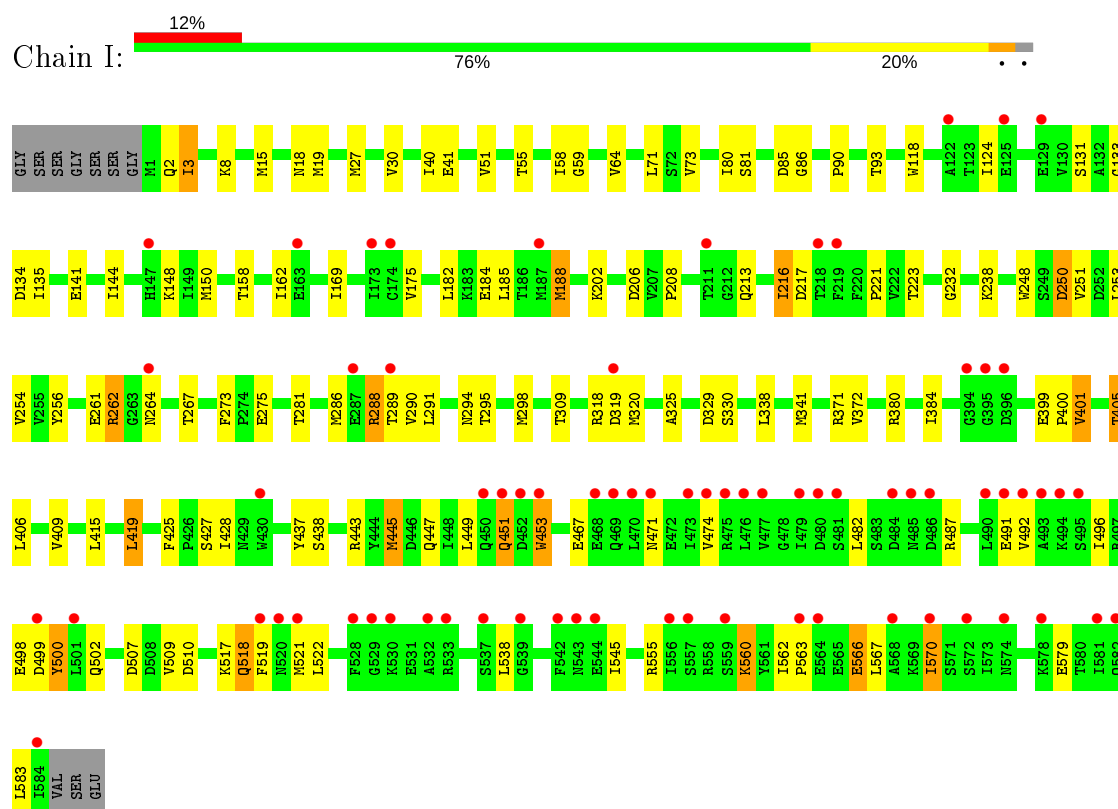


- Molecule 1: V-type sodium ATPase catalytic subunit A

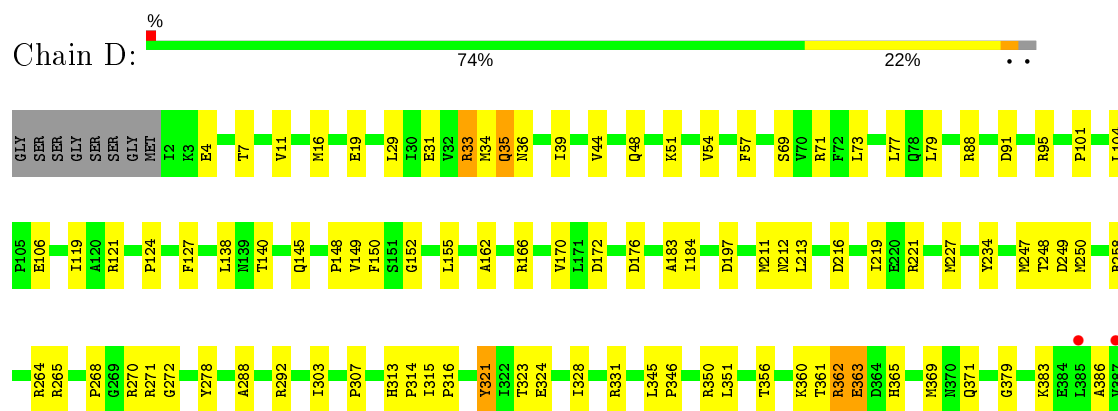




- Molecule 1: V-type sodium ATPase catalytic subunit A

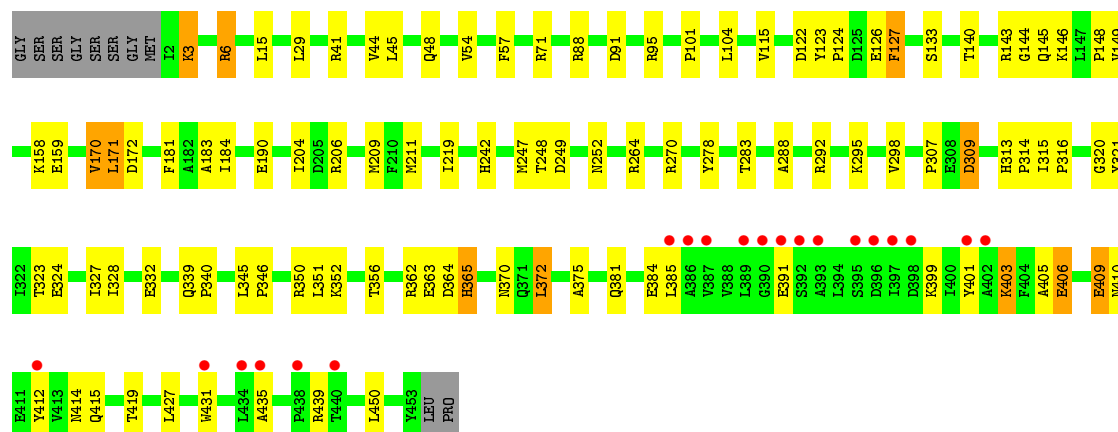
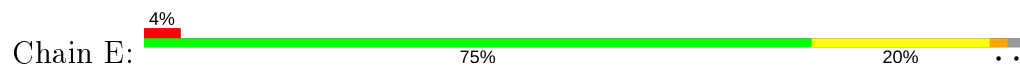


- Molecule 2: V-type sodium ATPase subunit B

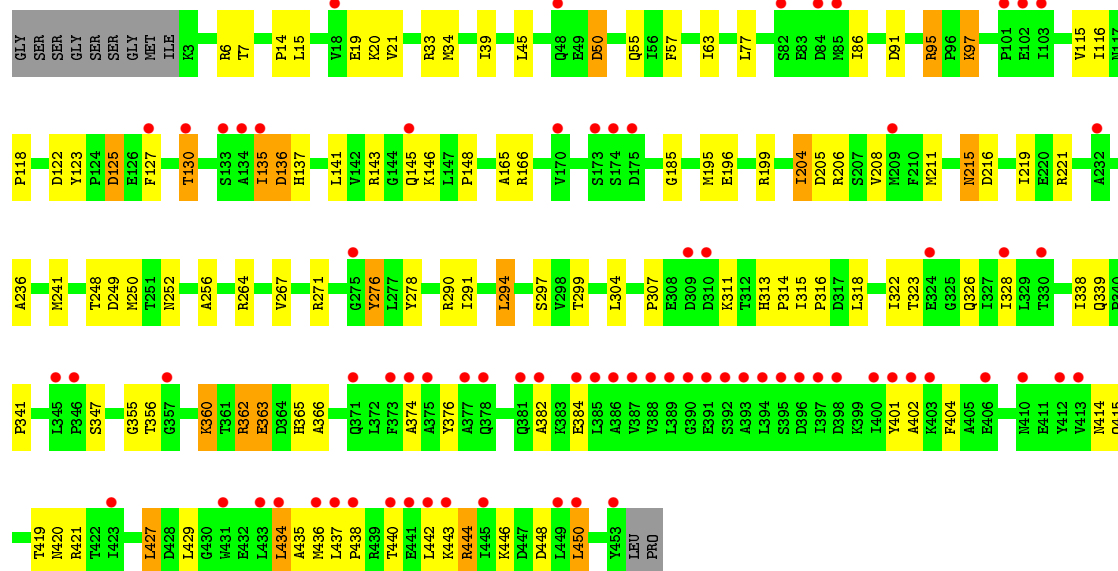
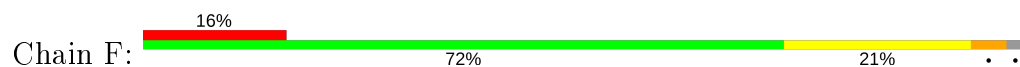




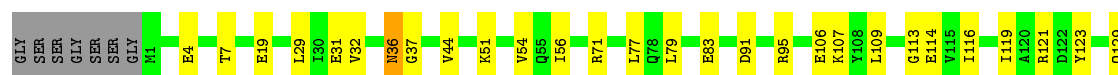
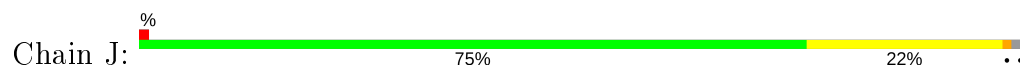
• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.84Å 107.77Å 193.37Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	48.20 – 3.38 48.72 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.20-3.38) 99.0 (48.72-3.38)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.215 , 0.258 0.215 , 0.257	Depositor DCC
$R_{free}$ test set	5088 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 81.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	47987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.24	0/4647	0.40	0/6287
1	B	0.24	0/4547	0.41	0/6166
1	C	0.24	0/4562	0.41	0/6183
1	G	0.24	0/4594	0.40	0/6222
1	H	0.24	0/4565	0.41	0/6187
1	I	0.25	0/4480	0.42	0/6085
2	D	0.25	0/3592	0.42	0/4864
2	E	0.25	0/3512	0.43	0/4762
2	F	0.25	0/3473	0.44	0/4714
2	J	0.25	0/3581	0.42	0/4853
2	K	0.24	0/3566	0.41	0/4835
2	L	0.25	0/3496	0.44	0/4750
All	All	0.24	0/48615	0.42	0/65908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4571	0	4534	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4471	0	4289	57	0
1	C	4486	0	4387	61	0
1	G	4519	0	4451	45	0
1	H	4489	0	4352	56	0
1	I	4406	0	4256	75	0
2	D	3528	0	3497	59	0
2	E	3449	0	3340	60	0
2	F	3412	0	3292	65	0
2	J	3517	0	3472	62	0
2	K	3502	0	3440	45	0
2	L	3435	0	3296	65	0
3	A	36	0	48	0	0
3	C	6	0	8	0	0
3	D	30	0	40	0	0
3	G	18	0	24	0	0
3	H	6	0	8	0	0
3	K	6	0	8	0	0
4	A	30	0	0	1	0
4	B	3	0	0	0	0
4	C	8	0	0	1	0
4	D	9	0	0	1	0
4	E	9	0	0	0	0
4	F	3	0	0	0	0
4	G	5	0	0	1	0
4	H	10	0	0	0	0
4	I	8	0	0	1	0
4	J	9	0	0	0	0
4	K	6	0	0	0	0
All	All	47987	0	46742	684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (684) 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)
2:F:404:PHE:HE2	2:F:436:MET:H	1.09	0.95
1:I:206:ASP:OD2	1:I:371:ARG:NH1	2.08	0.85
2:F:20:LYS:N	2:F:50:ASP:OD2	2.12	0.82
2:J:155:LEU:HD21	2:J:331:ARG:HG2	1.67	0.75
2:F:221:ARG:HE	2:F:256:ALA:HB2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:THR:OG1	2:F:19:GLU:O	2.05	0.74
2:K:48:GLN:HG2	2:K:51:LYS:HE3	1.69	0.74
1:C:476:LEU:HD23	1:C:477:VAL:HG13	1.68	0.74
1:I:250:ASP:N	1:I:250:ASP:OD1	2.22	0.73
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.72	0.72
2:F:404:PHE:HE2	2:F:436:MET:N	1.88	0.71
2:E:328:ILE:HG13	2:E:346:PRO:HB2	1.72	0.71
1:C:215:VAL:HG13	1:C:216:ILE:HD12	1.72	0.71
1:G:232:GLY:HA3	1:G:238:LYS:HD3	1.72	0.70
1:I:175:VAL:HG12	1:I:184:GLU:HB3	1.73	0.70
2:J:362:ARG:NH2	2:J:428:ASP:OD1	2.24	0.70
1:I:399:GLU:HG2	1:I:400:PRO:HD2	1.74	0.70
2:J:119:ILE:O	2:J:292:ARG:NH1	2.25	0.69
2:J:328:ILE:HG13	2:J:346:PRO:HB2	1.74	0.69
2:L:250:MET:HB2	2:L:304:LEU:HB3	1.73	0.69
1:H:571:SER:O	1:H:574:ASN:ND2	2.26	0.69
2:K:123:TYR:HD2	2:K:124:PRO:HD2	1.56	0.68
1:C:300:VAL:HG22	1:C:303:ARG:HH21	1.58	0.68
2:F:145:GLN:H	2:F:299:THR:HG23	1.59	0.67
1:B:574:ASN:O	1:B:578:LYS:NZ	2.27	0.67
1:C:488:LEU:HD23	1:C:533:ARG:HG3	1.77	0.67
1:I:401:VAL:O	1:I:405:THR:OG1	2.13	0.67
1:I:262:ARG:NH2	2:L:323:THR:O	2.27	0.67
1:B:38:GLU:OE1	1:B:52:TYR:OH	2.13	0.67
1:B:133:GLY:O	1:B:380:ARG:NH2	2.28	0.66
2:D:88:ARG:NH1	2:D:101:PRO:O	2.28	0.66
2:J:371:GLN:HG2	2:J:444:ARG:HB2	1.76	0.66
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.76	0.66
1:A:133:GLY:O	1:A:380:ARG:NH2	2.25	0.66
2:D:31:GLU:HG3	2:D:73:LEU:HD21	1.77	0.66
2:K:183:ALA:HB3	2:K:211:MET:HA	1.76	0.66
2:L:431:TRP:HA	2:L:434:LEU:HD23	1.76	0.66
2:L:137:HIS:NE2	2:L:368:THR:O	2.29	0.65
2:F:215:ASN:OD1	2:F:215:ASN:N	2.28	0.65
2:F:338:ILE:HA	2:F:414:ASN:HB2	1.78	0.65
2:J:149:VAL:HB	2:J:303:ILE:HG13	1.78	0.65
1:G:133:GLY:O	1:G:380:ARG:NH2	2.28	0.65
1:I:467:GLU:O	1:I:471:ASN:ND2	2.29	0.65
1:C:261:GLU:CD	1:C:330:SER:H	1.99	0.65
1:A:264:ASN:ND2	2:D:324:GLU:OE2	2.29	0.65
2:F:185:GLY:O	2:F:252:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ASP:O	1:B:511:THR:OG1	2.15	0.65
1:G:262:ARG:HB2	1:G:265:GLU:HB2	1.79	0.64
1:G:271:ASN:OD1	2:J:292:ARG:NH2	2.30	0.64
1:I:517:LYS:NZ	1:I:562:ILE:O	2.30	0.64
2:L:89:VAL:HG12	2:L:209:MET:HB2	1.80	0.64
2:J:333:LEU:HD12	2:J:338:ILE:HG13	1.79	0.64
2:L:133:SER:HB3	2:L:421:ARG:HD2	1.80	0.63
1:C:12:PRO:HG2	1:C:344:ARG:HD2	1.81	0.63
1:G:399:GLU:HG2	1:G:401:VAL:H	1.64	0.63
1:B:297:ASN:HD22	2:E:115:VAL:HG22	1.62	0.62
2:J:36:ASN:N	2:J:37:GLY:HA2	2.14	0.62
1:I:208:PRO:HA	1:I:223:THR:HA	1.81	0.62
2:D:361:THR:HG22	2:D:362:ARG:H	1.63	0.62
2:L:148:PRO:HB3	2:L:302:PRO:HG2	1.82	0.62
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.81	0.62
2:D:386:ALA:HB2	2:D:394:LEU:HD11	1.82	0.61
1:H:527:THR:HG21	1:H:574:ASN:HB2	1.80	0.61
1:A:556:ILE:HD11	1:A:577:ILE:HD11	1.82	0.61
1:C:489:THR:OG1	1:C:533:ARG:NH2	2.33	0.61
1:I:55:THR:HG22	1:I:58:ILE:HD12	1.81	0.61
2:L:133:SER:HB2	2:L:412:TYR:CE1	2.35	0.61
1:B:30:VAL:HA	1:B:64:VAL:HG22	1.82	0.61
1:B:221:PRO:HG3	1:B:441:VAL:HG11	1.82	0.61
2:E:183:ALA:HB3	2:E:211:MET:HA	1.82	0.61
2:F:137:HIS:HA	2:F:365:HIS:HE1	1.64	0.61
1:A:555:ARG:NH1	1:A:576:GLU:OE1	2.34	0.61
1:C:202:LYS:HG3	1:C:372:VAL:HG12	1.82	0.61
2:J:7:THR:OG1	2:J:19:GLU:O	2.14	0.61
1:C:214:ARG:NH2	1:C:502:GLN:O	2.34	0.61
1:G:440:GLU:OE1	1:G:443:ARG:NH1	2.34	0.60
1:A:271:ASN:OD1	2:D:292:ARG:NH2	2.34	0.60
1:G:232:GLY:HA2	1:G:415:LEU:HD12	1.83	0.60
2:D:149:VAL:HB	2:D:303:ILE:HG13	1.83	0.60
2:L:40:ARG:NH1	2:L:59:GLY:O	2.34	0.60
1:I:319:ASP:O	1:I:380:ARG:NH1	2.34	0.60
2:F:55:GLN:OE1	2:F:264:ARG:NH1	2.34	0.60
1:I:482:LEU:HD22	1:I:487:ARG:HH11	1.67	0.60
2:J:324:GLU:HB3	2:J:350:ARG:HB2	1.84	0.60
1:B:318:ARG:HB2	1:B:384:ILE:HD11	1.84	0.59
1:C:232:GLY:HA3	1:C:238:LYS:HD3	1.83	0.59
2:E:415:GLN:O	2:E:419:THR:OG1	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:ASP:OD1	1:G:86:GLY:N	2.35	0.59
2:E:45:LEU:HD13	2:E:264:ARG:HD3	1.84	0.59
2:K:250:MET:HB2	2:K:304:LEU:HB3	1.84	0.59
1:C:250:ASP:N	1:C:250:ASP:OD1	2.33	0.59
2:K:155:LEU:HD21	2:K:331:ARG:HG2	1.85	0.59
1:I:406:LEU:HA	1:I:409:VAL:HG22	1.85	0.59
1:I:232:GLY:HA3	1:I:238:LYS:HD3	1.84	0.59
1:H:549:THR:HA	1:H:552:VAL:HG12	1.84	0.58
1:G:24:ILE:HG22	1:G:25:GLN:HG2	1.85	0.58
2:J:185:GLY:O	2:J:252:ASN:ND2	2.36	0.58
2:L:221:ARG:HE	2:L:256:ALA:HB2	1.68	0.58
2:L:183:ALA:HB3	2:L:211:MET:HA	1.85	0.58
1:B:267:THR:O	1:B:271:ASN:ND2	2.36	0.58
1:H:39:ILE:HG12	1:H:49:ILE:HG12	1.86	0.58
2:F:165:ALA:O	2:F:206:ARG:NH1	2.36	0.58
2:K:450:LEU:HD22	2:K:454:LEU:HD12	1.86	0.58
2:E:364:ASP:OD2	2:E:431:TRP:NE1	2.36	0.57
2:K:82:SER:HB2	2:K:105:PRO:HA	1.86	0.57
1:C:406:LEU:HA	1:C:409:VAL:HG22	1.86	0.57
2:L:150:PHE:N	2:L:327:ILE:O	2.29	0.57
2:D:29:LEU:HD21	2:D:77:LEU:HG	1.86	0.57
2:J:31:GLU:OE2	2:J:71:ARG:NE	2.35	0.57
1:I:150:MET:HE1	1:I:320:MET:HA	1.86	0.57
2:L:82:SER:HB2	2:L:105:PRO:HA	1.87	0.57
2:J:176:ASP:OD1	2:J:176:ASP:N	2.37	0.57
2:J:324:GLU:HA	2:J:350:ARG:HD2	1.86	0.57
1:A:90:PRO:HD3	1:A:111:ALA:HA	1.85	0.57
1:B:333:ARG:NH1	2:E:278:TYR:OH	2.37	0.57
1:I:51:VAL:HG21	1:I:55:THR:HG23	1.87	0.57
1:I:40:ILE:HG13	1:I:41:GLU:HG2	1.86	0.56
2:L:55:GLN:OE1	2:L:264:ARG:NH2	2.37	0.56
1:I:451:GLN:HG3	1:I:519:PHE:CE2	2.40	0.56
1:B:130:VAL:HG13	1:B:134:ASP:HB2	1.88	0.56
1:C:198:PRO:HB2	1:C:375:LEU:HD11	1.88	0.56
2:E:171:LEU:HD12	2:E:171:LEU:H	1.70	0.56
1:A:124:ILE:HB	1:A:136:ILE:HA	1.87	0.56
1:B:565:GLU:OE1	1:B:565:GLU:N	2.39	0.56
1:G:85:ASP:HB3	1:G:89:ARG:H	1.70	0.56
2:L:166:ARG:NH2	2:L:417:PHE:O	2.39	0.56
1:H:346:GLU:O	2:L:265:ARG:NH2	2.34	0.56
2:D:170:VAL:HG12	2:D:172:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:ILE:O	2:D:292:ARG:NH1	2.39	0.56
1:A:400:PRO:O	1:A:404:ASN:ND2	2.38	0.56
1:B:477:VAL:HG13	1:B:481:SER:HB3	1.88	0.56
2:L:50:ASP:N	2:L:50:ASP:OD1	2.38	0.56
2:E:406:GLU:O	2:E:410:ASN:ND2	2.36	0.56
1:G:167:PHE:HB3	1:G:171:ASP:HB2	1.88	0.55
1:H:410:LYS:HB3	1:H:436:LEU:HB2	1.88	0.55
1:H:445:MET:HA	1:H:448:ILE:HG22	1.88	0.55
1:A:54:GLU:O	1:A:105:ARG:NH1	2.39	0.55
1:C:536:LEU:HA	1:C:540:ALA:HB3	1.88	0.55
1:G:208:PRO:HA	1:G:223:THR:HA	1.86	0.55
1:H:470:LEU:HD13	1:H:473:ILE:HD12	1.87	0.55
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.88	0.55
2:F:33:ARG:HG2	2:F:39:ILE:HG12	1.89	0.55
1:G:54:GLU:HB2	1:G:105:ARG:HD3	1.88	0.55
1:B:318:ARG:HD3	1:B:384:ILE:HG12	1.87	0.55
1:I:133:GLY:O	1:I:380:ARG:NH2	2.40	0.55
2:K:361:THR:HG22	2:K:362:ARG:H	1.72	0.55
2:L:166:ARG:HD3	2:L:201:THR:HG21	1.87	0.55
2:D:183:ALA:HB3	2:D:211:MET:HA	1.90	0.55
2:D:91:ASP:OD1	2:D:95:ARG:N	2.37	0.54
1:C:467:GLU:OE2	1:C:497:ARG:NH1	2.40	0.54
1:I:30:VAL:HA	1:I:64:VAL:HG22	1.89	0.54
1:I:567:LEU:HA	1:I:570:ILE:HD11	1.90	0.54
2:J:29:LEU:HD11	2:J:77:LEU:HD23	1.89	0.54
1:H:294:ASN:ND2	1:H:298:MET:SD	2.78	0.54
2:K:315:ILE:HB	2:K:316:PRO:HD3	1.90	0.54
2:J:315:ILE:HB	2:J:316:PRO:HD3	1.89	0.54
1:B:392:PRO:HG2	1:B:395:GLY:HA2	1.90	0.54
1:H:161:LYS:HB3	1:H:175:VAL:HB	1.90	0.54
1:H:453:TRP:HZ3	1:H:519:PHE:HA	1.72	0.54
1:H:528:PHE:HD1	1:H:577:ILE:HD12	1.73	0.54
2:J:338:ILE:HG23	2:J:414:ASN:HB2	1.89	0.54
1:C:73:VAL:HG11	1:C:309:THR:HG23	1.89	0.54
1:I:124:ILE:HG22	1:I:162:ILE:HD13	1.90	0.54
2:F:148:PRO:HD3	2:F:323:THR:HB	1.90	0.53
2:D:166:ARG:NH1	2:D:197:ASP:OD2	2.41	0.53
2:E:365:HIS:HB2	2:E:427:LEU:HD21	1.89	0.53
2:E:143:ARG:HH12	2:E:242:HIS:CE1	2.25	0.53
1:G:378:ASP:N	1:G:378:ASP:OD1	2.41	0.53
1:H:141:GLU:OE1	1:H:147:HIS:ND1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:ASP:OD1	1:I:86:GLY:N	2.40	0.53
2:D:155:LEU:HD21	2:D:331:ARG:HG2	1.89	0.53
1:A:297:ASN:N	1:A:297:ASN:OD1	2.32	0.53
2:E:124:PRO:HG3	2:E:351:LEU:HD13	1.89	0.53
1:I:148:LYS:NZ	4:I:601:HOH:O	2.41	0.53
2:E:133:SER:HB3	2:E:412:TYR:CE2	2.44	0.53
2:J:91:ASP:OD1	2:J:95:ARG:N	2.41	0.53
1:I:499:ASP:O	1:I:560:LYS:HG2	2.09	0.53
2:K:138:LEU:HD13	2:K:369:MET:HG3	1.90	0.53
1:B:256:TYR:HB3	1:B:291:LEU:HG	1.91	0.53
2:J:116:ILE:HD11	2:J:121:ARG:NH2	2.24	0.53
1:A:222:VAL:HG23	1:A:411:VAL:HG21	1.90	0.52
1:B:41:GLU:OE2	1:B:43:ARG:NH2	2.42	0.52
2:F:356:THR:HG21	2:F:366:ALA:HB2	1.91	0.52
1:I:518:GLN:NE2	1:I:522:LEU:HB2	2.24	0.52
2:K:91:ASP:OD1	2:K:95:ARG:N	2.42	0.52
1:B:218:THR:HG23	1:B:453:TRP:HZ2	1.74	0.52
2:J:271:ARG:HH11	2:J:314:PRO:HD3	1.74	0.52
2:J:407:ARG:NH2	2:J:411:GLU:OE2	2.43	0.52
1:G:565:GLU:OE1	1:G:565:GLU:N	2.42	0.52
1:A:562:ILE:HB	1:A:570:ILE:HD11	1.91	0.52
2:E:88:ARG:NH1	2:E:101:PRO:O	2.42	0.52
2:J:235:LEU:HB3	2:J:241:MET:HE2	1.92	0.52
1:C:400:PRO:O	1:C:404:ASN:ND2	2.29	0.52
2:L:57:PHE:HA	2:L:219:ILE:HD13	1.92	0.52
2:E:158:LYS:HD3	2:E:190:GLU:HG3	1.92	0.52
2:K:33:ARG:HE	2:K:71:ARG:HH11	1.56	0.52
2:L:408:PHE:O	2:L:413:VAL:HG13	2.10	0.52
2:D:406:GLU:O	2:D:410:ASN:ND2	2.40	0.52
2:D:438:PRO:HG2	2:D:441:GLU:HG2	1.92	0.52
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.91	0.52
2:F:415:GLN:O	2:F:419:THR:OG1	2.19	0.52
1:H:84:PHE:HB3	1:H:88:GLN:HA	1.92	0.52
2:D:324:GLU:HA	2:D:350:ARG:HD2	1.92	0.51
2:E:145:GLN:HG3	2:E:351:LEU:HD12	1.91	0.51
2:F:125:ASP:N	2:F:125:ASP:OD1	2.43	0.51
1:C:440:GLU:OE1	1:C:443:ARG:NH1	2.43	0.51
2:F:21:VAL:HG22	2:F:50:ASP:O	2.10	0.51
2:J:151:SER:OG	2:J:152:GLY:N	2.43	0.51
1:G:407:ARG:NH2	2:K:252:ASN:OD1	2.33	0.51
1:A:262:ARG:NH1	1:A:265:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:VAL:HA	1:C:64:VAL:HG22	1.92	0.51
1:I:425:PHE:H	1:I:502:GLN:HG2	1.75	0.51
1:A:144:ILE:HG21	1:A:288:ARG:HD3	1.91	0.51
1:B:39:ILE:HG12	1:B:49:ILE:HG12	1.91	0.51
2:E:242:HIS:NE2	2:E:295:LYS:O	2.39	0.51
2:F:442:LEU:HD23	2:F:450:LEU:HD22	1.92	0.51
1:H:257:VAL:HA	1:H:292:ILE:HB	1.90	0.51
1:I:85:ASP:OD1	1:I:294:ASN:ND2	2.40	0.51
1:H:378:ASP:OD2	1:H:380:ARG:NH2	2.44	0.51
1:I:202:LYS:HG3	1:I:372:VAL:HG12	1.91	0.51
1:A:8:LYS:HG3	2:D:48:GLN:HB3	1.92	0.51
2:F:315:ILE:HB	2:F:316:PRO:HD3	1.93	0.51
2:F:328:ILE:H	2:F:347:SER:HB3	1.75	0.51
1:G:263:GLY:N	4:G:701:HOH:O	2.44	0.51
1:I:507:ASP:HB3	1:I:510:ASP:HB3	1.93	0.51
2:K:372:LEU:HD23	2:K:408:PHE:HE1	1.76	0.51
1:B:286:MET:HA	1:B:289:THR:HG22	1.93	0.51
1:B:6:ILE:HD12	1:B:62:GLU:HB2	1.92	0.51
2:D:11:VAL:HG22	2:D:16:MET:HG3	1.92	0.51
2:L:434:LEU:HA	2:L:437:LEU:HD12	1.93	0.51
2:E:127:PHE:HE1	2:E:171:LEU:HD11	1.77	0.50
2:E:356:THR:HG22	2:E:365:HIS:CE1	2.46	0.50
1:I:261:GLU:OE2	1:I:330:SER:N	2.44	0.50
1:A:56:SER:O	1:A:105:ARG:NH2	2.35	0.50
1:C:40:ILE:HG13	1:C:41:GLU:HG2	1.94	0.50
2:D:315:ILE:HB	2:D:316:PRO:HD3	1.92	0.50
2:D:4:GLU:HG2	2:D:71:ARG:HG2	1.93	0.50
2:F:278:TYR:HB2	2:F:318:LEU:HD22	1.93	0.50
1:G:479:ILE:HD13	1:G:479:ILE:H	1.76	0.50
1:I:399:GLU:OE1	1:I:401:VAL:HG12	2.12	0.50
1:I:566:GLU:OE1	1:I:567:LEU:N	2.44	0.50
2:D:79:LEU:HD13	2:D:227:MET:HE1	1.94	0.50
1:I:27:MET:HE2	1:I:71:LEU:HB2	1.93	0.50
1:A:407:ARG:NH2	2:E:252:ASN:OD1	2.44	0.50
2:E:324:GLU:HA	2:E:350:ARG:HD2	1.94	0.50
1:G:332:SER:HB2	1:G:391:SER:HB3	1.94	0.50
1:C:51:VAL:HG21	1:C:55:THR:HG23	1.93	0.50
2:E:44:VAL:HG22	2:E:54:VAL:HG12	1.94	0.50
1:H:392:PRO:HG2	1:H:395:GLY:HA2	1.94	0.50
2:J:145:GLN:HG3	2:J:351:LEU:HD12	1.94	0.50
1:I:251:VAL:HG11	1:I:325:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:32:VAL:HG21	2:J:56:ILE:HD12	1.94	0.50
1:B:297:ASN:HB3	2:E:115:VAL:HG13	1.94	0.49
2:F:146:LYS:HD2	2:F:322:ILE:O	2.11	0.49
2:F:116:ILE:HD13	2:F:291:ILE:HD11	1.94	0.49
1:G:2:GLN:HE22	1:G:20:SER:H	1.59	0.49
1:H:256:TYR:HB3	1:H:291:LEU:HD22	1.94	0.49
2:J:121:ARG:NH1	2:J:288:ALA:O	2.45	0.49
2:J:44:VAL:HG22	2:J:54:VAL:HG12	1.94	0.49
1:C:399:GLU:HB3	1:C:401:VAL:HG12	1.95	0.49
2:L:406:GLU:O	2:L:410:ASN:ND2	2.45	0.49
1:B:271:ASN:OD1	2:E:292:ARG:NH2	2.45	0.49
2:L:127:PHE:CE2	2:L:140:THR:HG21	2.47	0.49
2:L:141:LEU:HD23	2:L:141:LEU:H	1.78	0.49
1:A:214:ARG:NH2	1:A:503:GLN:HB3	2.28	0.49
1:B:119:TRP:HA	1:B:166:SER:HA	1.94	0.49
1:G:455:ASP:N	1:G:455:ASP:OD1	2.46	0.49
1:H:271:ASN:OD1	2:K:292:ARG:NH2	2.45	0.49
1:I:451:GLN:HG3	1:I:519:PHE:CZ	2.47	0.49
2:J:313:HIS:HB3	2:J:316:PRO:HD2	1.95	0.49
1:I:144:ILE:HG12	1:I:281:THR:HG21	1.94	0.49
2:J:364:ASP:OD2	2:J:431:TRP:NE1	2.36	0.49
1:A:231:PRO:O	1:A:233:PRO:HD3	2.13	0.49
1:C:28:CYS:HB3	1:C:66:SER:HA	1.95	0.49
1:C:30:VAL:HB	1:C:35:VAL:HG23	1.94	0.49
2:E:133:SER:HB3	2:E:412:TYR:CZ	2.48	0.49
2:F:199:ARG:HG2	2:F:204:ILE:HG21	1.93	0.49
1:G:214:ARG:NH2	1:G:502:GLN:O	2.45	0.49
1:H:144:ILE:HG12	1:H:281:THR:HG21	1.93	0.49
1:I:496:ILE:HA	1:I:499:ASP:OD2	2.13	0.49
2:K:29:LEU:HB3	2:K:73:LEU:HD12	1.95	0.49
1:A:51:VAL:HG11	1:A:55:THR:HG22	1.94	0.49
1:C:251:VAL:HG11	1:C:325:ALA:HB2	1.94	0.49
1:G:513:THR:HG23	1:G:517:LYS:HD3	1.95	0.49
2:F:442:LEU:HD23	2:F:450:LEU:HD13	1.95	0.48
2:K:168:ALA:O	2:K:206:ARG:NH2	2.45	0.48
2:L:407:ARG:NE	2:L:411:GLU:OE1	2.45	0.48
1:B:550:VAL:HG22	1:B:553:ARG:HH21	1.78	0.48
2:E:143:ARG:HH21	2:E:170:VAL:HG11	1.77	0.48
1:H:202:LYS:HG3	1:H:372:VAL:HG12	1.95	0.48
1:I:73:VAL:HG11	1:I:309:THR:HG23	1.94	0.48
2:J:106:GLU:OE1	2:J:234:TYR:OH	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:NH2	2:E:320:GLY:O	2.46	0.48
2:F:248:THR:HA	2:F:249:ASP:HA	1.60	0.48
1:G:102:PHE:HA	2:J:116:ILE:HA	1.94	0.48
2:L:313:HIS:CD2	2:L:315:ILE:HG12	2.48	0.48
1:C:208:PRO:HA	1:C:223:THR:HA	1.95	0.48
1:C:253:LEU:HB3	1:C:324:VAL:HG13	1.95	0.48
1:C:482:LEU:HD11	1:C:487:ARG:HG2	1.96	0.48
2:D:152:GLY:H	2:D:155:LEU:HD12	1.78	0.48
2:J:345:LEU:HB2	2:J:346:PRO:HD3	1.96	0.48
2:J:36:ASN:N	2:J:36:ASN:OD1	2.46	0.48
1:B:414:GLY:H	1:B:433:SER:HB3	1.78	0.48
1:I:437:TYR:OH	2:J:189:GLU:OE1	2.23	0.48
1:C:542:PHE:HA	1:C:545:ILE:HG12	1.95	0.48
2:E:345:LEU:HB2	2:E:346:PRO:HD3	1.95	0.48
2:F:91:ASP:HB3	2:F:97:LYS:HD2	1.96	0.48
1:G:410:LYS:HB3	1:G:436:LEU:HB2	1.95	0.48
1:I:445:MET:HB3	1:I:453:TRP:CD1	2.49	0.48
2:J:107:LYS:HE3	2:J:109:LEU:HD21	1.95	0.48
2:J:159:GLU:N	2:J:159:GLU:OE1	2.45	0.48
2:L:288:ALA:HB2	2:L:300:GLN:HG3	1.96	0.48
1:H:286:MET:HA	1:H:289:THR:HG22	1.96	0.48
2:J:212:ASN:OD1	2:J:221:ARG:HG2	2.14	0.48
2:D:124:PRO:HG3	2:D:351:LEU:HD13	1.95	0.48
1:I:2:GLN:NE2	1:I:18:ASN:OD1	2.47	0.48
1:I:487:ARG:O	1:I:491:GLU:HG2	2.13	0.48
1:I:579:GLU:O	1:I:583:LEU:HG	2.14	0.48
2:L:126:GLU:OE1	2:L:143:ARG:NH2	2.45	0.48
1:B:582:GLN:N	1:B:582:GLN:OE1	2.33	0.48
2:J:137:HIS:HD1	2:J:412:TYR:HH	1.60	0.48
2:L:116:ILE:HD13	2:L:291:ILE:HD11	1.96	0.48
1:A:345:LEU:HB2	1:A:347:GLU:HG3	1.96	0.47
2:D:268:PRO:HB2	2:D:272:GLY:HA2	1.96	0.47
2:J:362:ARG:NH1	2:J:364:ASP:OD1	2.46	0.47
2:L:16:MET:HB3	2:L:54:VAL:HG23	1.95	0.47
2:F:57:PHE:HA	2:F:219:ILE:HD13	1.96	0.47
2:K:196:GLU:OE1	2:K:199:ARG:NH2	2.48	0.47
1:B:77:PRO:HG2	1:B:169:ILE:HG22	1.97	0.47
1:C:162:ILE:HD13	1:C:174:CYS:HB2	1.94	0.47
2:F:130:THR:HB	2:F:135:ILE:HB	1.95	0.47
1:G:504:ASN:OD1	1:G:507:ASP:N	2.48	0.47
1:H:351:ASP:N	1:H:351:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ASP:HB3	1:A:510:ASP:HB3	1.97	0.47
2:F:404:PHE:CZ	2:F:435:ALA:HB3	2.49	0.47
1:I:213:GLN:HB2	1:I:216:ILE:HG13	1.96	0.47
2:J:249:ASP:OD1	2:J:250:MET:N	2.47	0.47
1:B:212:GLY:N	1:B:217:ASP:OD2	2.48	0.47
1:B:84:PHE:HB2	1:B:88:GLN:HA	1.95	0.47
1:C:329:ASP:HA	1:C:330:SER:HA	1.61	0.47
2:K:249:ASP:OD1	2:K:304:LEU:HA	2.14	0.47
2:D:362:ARG:NH2	2:D:428:ASP:OD1	2.47	0.47
2:E:352:LYS:O	2:E:356:THR:HG23	2.15	0.47
2:E:29:LEU:HD21	2:E:41:ARG:HH21	1.79	0.47
2:F:195:MET:HE1	2:F:211:MET:HG3	1.97	0.47
1:H:140:ASP:OD1	1:H:140:ASP:N	2.38	0.47
1:H:214:ARG:O	1:H:218:THR:HB	2.14	0.47
2:E:143:ARG:HH12	2:E:242:HIS:CD2	2.33	0.47
1:H:204:ASN:O	1:H:371:ARG:NH2	2.43	0.47
1:H:531:GLU:HB3	1:H:581:ILE:HD12	1.97	0.47
1:H:264:ASN:ND2	2:K:324:GLU:OE2	2.47	0.47
1:A:212:GLY:N	1:A:217:ASP:OD2	2.48	0.47
1:A:333:ARG:NH1	2:D:278:TYR:OH	2.47	0.47
1:G:114:HIS:HA	1:G:169:ILE:HG12	1.97	0.47
1:I:256:TYR:HB3	1:I:291:LEU:HD12	1.97	0.47
2:J:129:GLN:OE1	2:J:423:ILE:N	2.47	0.47
2:E:248:THR:HA	2:E:249:ASP:HA	1.66	0.47
1:I:419:LEU:HB3	1:I:427:SER:HB2	1.95	0.47
1:C:5:LYS:NZ	4:C:701:HOH:O	2.48	0.46
2:E:143:ARG:HE	2:E:170:VAL:HG11	1.81	0.46
1:G:494:LYS:NZ	1:G:498:GLU:OE2	2.46	0.46
1:I:499:ASP:HA	1:I:560:LYS:HE2	1.97	0.46
1:A:484:ASP:HB2	1:A:536:LEU:HD21	1.97	0.46
2:F:434:LEU:HD13	2:F:434:LEU:N	2.30	0.46
1:I:492:VAL:O	1:I:496:ILE:HG23	2.15	0.46
1:I:518:GLN:NE2	1:I:518:GLN:O	2.48	0.46
2:D:184:ILE:N	2:D:248:THR:O	2.43	0.46
2:E:149:VAL:HG22	2:E:327:ILE:HB	1.97	0.46
2:L:136:ASP:O	2:L:140:THR:OG1	2.33	0.46
2:L:73:LEU:HB3	2:L:75:HIS:CD2	2.50	0.46
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.79	0.46
2:E:315:ILE:HB	2:E:316:PRO:HD3	1.96	0.46
2:F:374:ALA:HB2	2:F:444:ARG:HH12	1.81	0.46
2:K:221:ARG:HD2	2:K:256:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:GLU:O	1:B:470:LEU:HB2	2.16	0.46
1:B:534:LYS:O	1:B:538:LEU:HG	2.15	0.46
1:C:130:VAL:HG21	1:C:176:ILE:HD13	1.98	0.46
2:E:372:LEU:HA	2:E:375:ALA:HB3	1.96	0.46
1:I:90:PRO:HB2	1:I:93:THR:HB	1.98	0.46
2:D:121:ARG:NH1	2:D:288:ALA:O	2.49	0.46
2:E:309:ASP:N	2:E:309:ASP:OD1	2.46	0.46
1:G:556:ILE:HD11	1:G:577:ILE:HD11	1.97	0.46
2:J:270:ARG:HD2	2:J:314:PRO:HG3	1.97	0.46
2:J:454:LEU:HD12	2:J:455:PRO:HD2	1.96	0.46
1:B:79:ILE:HD11	1:B:313:ILE:HD13	1.98	0.46
2:D:212:ASN:OD1	2:D:221:ARG:HG2	2.15	0.46
2:E:307:PRO:HG2	2:E:313:HIS:CE1	2.51	0.46
2:E:148:PRO:HD3	2:E:323:THR:HB	1.97	0.46
2:E:91:ASP:OD1	2:E:95:ARG:N	2.49	0.46
2:K:33:ARG:HE	2:K:71:ARG:NH1	2.14	0.46
1:A:73:VAL:HG23	1:A:88:GLN:CD	2.37	0.46
1:B:314:ALA:HB1	1:B:384:ILE:HD12	1.97	0.46
2:D:248:THR:HA	2:D:249:ASP:HA	1.68	0.46
2:D:258:ARG:NH2	2:D:271:ARG:O	2.49	0.46
1:I:570:ILE:HD13	1:I:570:ILE:H	1.81	0.46
1:I:80:ILE:HA	1:I:290:VAL:HG22	1.98	0.46
2:L:137:HIS:HE2	2:L:368:THR:HB	1.81	0.46
2:L:410:ASN:O	2:L:414:ASN:HB3	2.16	0.46
2:E:3:LYS:HG3	2:E:3:LYS:H	1.45	0.45
2:F:86:ILE:HA	2:F:208:VAL:HG22	1.98	0.45
2:F:339:GLN:HA	2:F:341:PRO:HD3	1.98	0.45
2:E:127:PHE:CE1	2:E:171:LEU:HD11	2.50	0.45
1:C:298:MET:HG3	2:F:115:VAL:HG11	1.98	0.45
2:F:360:LYS:H	2:F:360:LYS:HG3	1.49	0.45
1:G:262:ARG:NH1	1:G:265:GLU:OE2	2.50	0.45
1:H:83:MET:HG2	1:H:291:LEU:HB3	1.98	0.45
2:K:102:GLU:HA	2:K:103:ILE:HA	1.73	0.45
2:L:307:PRO:O	2:L:308:GLU:HG2	2.16	0.45
2:L:328:ILE:HD12	2:L:346:PRO:HG2	1.98	0.45
1:A:30:VAL:HA	1:A:64:VAL:HG22	1.98	0.45
2:E:57:PHE:CE1	2:E:219:ILE:HG21	2.51	0.45
1:G:329:ASP:HA	1:G:330:SER:HA	1.54	0.45
1:G:332:SER:HA	1:G:401:VAL:HG11	1.98	0.45
2:K:106:GLU:OE1	2:K:234:TYR:OH	2.32	0.45
1:A:6:ILE:HD12	1:A:62:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:SER:N	1:I:134:ASP:OD2	2.49	0.45
2:K:152:GLY:H	2:K:155:LEU:HD12	1.81	0.45
2:K:45:LEU:HD11	2:K:55:GLN:HB2	1.98	0.45
1:A:98:THR:HG22	1:A:100:SER:HB3	1.99	0.45
2:D:106:GLU:OE1	2:D:234:TYR:OH	2.34	0.45
2:F:362:ARG:NE	2:F:427:LEU:HG	2.31	0.45
2:J:183:ALA:HB3	2:J:211:MET:HA	1.98	0.45
2:K:278:TYR:HB2	2:K:318:LEU:HD22	1.99	0.45
2:L:8:ILE:HG21	2:L:16:MET:HE2	1.97	0.45
1:A:274:PRO:HA	1:A:286:MET:HG2	1.99	0.45
1:A:304:GLU:O	1:A:334:TRP:NE1	2.47	0.45
1:B:214:ARG:HD2	1:B:500:TYR:CD1	2.52	0.45
1:G:327:MET:HG2	1:G:387:ILE:HB	1.99	0.45
1:H:54:GLU:HG3	1:H:56:SER:H	1.81	0.45
1:I:500:TYR:HE1	1:I:518:GLN:CD	2.20	0.45
2:K:328:ILE:H	2:K:347:SER:HB3	1.80	0.45
1:C:90:PRO:HB2	1:C:93:THR:HB	1.99	0.45
2:D:450:LEU:HD12	2:D:454:LEU:HD22	1.98	0.45
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.52	0.45
1:H:528:PHE:HA	1:H:577:ILE:HG21	1.99	0.45
2:J:4:GLU:OE2	2:J:71:ARG:NH2	2.44	0.45
2:K:10:GLU:H	2:K:17:ALA:HB3	1.80	0.45
1:B:497:ARG:HA	1:B:501:LEU:HB2	1.98	0.45
1:G:124:ILE:HG22	1:G:162:ILE:HD13	1.98	0.45
1:H:251:VAL:O	1:H:288:ARG:NH1	2.47	0.45
1:H:269:VAL:O	1:H:273:PHE:HB2	2.17	0.45
2:J:379:GLY:HA2	2:J:401:TYR:HB3	1.97	0.45
2:D:7:THR:OG1	2:D:19:GLU:O	2.28	0.45
2:D:29:LEU:HD11	2:D:77:LEU:HD23	1.98	0.45
1:C:91:LEU:HD13	2:F:118:PRO:HG2	1.99	0.45
2:F:382:ALA:HB3	2:F:402:ALA:HB2	1.99	0.45
1:I:81:SER:HA	1:I:286:MET:HG3	1.99	0.45
2:L:137:HIS:HB2	2:L:412:TYR:OH	2.17	0.45
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.99	0.45
1:C:559:SER:HA	1:C:562:ILE:HD13	1.97	0.45
2:F:250:MET:HB2	2:F:304:LEU:HB3	1.99	0.45
1:A:399:GLU:OE2	1:A:402:THR:N	2.43	0.44
2:F:34:MET:SD	2:F:63:ILE:HG12	2.56	0.44
2:L:163:GLN:OE1	2:L:415:GLN:NE2	2.50	0.44
1:A:513:THR:HG23	1:A:517:LYS:HD3	1.98	0.44
1:C:261:GLU:OE2	1:C:330:SER:N	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD13	1:C:316:TYR:HB2	1.98	0.44
1:G:453:TRP:HZ3	1:G:519:PHE:HA	1.82	0.44
2:J:113:GLY:HA2	2:J:114:GLU:HA	1.75	0.44
2:J:146:LYS:HD3	2:J:285:PHE:O	2.16	0.44
2:J:172:ASP:N	2:J:172:ASP:OD1	2.48	0.44
1:A:201:GLN:HB3	1:A:373:ILE:HD12	1.98	0.44
2:K:6:ARG:HD3	2:K:69:SER:HB3	2.00	0.44
2:L:145:GLN:HB2	2:L:351:LEU:HD12	2.00	0.44
1:C:167:PHE:HB3	1:C:171:ASP:HB2	2.00	0.44
2:F:125:ASP:O	2:F:360:LYS:NZ	2.50	0.44
1:H:526:LEU:HB3	1:H:530:LYS:HE2	1.98	0.44
1:A:474:VAL:HG13	1:A:479:ILE:HG13	2.00	0.44
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.98	0.44
2:D:391:GLU:O	2:D:399:LYS:NZ	2.49	0.44
1:G:342:SER:HB2	1:G:355:PRO:HG3	2.00	0.44
1:G:410:LYS:HG2	1:G:436:LEU:HD12	1.99	0.44
1:H:204:ASN:OD1	1:H:204:ASN:N	2.48	0.44
1:H:446:ASP:OD1	1:H:453:TRP:N	2.47	0.44
1:H:77:PRO:HA	1:H:78:GLY:HA2	1.50	0.44
2:J:248:THR:HA	2:J:249:ASP:HA	1.65	0.44
2:L:409:GLU:O	2:L:413:VAL:HG22	2.18	0.44
1:B:582:GLN:CD	1:B:582:GLN:H	2.19	0.44
2:F:45:LEU:HD11	2:F:55:GLN:HB2	1.99	0.44
1:G:488:LEU:HD22	1:G:536:LEU:HD12	2.00	0.44
1:I:329:ASP:HA	1:I:330:SER:HA	1.53	0.44
2:L:132:ILE:HA	2:L:415:GLN:HE22	1.83	0.44
1:A:479:ILE:HG22	1:A:487:ARG:HH11	1.83	0.44
1:B:139:VAL:HG21	1:B:187:MET:HE3	1.99	0.44
1:C:197:ARG:HG3	1:C:315:GLU:HB3	2.00	0.44
2:D:313:HIS:HB3	2:D:316:PRO:HD2	2.00	0.44
2:E:171:LEU:HA	2:E:172:ASP:HA	1.77	0.44
1:H:327:MET:HG2	1:H:387:ILE:HB	1.99	0.44
2:J:19:GLU:HG3	2:J:51:LYS:HG2	1.99	0.44
2:K:151:SER:OG	2:K:152:GLY:N	2.51	0.44
2:K:270:ARG:HE	2:K:314:PRO:HG3	1.82	0.44
2:D:407:ARG:NE	2:D:436:MET:SD	2.79	0.43
2:E:324:GLU:HB3	2:E:350:ARG:HB2	1.99	0.43
1:G:266:MET:HE3	1:G:294:ASN:H	1.83	0.43
1:H:536:LEU:HD22	1:H:540:ALA:HB3	2.00	0.43
1:I:169:ILE:HB	1:I:188:MET:HG2	1.99	0.43
1:I:295:THR:OG1	1:I:298:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:248:THR:HA	2:K:249:ASP:HA	1.66	0.43
1:A:231:PRO:HA	1:A:390:VAL:O	2.19	0.43
2:E:6:ARG:HE	2:E:6:ARG:HB2	1.51	0.43
1:I:135:ILE:HD13	1:I:148:LYS:HD3	2.00	0.43
1:I:318:ARG:HD3	1:I:384:ILE:HG13	1.99	0.43
1:I:471:ASN:HA	1:I:474:VAL:HG22	2.00	0.43
2:E:126:GLU:CB	2:E:143:ARG:HD2	2.48	0.43
2:J:83:GLU:N	2:J:83:GLU:OE1	2.47	0.43
2:L:246:ILE:HD13	2:L:301:ILE:HB	1.98	0.43
2:J:116:ILE:H	2:J:116:ILE:HG13	1.61	0.43
2:L:150:PHE:HB3	2:L:306:MET:SD	2.59	0.43
2:D:138:LEU:HA	2:D:369:MET:HG3	2.01	0.43
2:D:148:PRO:HD3	2:D:323:THR:HB	2.00	0.43
2:F:122:ASP:OD1	2:F:123:TYR:N	2.51	0.43
1:I:562:ILE:HD12	1:I:563:PRO:HD2	2.00	0.43
1:A:123:THR:HG23	1:A:137:GLY:HA2	2.00	0.43
2:D:35:GLN:CD	2:D:35:GLN:H	2.15	0.43
1:H:418:SER:O	1:H:422:LYS:HG2	2.18	0.43
1:I:221:PRO:HD2	1:I:438:SER:HB3	1.99	0.43
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.36	0.43
1:C:410:LYS:HB3	1:C:436:LEU:HB2	2.01	0.43
2:D:363:GLU:H	2:D:363:GLU:HG3	1.50	0.43
2:F:415:GLN:HB2	2:F:421:ARG:HD3	1.99	0.43
1:H:362:LEU:HD13	1:H:405:THR:HG23	2.00	0.43
1:I:118:TRP:CZ3	1:I:141:GLU:HA	2.53	0.43
2:K:446:LYS:HA	2:K:446:LYS:HD3	1.81	0.43
2:F:363:GLU:HG3	2:F:363:GLU:H	1.41	0.43
1:H:135:ILE:HG12	1:H:148:LYS:HB3	2.00	0.43
1:H:536:LEU:HA	1:H:540:ALA:HB3	1.99	0.43
1:H:87:ILE:HG13	1:H:89:ARG:HG3	2.01	0.43
2:K:338:ILE:HG23	2:K:414:ASN:HB2	2.00	0.43
2:K:362:ARG:HD3	2:K:453:TYR:CE1	2.54	0.43
1:B:486:ASP:N	1:B:486:ASP:OD1	2.50	0.43
1:H:153:ASN:OD1	1:H:154:GLY:N	2.52	0.43
1:C:470:LEU:HB2	1:C:490:LEU:HD21	1.99	0.42
2:E:181:PHE:HB3	2:E:209:MET:HG2	2.01	0.42
2:F:313:HIS:CG	2:F:314:PRO:HD2	2.54	0.42
1:H:491:GLU:OE1	1:H:553:ARG:NH2	2.52	0.42
2:K:361:THR:HG21	2:K:365:HIS:ND1	2.34	0.42
1:A:5:LYS:HE3	1:A:5:LYS:HB3	1.81	0.42
1:B:141:GLU:HG3	1:B:142:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:PHE:CE1	2:D:219:ILE:HG21	2.54	0.42
2:F:95:ARG:HG2	2:F:95:ARG:H	1.55	0.42
1:I:518:GLN:O	1:I:521:MET:HG2	2.19	0.42
2:L:155:LEU:HD13	2:L:156:PRO:HD2	2.02	0.42
1:A:257:VAL:HG22	1:A:292:ILE:HD12	2.00	0.42
1:A:378:ASP:HB2	1:A:380:ARG:HH11	1.84	0.42
1:B:329:ASP:HA	1:B:330:SER:HA	1.56	0.42
1:C:259:CYS:HB2	1:C:334:TRP:HB2	2.00	0.42
2:D:356:THR:HG22	2:D:365:HIS:CE1	2.54	0.42
2:E:405:ALA:O	2:E:409:GLU:HG2	2.19	0.42
1:H:400:PRO:O	1:H:404:ASN:ND2	2.40	0.42
2:J:138:LEU:HA	2:J:369:MET:HG3	2.01	0.42
2:L:248:THR:HA	2:L:249:ASP:HA	1.61	0.42
1:A:399:GLU:HG2	1:A:400:PRO:HD2	2.01	0.42
1:C:169:ILE:HA	1:C:187:MET:HG3	2.02	0.42
1:C:273:PHE:H	1:C:274:PRO:HD2	1.84	0.42
2:F:434:LEU:HD22	2:F:434:LEU:H	1.85	0.42
1:G:231:PRO:HD2	1:G:415:LEU:H	1.85	0.42
2:J:339:GLN:H	2:J:414:ASN:ND2	2.17	0.42
2:K:339:GLN:HA	2:K:340:PRO:HA	1.89	0.42
2:L:132:ILE:HA	2:L:415:GLN:NE2	2.34	0.42
1:C:105:ARG:HG2	1:C:105:ARG:H	1.61	0.42
1:C:261:GLU:CD	1:C:330:SER:N	2.70	0.42
1:I:415:LEU:HD23	1:I:428:ILE:HG12	2.02	0.42
1:C:92:ASP:OD1	1:C:93:THR:N	2.49	0.42
2:F:136:ASP:OD1	2:F:136:ASP:N	2.53	0.42
1:H:329:ASP:HA	1:H:330:SER:HA	1.52	0.42
1:H:41:GLU:HB2	1:H:48:SER:HB2	2.00	0.42
2:K:268:PRO:HA	2:K:269:GLY:HA3	1.80	0.42
2:L:249:ASP:OD1	2:L:251:THR:N	2.42	0.42
2:L:285:PHE:HE2	2:L:319:THR:HG22	1.85	0.42
1:A:245:ILE:O	1:A:249:SER:OG	2.29	0.42
1:A:517:LYS:HE2	1:A:521:MET:HE1	2.02	0.42
1:B:261:GLU:HB2	1:B:266:MET:HB2	2.02	0.42
2:F:276:TYR:HD1	2:F:276:TYR:H	1.68	0.42
2:F:291:ILE:HG22	2:F:294:LEU:HB2	2.01	0.42
2:L:182:ALA:HB3	2:L:247:MET:HG2	2.02	0.42
1:H:199:ILE:HD13	1:H:199:ILE:H	1.85	0.42
2:J:198:PHE:HB3	2:J:204:ILE:HB	2.01	0.42
2:L:219:ILE:HG13	2:L:260:ILE:HD11	2.01	0.42
1:A:156:LYS:NZ	4:A:701:HOH:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:SER:HA	1:B:384:ILE:HB	2.02	0.42
2:F:14:PRO:HG2	2:F:15:LEU:HD12	2.02	0.42
2:F:437:LEU:HD13	2:F:438:PRO:HD2	2.01	0.42
1:A:2:GLN:NE2	1:A:18:ASN:O	2.53	0.42
2:D:270:ARG:HH21	2:D:314:PRO:HA	1.84	0.42
1:H:543:ASN:N	1:H:543:ASN:OD1	2.53	0.42
1:I:264:ASN:HA	1:I:267:THR:HG22	2.01	0.41
2:L:339:GLN:HA	2:L:340:PRO:HA	1.78	0.41
1:C:259:CYS:O	1:C:333:ARG:HB2	2.21	0.41
1:C:85:ASP:HB3	1:C:91:LEU:HD21	2.02	0.41
2:D:371:GLN:OE1	2:D:444:ARG:HG2	2.20	0.41
2:E:159:GLU:N	2:E:159:GLU:OE1	2.50	0.41
2:F:355:GLY:O	2:F:360:LYS:HD3	2.21	0.41
2:K:222:ILE:HD12	2:K:260:ILE:HD12	2.01	0.41
2:L:88:ARG:CZ	2:L:100:GLY:HA3	2.50	0.41
2:L:249:ASP:OD1	2:L:250:MET:N	2.53	0.41
1:A:449:LEU:HD13	1:A:451:GLN:HB2	2.02	0.41
1:B:257:VAL:HA	1:B:292:ILE:HB	2.02	0.41
1:C:258:GLY:HA2	1:C:329:ASP:O	2.20	0.41
1:C:498:GLU:O	1:C:560:LYS:NZ	2.54	0.41
2:F:290:ARG:HG2	2:F:297:SER:HB3	2.01	0.41
2:K:145:GLN:HG3	2:K:351:LEU:HD12	2.01	0.41
2:L:13:GLY:O	2:L:60:THR:OG1	2.31	0.41
2:L:433:LEU:O	2:L:433:LEU:HD22	2.20	0.41
1:C:264:ASN:O	1:C:267:THR:HG22	2.21	0.41
2:E:399:LYS:O	2:E:403:LYS:HB2	2.21	0.41
1:G:251:VAL:HG11	1:G:325:ALA:HB2	2.02	0.41
1:I:518:GLN:CA	1:I:518:GLN:HE21	2.33	0.41
2:L:92:GLY:O	2:L:227:MET:HG3	2.19	0.41
2:L:326:GLN:O	2:L:347:SER:OG	2.25	0.41
1:C:93:THR:O	1:C:97:VAL:HG12	2.20	0.41
2:D:379:GLY:HA3	2:D:405:ALA:HB2	2.00	0.41
2:E:122:ASP:OD1	2:E:123:TYR:N	2.54	0.41
2:F:236:ALA:HA	2:F:241:MET:H	1.85	0.41
1:I:3:ILE:HD13	1:I:3:ILE:H	1.84	0.41
1:I:59:GLY:N	2:L:25:LYS:HG3	2.36	0.41
1:C:307:ILE:HD11	1:C:328:ALA:HB1	2.02	0.41
1:H:125:GLU:O	1:H:128:THR:OG1	2.37	0.41
2:K:123:TYR:CD2	2:K:124:PRO:HD2	2.46	0.41
2:L:340:PRO:HG2	2:L:342:ILE:HD11	2.03	0.41
2:D:307:PRO:HG2	2:D:313:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:SER:OG	2:D:321:TYR:OH	2.36	0.41
2:D:33:ARG:HD3	2:D:69:SER:OG	2.20	0.41
2:E:431:TRP:O	2:E:435:ALA:N	2.54	0.41
2:F:135:ILE:HG12	2:F:135:ILE:H	1.72	0.41
1:A:192:PRO:HG2	1:A:195:ARG:HB3	2.03	0.41
2:D:264:ARG:NH2	4:D:602:HOH:O	2.39	0.41
2:D:345:LEU:HB2	2:D:346:PRO:HD3	2.03	0.41
2:F:219:ILE:H	2:F:219:ILE:HD12	1.85	0.41
2:F:404:PHE:CE2	2:F:436:MET:N	2.74	0.41
2:K:150:PHE:HB3	2:K:306:MET:SD	2.61	0.41
1:A:555:ARG:CZ	1:A:573:ILE:HD13	2.50	0.41
1:C:346:GLU:O	2:D:265:ARG:NH1	2.42	0.41
2:K:162:ALA:O	2:K:166:ARG:HG3	2.21	0.41
2:K:313:HIS:HB3	2:K:316:PRO:HD2	2.02	0.41
2:L:397:ILE:HD12	2:L:398:ASP:N	2.36	0.41
1:B:90:PRO:HG2	1:B:93:THR:HB	2.02	0.41
1:C:77:PRO:HG2	1:C:169:ILE:HG22	2.03	0.41
2:D:162:ALA:O	2:D:166:ARG:HG3	2.21	0.41
2:D:150:PHE:HB2	2:D:328:ILE:HD13	2.03	0.41
2:E:144:GLY:HA2	2:E:298:VAL:O	2.21	0.41
1:H:156:LYS:HE2	1:H:156:LYS:HB2	1.62	0.41
1:H:202:LYS:NZ	1:H:367:GLU:O	2.51	0.41
2:L:134:ALA:HB2	2:L:413:VAL:HB	2.02	0.41
1:H:467:GLU:O	1:H:471:ASN:N	2.50	0.41
2:J:184:ILE:HD13	2:J:225:PRO:HG3	2.02	0.41
2:L:245:VAL:HB	2:L:300:GLN:HA	2.03	0.41
1:A:9:VAL:HG22	1:A:14:VAL:HG22	2.02	0.40
1:B:278:ASP:N	1:B:283:GLU:O	2.43	0.40
1:B:536:LEU:HA	1:B:540:ALA:HB3	2.02	0.40
2:D:44:VAL:HG22	2:D:54:VAL:HG12	2.03	0.40
2:E:403:LYS:HG3	2:E:403:LYS:HZ2	1.77	0.40
2:F:307:PRO:HG2	2:F:313:HIS:CE1	2.56	0.40
1:G:563:PRO:HD2	1:G:566:GLU:HG3	2.03	0.40
1:I:253:LEU:HG	1:I:288:ARG:O	2.21	0.40
2:L:434:LEU:H	2:L:434:LEU:HD22	1.86	0.40
1:B:81:SER:HA	1:B:286:MET:HG3	2.02	0.40
1:B:397:ILE:O	1:B:403:GLN:NE2	2.50	0.40
1:B:507:ASP:HB3	1:B:510:ASP:HB3	2.03	0.40
2:E:143:ARG:HH21	2:E:170:VAL:HG21	1.84	0.40
2:E:270:ARG:HD2	2:E:314:PRO:HG3	2.03	0.40
1:G:88:GLN:HE21	1:G:88:GLN:HB3	1.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:254:VAL:O	1:I:289:THR:HA	2.21	0.40
1:I:500:TYR:HA	1:I:500:TYR:HD2	1.61	0.40
2:J:386:ALA:HB1	2:J:391:GLU:HA	2.02	0.40
2:J:397:ILE:HG13	2:J:397:ILE:H	1.56	0.40
2:J:415:GLN:HE21	2:J:415:GLN:HB2	1.75	0.40
1:B:2:GLN:NE2	1:B:18:ASN:O	2.54	0.40
1:B:209:MET:SD	1:B:385:THR:HG21	2.61	0.40
1:C:173:ILE:HD13	1:C:173:ILE:H	1.87	0.40
2:D:213:LEU:N	2:D:216:ASP:OD2	2.45	0.40
2:E:339:GLN:HA	2:E:340:PRO:HA	1.94	0.40
1:G:122:ALA:H	1:G:164:SER:HB2	1.86	0.40
1:H:464:LEU:HD21	1:H:496:ILE:HG21	2.03	0.40
2:L:415:GLN:HB3	2:L:421:ARG:HH21	1.86	0.40
1:B:396:ASP:OD1	1:B:397:ILE:N	2.54	0.40
2:D:145:GLN:HG3	2:D:351:LEU:HD12	2.04	0.40
2:E:146:LYS:HD2	2:E:288:ALA:HB3	2.04	0.40
2:E:184:ILE:N	2:E:248:THR:O	2.42	0.40
1:I:8:LYS:HB3	1:I:15:MET:HB2	2.04	0.40
1:B:489:THR:O	1:B:493:ALA:N	2.45	0.40
1:C:332:SER:OG	1:C:391:SER:N	2.54	0.40
2:F:127:PHE:HB3	2:F:360:LYS:HB2	2.03	0.40
1:G:173:ILE:HD13	1:G:187:MET:HG2	2.03	0.40
2:J:140:THR:HB	2:J:352:LYS:HG3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/594 (98%)	569 (97%)	16 (3%)	0	100	100
1	B	584/594 (98%)	576 (99%)	8 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	582/594 (98%)	564 (97%)	18 (3%)	0	100	100
1	G	585/594 (98%)	563 (96%)	21 (4%)	1 (0%)	47	78
1	H	584/594 (98%)	569 (97%)	15 (3%)	0	100	100
1	I	582/594 (98%)	569 (98%)	13 (2%)	0	100	100
2	D	452/462 (98%)	441 (98%)	11 (2%)	0	100	100
2	E	450/462 (97%)	438 (97%)	12 (3%)	0	100	100
2	F	449/462 (97%)	429 (96%)	20 (4%)	0	100	100
2	J	453/462 (98%)	444 (98%)	9 (2%)	0	100	100
2	K	452/462 (98%)	445 (98%)	7 (2%)	0	100	100
2	L	453/462 (98%)	430 (95%)	22 (5%)	1 (0%)	47	78
All	All	6211/6336 (98%)	6037 (97%)	172 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	393	ALA
1	G	397	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	503/507 (99%)	482 (96%)	21 (4%)	30	60
1	B	466/507 (92%)	434 (93%)	32 (7%)	15	46
1	C	482/507 (95%)	459 (95%)	23 (5%)	25	57
1	G	490/507 (97%)	474 (97%)	16 (3%)	38	67
1	H	476/507 (94%)	453 (95%)	23 (5%)	25	57
1	I	465/507 (92%)	430 (92%)	35 (8%)	13	42
2	D	367/385 (95%)	348 (95%)	19 (5%)	23	54
2	E	344/385 (89%)	311 (90%)	33 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	340/385 (88%)	301 (88%)	39 (12%)	5	22
2	J	364/385 (94%)	347 (95%)	17 (5%)	26	58
2	K	360/385 (94%)	343 (95%)	17 (5%)	26	58
2	L	343/385 (89%)	318 (93%)	25 (7%)	14	43
All	All	5000/5352 (93%)	4700 (94%)	300 (6%)	19	50

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	33	LEU
1	A	43	ARG
1	A	73	VAL
1	A	150	MET
1	A	222	VAL
1	A	273	PHE
1	A	297	ASN
1	A	327	MET
1	A	339	ARG
1	A	348	MET
1	A	396	ASP
1	A	399	GLU
1	A	449	LEU
1	A	465	GLN
1	A	480	ASP
1	A	485	ASN
1	A	533	ARG
1	A	543	ASN
1	A	552	VAL
1	A	573	ILE
1	B	24	ILE
1	B	25	GLN
1	B	44	GLN
1	B	79	ILE
1	B	83	MET
1	B	84	PHE
1	B	145	ILE
1	B	159	VAL
1	B	160	GLN
1	B	162	ILE
1	B	182	LEU

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Mol	Chain	Res	Type
1	B	188	MET
1	B	230	VAL
1	B	259	CYS
1	B	273	PHE
1	B	275	GLU
1	B	348	MET
1	B	455	ASP
1	B	461	MET
1	B	465	GLN
1	B	470	LEU
1	B	475	ARG
1	B	480	ASP
1	B	482	LEU
1	B	487	ARG
1	B	500	TYR
1	B	511	THR
1	B	533	ARG
1	B	536	LEU
1	B	541	TYR
1	B	542	PHE
1	B	585	VAL
1	C	3	ILE
1	C	19	MET
1	C	69	GLU
1	C	87	ILE
1	C	99	GLN
1	C	105	ARG
1	C	143	LYS
1	C	173	ILE
1	C	177	GLU
1	C	179	GLU
1	C	185	LEU
1	C	188	MET
1	C	204	ASN
1	C	250	ASP
1	C	253	LEU
1	C	259	CYS
1	C	273	PHE
1	C	288	ARG
1	C	295	THR
1	C	399	GLU
1	C	445	MET

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Mol	Chain	Res	Type
1	C	476	LEU
1	C	482	LEU
2	D	33	ARG
2	D	34	MET
2	D	35	GLN
2	D	36	ASN
2	D	39	ILE
2	D	51	LYS
2	D	104	LEU
2	D	127	PHE
2	D	140	THR
2	D	176	ASP
2	D	247	MET
2	D	250	MET
2	D	321	TYR
2	D	360	LYS
2	D	362	ARG
2	D	363	GLU
2	D	383	LYS
2	D	444	ARG
2	D	450	LEU
2	E	3	LYS
2	E	6	ARG
2	E	15	LEU
2	E	48	GLN
2	E	71	ARG
2	E	104	LEU
2	E	127	PHE
2	E	140	THR
2	E	170	VAL
2	E	171	LEU
2	E	204	ILE
2	E	206	ARG
2	E	247	MET
2	E	283	THR
2	E	309	ASP
2	E	321	TYR
2	E	332	GLU
2	E	362	ARG
2	E	363	GLU
2	E	365	HIS
2	E	370	ASN

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Mol	Chain	Res	Type
2	E	372	LEU
2	E	381	GLN
2	E	384	GLU
2	E	385	LEU
2	E	391	GLU
2	E	401	TYR
2	E	403	LYS
2	E	406	GLU
2	E	409	GLU
2	E	414	ASN
2	E	439	ARG
2	E	450	LEU
2	F	6	ARG
2	F	50	ASP
2	F	77	LEU
2	F	95	ARG
2	F	97	LYS
2	F	125	ASP
2	F	130	THR
2	F	135	ILE
2	F	136	ASP
2	F	141	LEU
2	F	143	ARG
2	F	166	ARG
2	F	196	GLU
2	F	204	ILE
2	F	205	ASP
2	F	215	ASN
2	F	216	ASP
2	F	267	VAL
2	F	271	ARG
2	F	276	TYR
2	F	294	LEU
2	F	311	LYS
2	F	326	GLN
2	F	360	LYS
2	F	362	ARG
2	F	363	GLU
2	F	376	TYR
2	F	384	GLU
2	F	401	TYR
2	F	420	ASN

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Mol	Chain	Res	Type
2	F	427	LEU
2	F	429	LEU
2	F	434	LEU
2	F	440	THR
2	F	443	LYS
2	F	444	ARG
2	F	446	LYS
2	F	448	ASP
2	F	450	LEU
1	G	88	GLN
1	G	268	ASP
1	G	273	PHE
1	G	297	ASN
1	G	378	ASP
1	G	424	HIS
1	G	455	ASP
1	G	479	ILE
1	G	536	LEU
1	G	543	ASN
1	G	546	MET
1	G	566	GLU
1	G	579	GLU
1	G	581	ILE
1	G	582	GLN
1	G	584	ILE
1	H	2	GLN
1	H	13	LEU
1	H	21	GLU
1	H	128	THR
1	H	143	LYS
1	H	158	THR
1	H	199	ILE
1	H	203	LEU
1	H	218	THR
1	H	259	CYS
1	H	273	PHE
1	H	275	GLU
1	H	291	LEU
1	H	401	VAL
1	H	407	ARG
1	H	462	ARG
1	H	488	LEU

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Mol	Chain	Res	Type
1	H	511	THR
1	H	536	LEU
1	H	543	ASN
1	H	545	ILE
1	H	552	VAL
1	H	574	ASN
1	I	3	ILE
1	I	19	MET
1	I	158	THR
1	I	182	LEU
1	I	185	LEU
1	I	188	MET
1	I	216	ILE
1	I	217	ASP
1	I	248	TRP
1	I	250	ASP
1	I	262	ARG
1	I	273	PHE
1	I	275	GLU
1	I	288	ARG
1	I	338	LEU
1	I	341	MET
1	I	401	VAL
1	I	405	THR
1	I	419	LEU
1	I	443	ARG
1	I	445	MET
1	I	447	GLN
1	I	449	LEU
1	I	451	GLN
1	I	453	TRP
1	I	498	GLU
1	I	500	TYR
1	I	509	VAL
1	I	518	GLN
1	I	538	LEU
1	I	545	ILE
1	I	555	ARG
1	I	560	LYS
1	I	566	GLU
1	I	570	ILE
2	J	36	ASN

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Mol	Chain	Res	Type
2	J	79	LEU
2	J	123	TYR
2	J	155	LEU
2	J	206	ARG
2	J	250	MET
2	J	360	LYS
2	J	361	THR
2	J	362	ARG
2	J	371	GLN
2	J	403	LYS
2	J	415	GLN
2	J	422	THR
2	J	429	LEU
2	J	432	GLU
2	J	439	ARG
2	J	446	LYS
2	K	21	VAL
2	K	51	LYS
2	K	97	LYS
2	K	104	LEU
2	K	119	ILE
2	K	123	TYR
2	K	129	GLN
2	K	205	ASP
2	K	241	MET
2	K	247	MET
2	K	257	LEU
2	K	294	LEU
2	K	360	LYS
2	K	401	TYR
2	K	429	LEU
2	K	442	LEU
2	K	444	ARG
2	L	25	LYS
2	L	48	GLN
2	L	90	PHE
2	L	97	LYS
2	L	146	LYS
2	L	174	SER
2	L	204	ILE
2	L	244	LEU
2	L	364	ASP

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Mol	Chain	Res	Type
2	L	373	PHE
2	L	388	VAL
2	L	391	GLU
2	L	400	ILE
2	L	413	VAL
2	L	415	GLN
2	L	425	GLU
2	L	429	LEU
2	L	431	TRP
2	L	433	LEU
2	L	440	THR
2	L	443	LYS
2	L	444	ARG
2	L	447	ASP
2	L	448	ASP
2	L	449	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	67	ASN
2	E	381	GLN
1	G	88	GLN
1	H	574	ASN
1	I	471	ASN
1	I	518	GLN
2	J	167	GLN
2	J	414	ASN
2	L	313	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
3	GOL	A	601	-	5,5,5	0.80	0	5,5,5	1.13	0
3	GOL	G	601	-	5,5,5	0.92	0	5,5,5	1.01	0
3	GOL	H	601	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	D	503	-	5,5,5	0.91	0	5,5,5	1.00	0
3	GOL	A	605	-	5,5,5	0.93	0	5,5,5	0.99	0
3	GOL	A	603	-	5,5,5	0.90	0	5,5,5	1.01	0
3	GOL	D	502	-	5,5,5	0.93	0	5,5,5	0.96	0
3	GOL	D	501	-	5,5,5	0.90	0	5,5,5	1.03	0
3	GOL	G	603	-	5,5,5	0.90	0	5,5,5	1.02	0
3	GOL	D	505	-	5,5,5	0.90	0	5,5,5	1.02	0
3	GOL	A	602	-	5,5,5	0.94	0	5,5,5	0.98	0
3	GOL	D	504	-	5,5,5	0.93	0	5,5,5	0.98	0
3	GOL	A	604	-	5,5,5	0.91	0	5,5,5	1.00	0
3	GOL	K	501	-	5,5,5	0.91	0	5,5,5	0.98	0
3	GOL	A	606	-	5,5,5	0.91	0	5,5,5	1.03	0
3	GOL	C	601	-	5,5,5	0.94	0	5,5,5	0.96	0
3	GOL	G	602	-	5,5,5	0.92	0	5,5,5	0.98	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
3	GOL	A	601	-	-	4/4/4/4	-
3	GOL	G	601	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	H	601	-	-	0/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	A	605	-	-	0/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	G	603	-	-	2/4/4/4	-
3	GOL	D	505	-	-	0/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	D	504	-	-	0/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	K	501	-	-	0/4/4/4	-
3	GOL	A	606	-	-	4/4/4/4	-
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	G	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	O1-C1-C2-C3
3	G	601	GOL	O1-C1-C2-C3
3	D	503	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-C3
3	A	606	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3
3	A	604	GOL	O1-C1-C2-C3
3	G	603	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3
3	C	601	GOL	O1-C1-C2-C3
3	G	602	GOL	O1-C1-C2-C3
3	A	601	GOL	O1-C1-C2-O2
3	G	601	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	502	GOL	O1-C1-C2-O2
3	A	606	GOL	O1-C1-C2-O2
3	G	602	GOL	O1-C1-C2-O2
3	D	503	GOL	O1-C1-C2-O2
3	A	601	GOL	O2-C2-C3-O3
3	G	603	GOL	O1-C1-C2-O2
3	C	601	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	587/594 (98%)	0.08	4 (0%) 87 91	42, 67, 119, 162	0
1	B	586/594 (98%)	0.48	33 (5%) 24 28	51, 126, 183, 248	0
1	C	584/594 (98%)	0.47	33 (5%) 23 27	68, 110, 169, 252	0
1	G	587/594 (98%)	0.35	22 (3%) 41 45	45, 85, 165, 251	0
1	H	586/594 (98%)	0.42	43 (7%) 15 18	62, 101, 165, 225	0
1	I	584/594 (98%)	0.77	72 (12%) 4 5	73, 119, 212, 238	0
2	D	454/462 (98%)	0.10	5 (1%) 80 84	43, 76, 124, 161	0
2	E	452/462 (97%)	0.31	20 (4%) 34 38	56, 93, 186, 266	0
2	F	451/462 (97%)	0.96	75 (16%) 1 2	73, 136, 232, 279	0
2	J	455/462 (98%)	0.25	5 (1%) 80 84	58, 93, 152, 229	0
2	K	454/462 (98%)	0.24	10 (2%) 62 66	54, 88, 139, 202	0
2	L	455/462 (98%)	0.51	42 (9%) 9 11	68, 123, 213, 305	0
All	All	6235/6336 (98%)	0.41	364 (5%) 23 27	42, 101, 188, 305	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	435	ALA	10.9
2	L	445	ILE	8.2
2	F	437	LEU	7.7
2	L	436	MET	7.7
1	C	539	GLY	6.8
2	F	436	MET	6.7
2	F	389	LEU	6.6
1	I	476	LEU	6.5
2	F	385	LEU	6.2
1	I	539	GLY	6.0
1	I	529	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
2	F	133	SER	5.9
2	L	441	GLU	5.6
1	H	177	GLU	5.5
2	F	382	ALA	5.4
1	H	577	ILE	5.3
1	H	479	ILE	5.3
2	F	403	LYS	5.3
2	J	388	VAL	5.3
1	I	581	ILE	5.0
1	I	491	GLU	5.0
2	L	365	HIS	5.0
1	H	174	CYS	4.9
1	B	536	LEU	4.8
1	H	173	ILE	4.7
1	I	542	PHE	4.7
1	G	500	TYR	4.6
1	B	541	TYR	4.6
2	F	413	VAL	4.6
1	I	473	ILE	4.6
2	E	393	ALA	4.5
2	F	330	THR	4.5
1	B	174	CYS	4.5
2	F	398	ASP	4.5
2	F	392	SER	4.4
2	K	394	LEU	4.4
2	F	388	VAL	4.4
1	B	477	VAL	4.4
2	E	385	LEU	4.3
2	E	386	ALA	4.3
1	I	528	PHE	4.3
2	K	393	ALA	4.3
2	F	275	GLY	4.3
1	C	540	ALA	4.2
2	F	442	LEU	4.2
2	K	388	VAL	4.2
1	I	533	ARG	4.2
1	C	476	LEU	4.2
2	L	397	ILE	4.2
1	H	184	GLU	4.1
1	H	162	ILE	4.1
2	F	386	ALA	4.1
2	E	401	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	478	GLY	4.0
2	L	428	ASP	4.0
1	H	477	VAL	4.0
2	F	438	PRO	4.0
2	E	392	SER	4.0
1	I	530	LYS	4.0
2	F	390	GLY	3.9
1	I	174	CYS	3.9
1	B	479	ILE	3.9
1	C	570	ILE	3.9
1	I	450	GLN	3.9
1	I	574	ASN	3.9
1	I	477	VAL	3.9
1	B	481	SER	3.8
2	L	400	ILE	3.8
1	C	182	LEU	3.8
1	B	478	GLY	3.8
2	F	402	ALA	3.8
1	I	499	ASP	3.8
1	C	480	ASP	3.7
1	I	582	GLN	3.7
2	E	390	GLY	3.7
2	K	389	LEU	3.7
2	F	393	ALA	3.7
2	L	382	ALA	3.7
1	I	452	ASP	3.7
2	L	442	LEU	3.6
2	L	449	LEU	3.6
1	I	470	LEU	3.6
2	F	387	VAL	3.6
1	I	564	GLU	3.6
1	I	187	MET	3.6
1	G	479	ILE	3.6
1	I	430	TRP	3.6
1	H	543	ASN	3.6
2	F	134	ALA	3.6
2	L	385	LEU	3.6
1	B	484	ASP	3.6
1	I	486	ASP	3.6
2	E	396	ASP	3.6
1	I	493	ALA	3.5
2	F	127	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	364	ASP	3.5
2	F	434	LEU	3.5
2	F	412	TYR	3.5
1	H	164	SER	3.5
1	H	483	SER	3.5
2	L	455	PRO	3.5
1	C	187	MET	3.5
2	F	396	ASP	3.4
2	F	103	ILE	3.4
1	C	544	GLU	3.4
2	F	130	THR	3.4
2	E	402	ALA	3.4
1	I	521	MET	3.4
1	A	479	ILE	3.3
2	F	374	ALA	3.3
1	I	543	ASN	3.3
2	K	172	ASP	3.3
2	E	397	ILE	3.3
2	L	454	LEU	3.3
1	G	572	SER	3.3
2	F	377	ALA	3.3
2	L	401	TYR	3.3
1	B	482	LEU	3.2
1	C	492	VAL	3.2
1	H	136	ILE	3.2
1	H	167	PHE	3.2
2	F	401	TYR	3.2
2	L	373	PHE	3.2
2	J	387	VAL	3.2
1	I	578	LYS	3.2
1	G	552	VAL	3.2
1	G	477	VAL	3.2
2	F	395	SER	3.2
2	F	440	THR	3.2
2	F	373	PHE	3.2
1	C	173	ILE	3.2
2	E	387	VAL	3.2
2	F	378	GLN	3.2
2	F	441	GLU	3.2
1	I	319	ASP	3.1
1	A	477	VAL	3.1
1	B	184	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	474	VAL	3.1
2	L	438	PRO	3.1
2	E	389	LEU	3.1
2	F	384	GLU	3.1
2	F	309	ASP	3.1
1	B	453	TRP	3.1
2	F	371	GLN	3.1
1	B	539	GLY	3.1
1	A	476	LEU	3.1
2	F	433	LEU	3.1
2	F	145	GLN	3.0
2	F	394	LEU	3.0
2	D	393	ALA	3.0
1	I	173	ILE	3.0
1	C	481	SER	3.0
1	H	583	LEU	3.0
2	L	432	GLU	3.0
1	C	477	VAL	3.0
1	I	474	VAL	3.0
1	I	481	SER	3.0
2	F	443	LYS	3.0
2	L	368	THR	3.0
1	I	520	ASN	3.0
2	F	381	GLN	3.0
1	I	480	ASP	3.0
1	I	471	ASN	3.0
2	F	170	VAL	2.9
2	F	82	SER	2.9
2	E	391	GLU	2.9
1	I	469	GLN	2.9
1	H	581	ILE	2.9
2	F	328	ILE	2.9
2	L	446	LYS	2.9
1	I	485	ASN	2.9
1	C	262	ARG	2.9
1	G	577	ILE	2.9
1	B	577	ILE	2.9
1	C	545	ILE	2.9
2	K	387	VAL	2.9
2	L	137	HIS	2.9
1	C	478	GLY	2.9
1	B	463	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	387	VAL	2.9
2	F	410	ASN	2.9
1	C	535	ALA	2.9
1	H	120	PHE	2.8
1	I	495	SER	2.8
1	C	559	SER	2.8
2	L	5	TYR	2.8
2	L	388	VAL	2.8
1	B	77	PRO	2.8
1	G	496	ILE	2.8
1	I	570	ILE	2.8
2	F	310	ASP	2.8
1	H	484	ASP	2.7
1	I	484	ASP	2.7
1	I	147	HIS	2.7
1	I	479	ILE	2.7
2	K	390	GLY	2.7
2	L	393	ALA	2.7
2	F	345	LEU	2.7
1	H	585	VAL	2.7
1	B	493	ALA	2.7
1	B	557	SER	2.7
2	E	434	LEU	2.7
2	F	346	PRO	2.7
2	F	375	ALA	2.7
1	C	549	THR	2.6
1	I	219	PHE	2.6
1	B	565	GLU	2.6
1	H	185	LEU	2.6
2	F	431	TRP	2.6
1	B	488	LEU	2.6
1	I	556	ILE	2.6
1	H	176	ILE	2.6
1	H	123	THR	2.6
2	F	102	GLU	2.6
1	G	478	GLY	2.6
1	G	547	GLU	2.6
1	H	536	LEU	2.6
1	I	475	ARG	2.6
1	H	163	GLU	2.6
1	I	519	PHE	2.5
1	H	541	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	450	LEU	2.5
1	I	537	SER	2.5
1	H	524	VAL	2.5
1	I	122	ALA	2.5
1	B	499	ASP	2.5
2	F	357	GLY	2.5
2	L	431	TRP	2.5
1	B	468	GLU	2.5
1	B	430	TRP	2.5
2	F	397	ILE	2.5
2	J	440	THR	2.5
1	H	538	LEU	2.5
1	I	501	LEU	2.5
2	L	386	ALA	2.5
1	G	522	LEU	2.5
1	I	557	SER	2.4
1	C	259	CYS	2.4
1	C	542	PHE	2.4
2	F	445	ILE	2.4
1	I	490	LEU	2.4
1	I	492	VAL	2.4
2	E	440	THR	2.4
1	G	570	ILE	2.4
1	G	573	ILE	2.4
1	C	486	ASP	2.4
1	I	584	ILE	2.4
1	I	572	SER	2.4
1	H	472	GLU	2.4
1	I	568	ALA	2.4
2	F	406	GLU	2.4
2	F	84	ASP	2.4
2	L	453	TYR	2.4
1	C	160	GLN	2.4
1	G	476	LEU	2.4
2	L	93	LEU	2.4
2	F	209	MET	2.3
1	C	126	GLU	2.3
1	I	129	GLU	2.3
1	G	528	PHE	2.3
2	E	431	TRP	2.3
1	I	396	ASP	2.3
1	C	470	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	476	LEU	2.3
2	L	375	ALA	2.3
1	I	563	PRO	2.3
2	F	101	PRO	2.3
1	I	468	GLU	2.3
1	C	183	LYS	2.3
1	I	453	TRP	2.3
1	C	124	ILE	2.3
2	F	18	VAL	2.3
2	L	404	PHE	2.3
2	F	85	MET	2.3
1	C	393	SER	2.3
2	F	391	GLU	2.3
1	H	149	ILE	2.3
1	G	568	ALA	2.3
1	B	584	ILE	2.2
1	I	494	LYS	2.2
2	E	438	PRO	2.2
1	G	260	GLY	2.2
2	D	392	SER	2.2
2	L	434	LEU	2.2
1	G	545	ILE	2.2
2	F	423	ILE	2.2
1	I	289	THR	2.2
2	F	175	ASP	2.2
1	C	137	GLY	2.2
1	G	554	GLU	2.2
1	H	160	GLN	2.2
2	E	412	TYR	2.2
2	K	433	LEU	2.2
2	E	395	SER	2.2
1	G	351	ASP	2.2
1	I	287	GLU	2.2
1	H	122	ALA	2.2
1	I	264	ASN	2.2
1	B	470	LEU	2.2
1	B	526	LEU	2.2
2	D	385	LEU	2.2
2	K	171	LEU	2.2
1	C	176	ILE	2.2
1	G	585	VAL	2.2
1	I	395	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	324	GLU	2.2
1	C	581	ILE	2.2
1	H	175	VAL	2.2
2	L	392	SER	2.2
1	H	540	ALA	2.2
2	F	135	ILE	2.2
1	B	172	PRO	2.2
1	H	187	MET	2.2
1	C	490	LEU	2.2
1	H	535	ALA	2.2
2	J	435	ALA	2.2
1	B	566	GLU	2.1
2	F	400	ILE	2.1
2	J	384	GLU	2.1
1	G	527	THR	2.1
1	H	130	VAL	2.1
1	H	539	GLY	2.1
2	L	389	LEU	2.1
2	F	48	GLN	2.1
2	L	363	GLU	2.1
1	A	490	LEU	2.1
1	G	565	GLU	2.1
2	L	355	GLY	2.1
1	B	252	ASP	2.1
2	E	398	ASP	2.1
1	B	452	ASP	2.1
1	H	396	ASP	2.1
2	E	435	ALA	2.1
1	B	581	ILE	2.1
2	F	173	SER	2.1
2	L	411	GLU	2.1
2	L	176	ASP	2.1
2	L	381	GLN	2.1
1	H	121	GLU	2.1
1	I	163	GLU	2.1
1	I	211	THR	2.1
1	I	125	GLU	2.1
2	D	388	VAL	2.1
1	C	543	ASN	2.1
1	I	544	GLU	2.1
2	L	377	ALA	2.1
1	B	464	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	162	ILE	2.1
1	H	158	THR	2.0
1	I	532	ALA	2.0
2	F	449	LEU	2.0
1	I	559	SER	2.0
2	F	453	TYR	2.0
1	B	466	GLU	2.0
1	I	451	GLN	2.0
2	F	174	SER	2.0
2	L	398	ASP	2.0
2	F	232	ALA	2.0
1	I	218	THR	2.0
1	H	148	LYS	2.0
1	H	453	TRP	2.0
1	I	394	GLY	2.0
2	K	356	THR	2.0
2	L	384	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	602	6/6	0.63	0.31	102,103,104,105	0
3	GOL	A	601	6/6	0.78	0.48	108,110,110,112	0
3	GOL	G	602	6/6	0.78	0.25	91,92,93,95	0
3	GOL	K	501	6/6	0.80	0.25	104,105,105,105	0
3	GOL	C	601	6/6	0.83	0.25	116,118,119,120	0
3	GOL	A	606	6/6	0.84	0.36	110,110,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	503	6/6	0.85	0.33	137,137,138,138	0
3	GOL	G	603	6/6	0.85	0.40	92,94,94,94	0
3	GOL	H	601	6/6	0.86	0.32	89,90,91,92	0
3	GOL	A	603	6/6	0.86	0.35	93,95,96,96	0
3	GOL	D	502	6/6	0.86	0.44	84,86,86,86	0
3	GOL	A	605	6/6	0.87	0.16	94,96,96,97	0
3	GOL	D	505	6/6	0.88	0.23	116,117,117,118	0
3	GOL	G	601	6/6	0.89	0.19	95,95,95,96	0
3	GOL	D	501	6/6	0.90	0.23	74,76,77,77	0
3	GOL	A	604	6/6	0.91	0.21	77,79,80,80	0
3	GOL	D	504	6/6	0.93	0.17	114,115,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.