



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:42 PM UTC

PDB ID : 5ZEA / pdb_00005zea
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

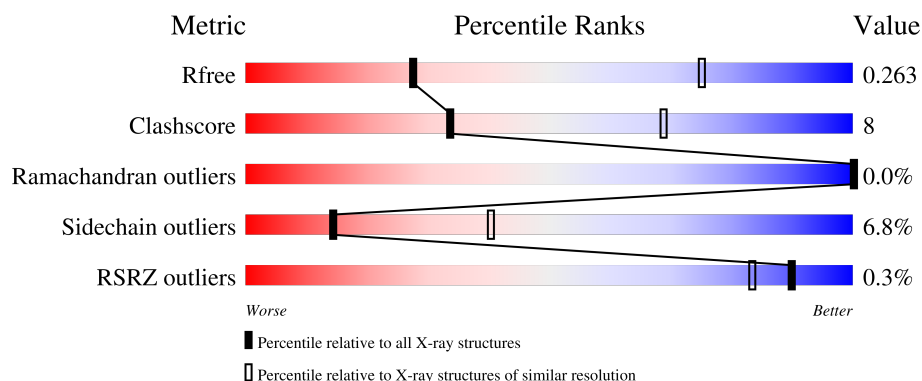
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	78% 19% ..
1	B	594	77% 20% ..
1	C	594	77% 20% ..
1	G	594	83% 15% ..
1	H	594	79% 18% ..

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Mol	Chain	Length	Quality of chain
1	I	594	% 75% 21%
2	D	462	74% 23%
2	E	462	74% 21%
2	F	462	% 72% 22%
2	J	462	74% 23%
2	K	462	78% 20%
2	L	462	% 73% 25%

2 Entry composition [i](#)

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:

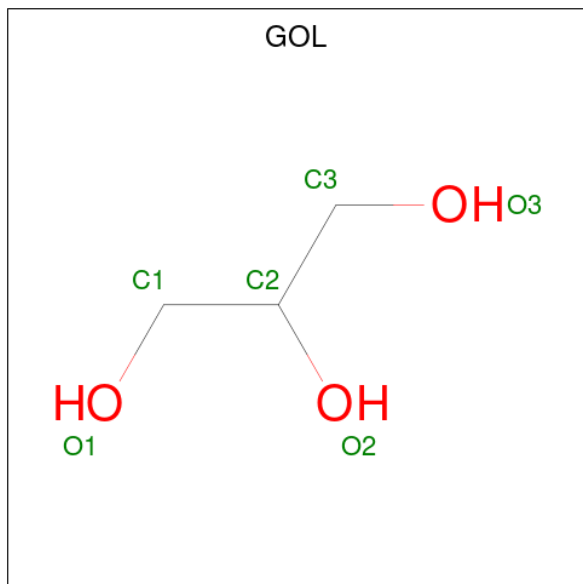
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	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		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		

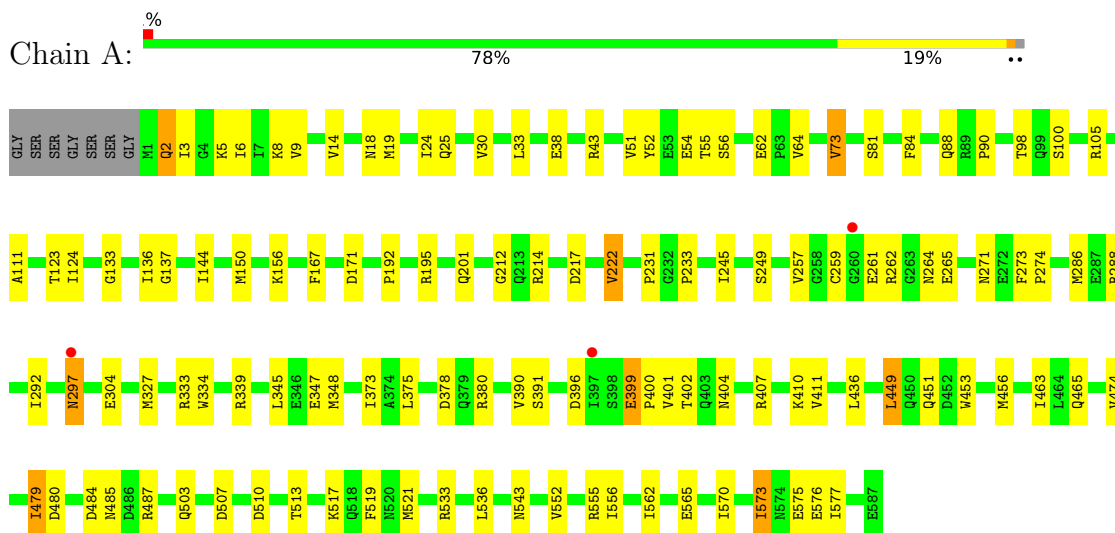
- Molecule 4 is water.

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

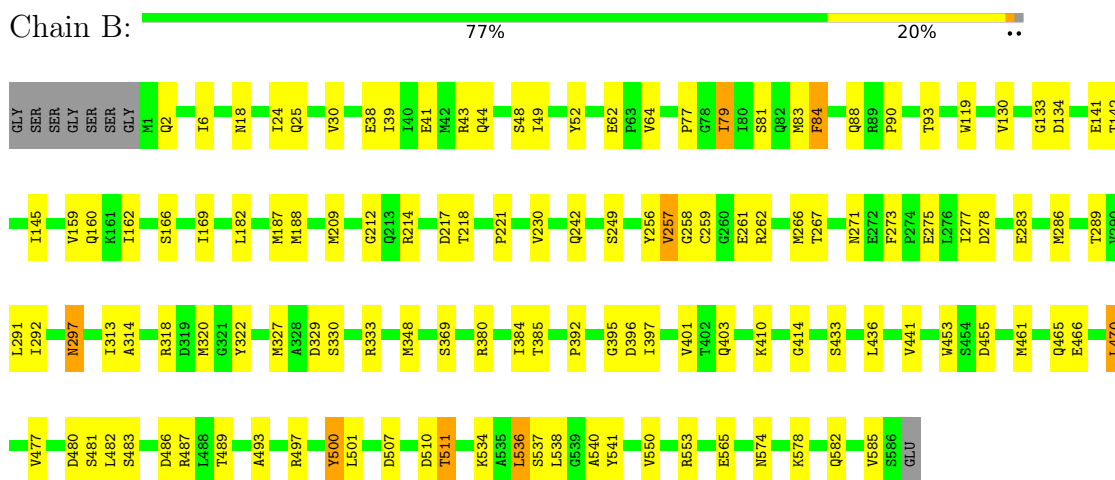
3 Residue-property plots

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 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

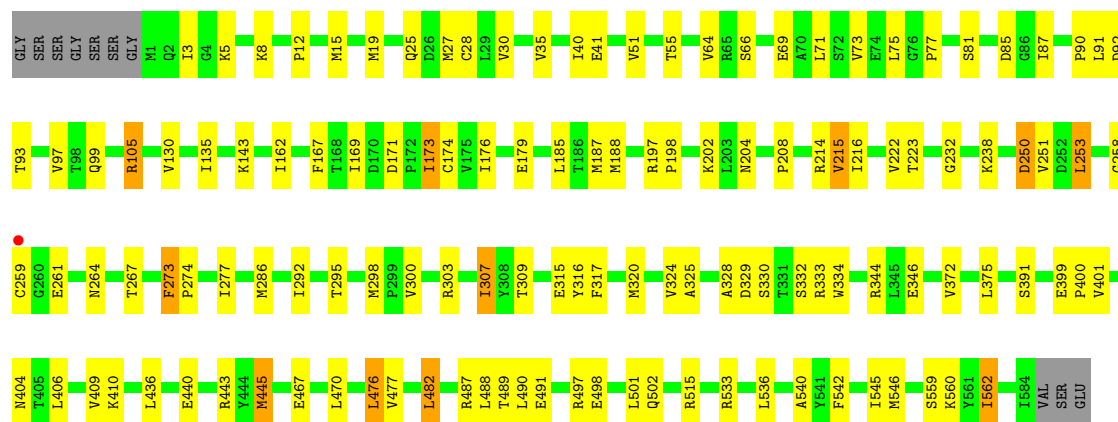


• Molecule 1: V-type sodium ATPase catalytic subunit A



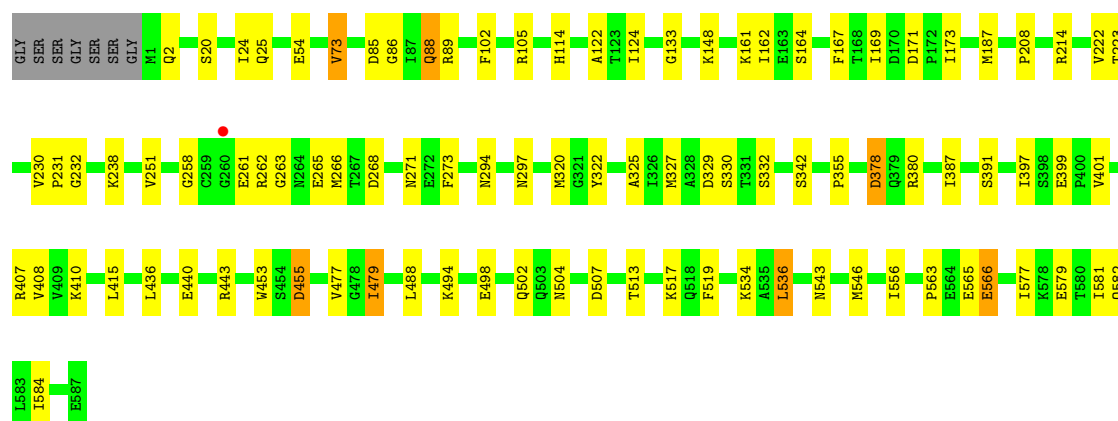
• Molecule 1: V-type sodium ATPase catalytic subunit A





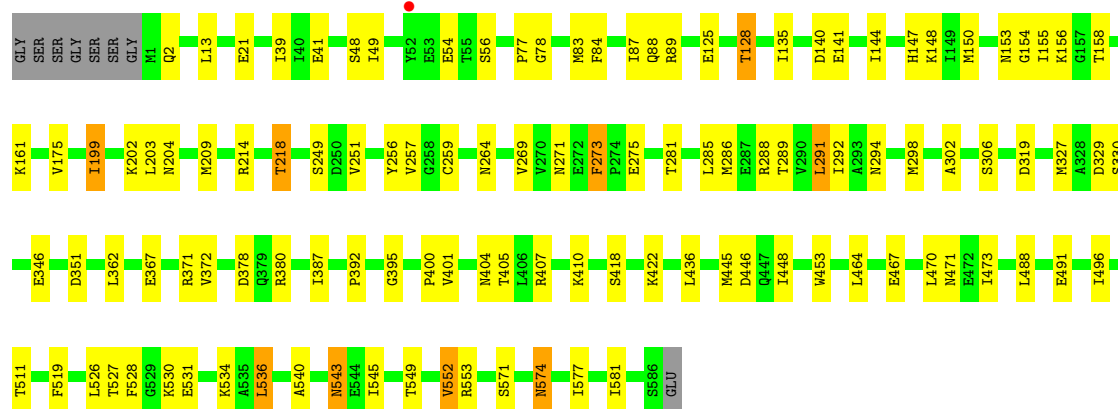
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain G: 83% 15% ..



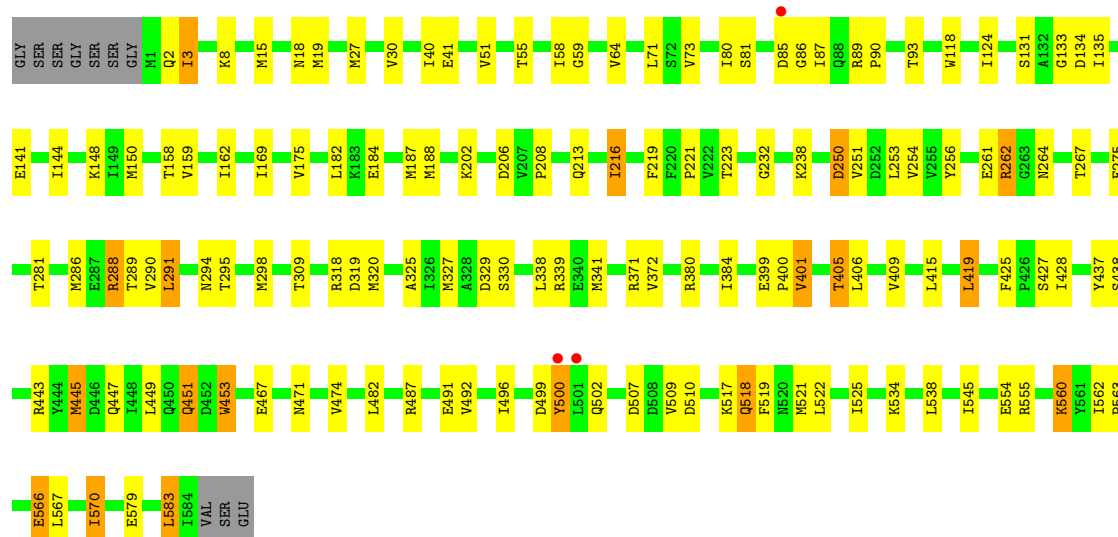
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain H: 79% 18% ..



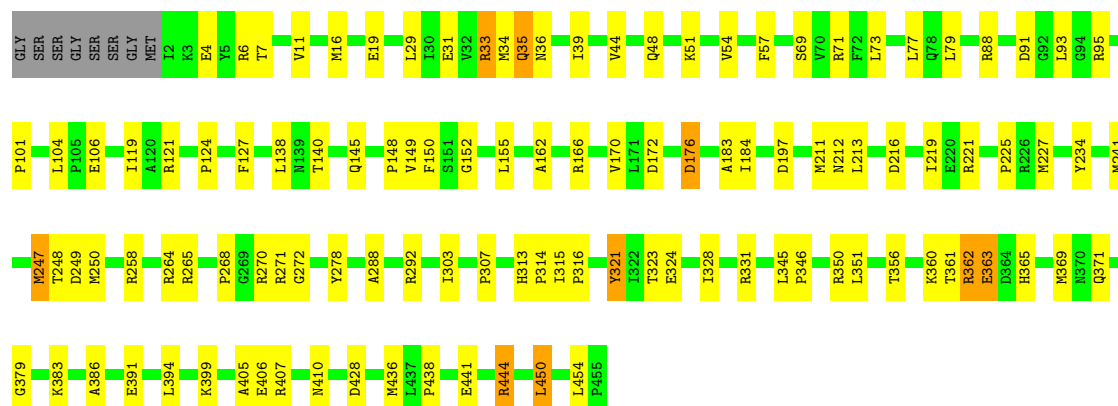
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain I: 75% 21% ..



• Molecule 2: V-type sodium ATPase subunit B

Chain D: 74% 23% . .

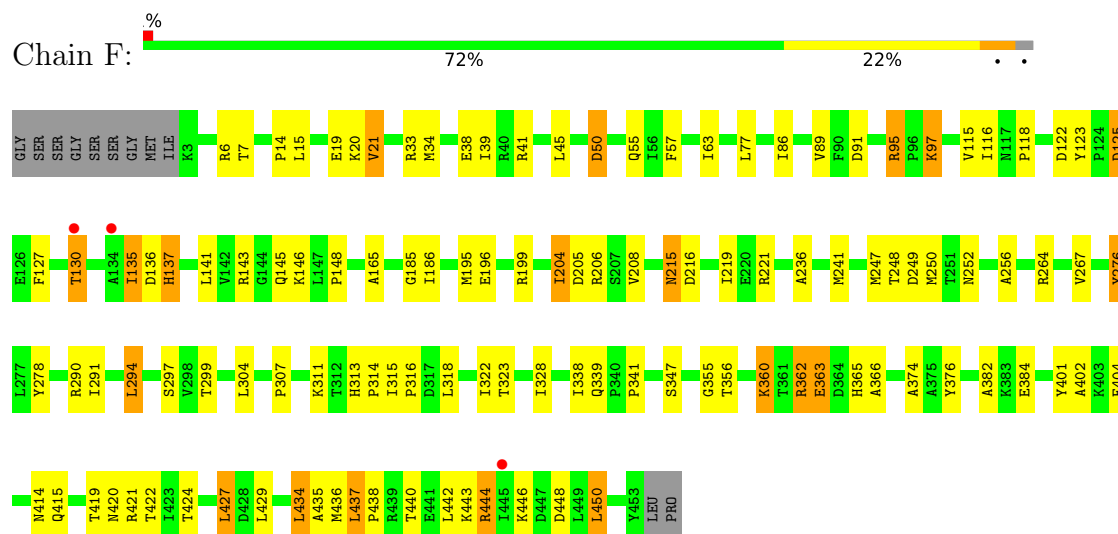


• Molecule 2: V-type sodium ATPase subunit B

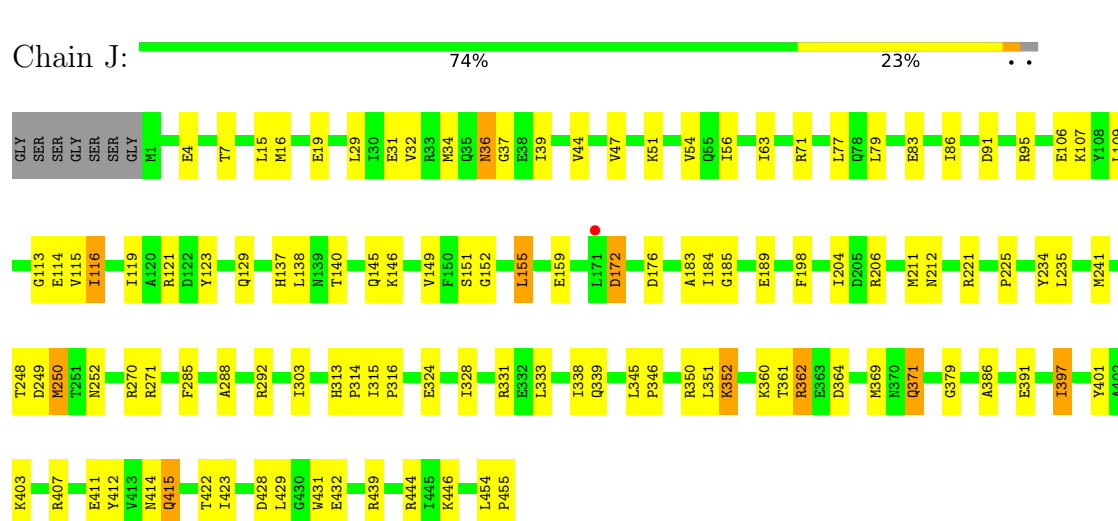
Chain E: 74% 21% . .



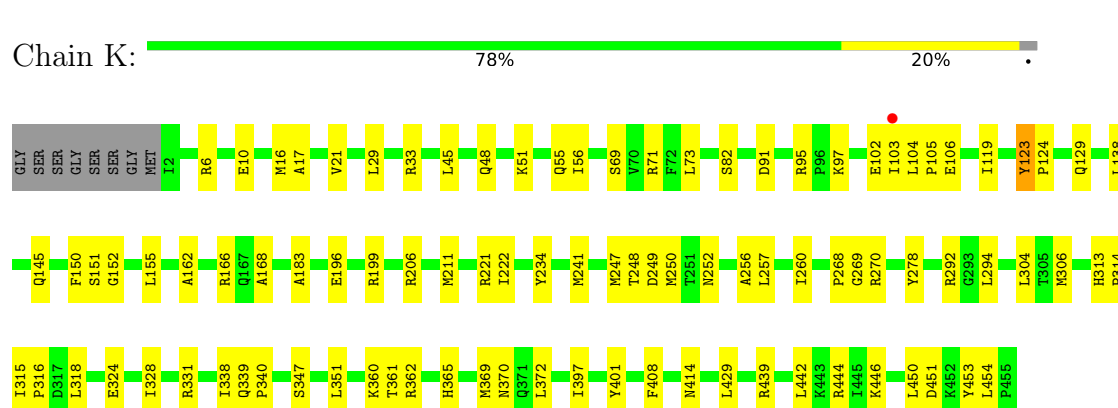
• Molecule 2: V-type sodium ATPase subunit B



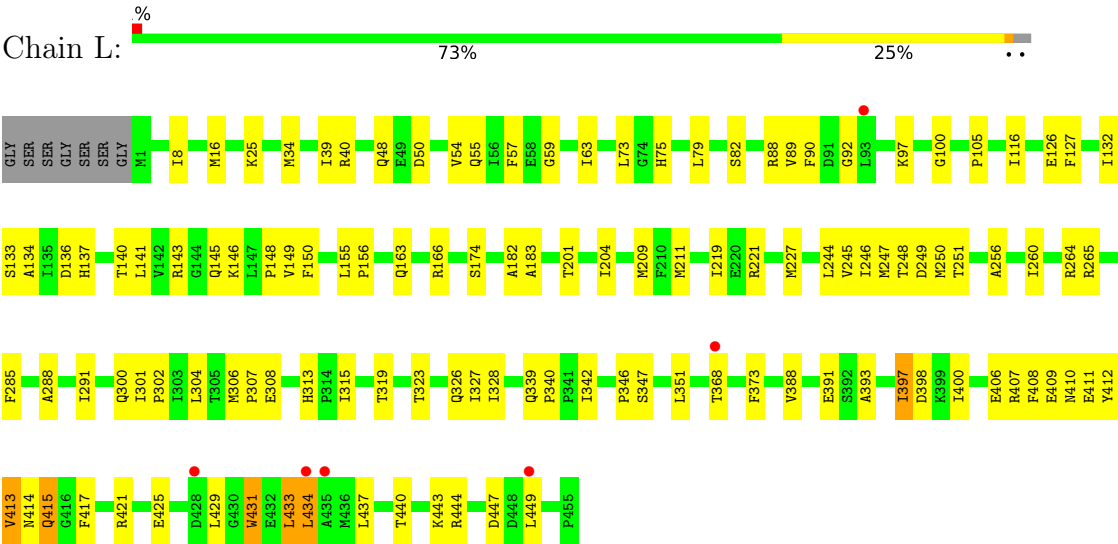
• Molecule 2: V-type sodium ATPase subunit B



• 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, α , β , γ	180.84Å 107.77Å 193.37Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	48.20 – 3.38 48.20 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.20-3.38) 99.0 (48.20-3.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.215 , 0.258 0.223 , 0.263	Depositor DCC
R_{free} test set	5088 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.10	0/4647	0.27	0/6287
1	B	0.09	0/4547	0.25	0/6166
1	C	0.09	0/4562	0.27	0/6183
1	G	0.09	0/4594	0.26	0/6222
1	H	0.09	0/4565	0.26	0/6187
1	I	0.11	0/4480	0.28	0/6085
2	D	0.10	0/3592	0.28	0/4864
2	E	0.10	0/3512	0.29	0/4762
2	F	0.12	0/3473	0.31	0/4714
2	J	0.10	0/3581	0.30	0/4853
2	K	0.10	0/3566	0.28	0/4835
2	L	0.12	0/3496	0.31	0/4750
All	All	0.10	0/48615	0.28	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	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4471	0	4289	63	0
1	C	4486	0	4387	69	0
1	G	4519	0	4451	51	0
1	H	4489	0	4352	59	0
1	I	4406	0	4256	82	0
2	D	3528	0	3497	62	0
2	E	3449	0	3340	64	0
2	F	3412	0	3292	66	0
2	J	3517	0	3472	65	0
2	K	3502	0	3440	47	0
2	L	3435	0	3296	67	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	732	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 8.

All (732) 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
1:G:148:LYS:H	1:G:320:MET:HE3	1.47	0.79
2:J:155:LEU:HD21	2:J:331:ARG:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:221:ARG:HE	2:F:256:ALA:HB2	1.52	0.75
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:OD1	1:I:250:ASP:N	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
1:G:266:MET:HE3	1:G:294:ASN:H	1.55	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
1:C:261:GLU:CD	1:C:330:SER:H	1.99	0.69
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
2:L:137:HIS:NE2	2:L:368:THR:O	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:MET:HE2	1:G:322:TYR:HE2	1.61	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
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:79:LEU:HD13	2:D:227:MET:HE1	1.82	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	1:C:250:ASP:N	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:C:27:MET:HE3	1:C:71:LEU:HB2	1.84	0.59
1:I:232:GLY:HA3	1:I:238:LYS:HD3	1.84	0.59
2:L:247:MET:HE3	2:L:302:PRO:HB3	1.83	0.59
1:H:549:THR:HA	1:H:552:VAL:HG12	1.84	0.58
2:J:16:MET:HE1	2:J:63:ILE:HG21	1.85	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
2:L:82:SER:HB2	2:L:105:PRO:HA	1.87	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
2:J:176:ASP:N	2:J:176:ASP:OD1	2.37	0.57
2:F:89:VAL:HG11	2:F:195:MET:HE1	1.85	0.57
1:I:40:ILE:HG13	1:I:41:GLU:HG2	1.86	0.56
2:E:16:MET:HE2	2:E:56:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PRO:HB2	1:C:375:LEU:HD11	1.88	0.56
2:E:171:LEU:H	2:E:171:LEU:HD12	1.70	0.56
1:A:124:ILE:HB	1:A:136:ILE:HA	1.87	0.56
1:B:565:GLU:N	1:B:565:GLU:OE1	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:119:ILE:O	2:D:292:ARG:NH1	2.39	0.56
2:D:170:VAL:HG12	2:D:172:ASP:H	1.71	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
1:C:491:GLU:HG3	1:C:546:MET:HE1	1.88	0.56
2:L:50:ASP:OD1	2:L:50:ASP:N	2.38	0.56
2:E:406:GLU:O	2:E:410:ASN:ND2	2.36	0.56
2:K:16:MET:HE2	2:K:56:ILE:HD11	1.87	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
2:E:89:VAL:HG22	2:E:209:MET:HE3	1.89	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
1:B:77:PRO:HG3	1:B:187:MET:HE2	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:D:176:ASP:HB3	2:D:241:MET:HE3	1.90	0.54
2:J:315:ILE:HB	2:J:316:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:141:GLU:OE1	1:H:147:HIS:ND1	2.42	0.53
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:G:258:GLY:HA3	1:G:266:MET:HE1	1.90	0.53
1:A:297:ASN:OD1	1:A:297:ASN:N	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
1:C:317:PHE:HA	1:C:320:MET:HE2	1.88	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
1:G:378:ASP:N	1:G:378:ASP:OD1	2.41	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:N	1:G:565:GLU:OE1	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
1:C:85:ASP:HB2	1:C:298:MET:HE1	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:86:ILE:HD11	2:J:241:MET:HE1	1.92	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
1:G:407:ARG:NH2	2:K:252:ASN:OD1	2.33	0.51
2:J:151:SER:OG	2:J:152:GLY:N	2.43	0.51
1:A:262:ARG:NH1	1:A:265:GLU:OE2	2.44	0.51
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:C:81:SER:HA	1:C:286:MET:HE3	1.92	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:6:ILE:HD12	1:B:62:GLU:HB2	1.92	0.51
1:B:286:MET:HA	1:B:289:THR:HG22	1.93	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:A:73:VAL:HG23	1:A:88:GLN:CD	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:ILE:HD13	2:L:16:MET:HE2	1.93	0.50
1:C:40:ILE:HG13	1:C:41:GLU:HG2	1.94	0.50
2:D:4:GLU:HG2	2:D:71:ARG:HG2	1.93	0.50
2:D:315:ILE:HB	2:D:316:PRO:HD3	1.92	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
1:I:256:TYR:HD2	1:I:327:MET:HE3	1.76	0.50
1:I:500:TYR:HE1	1:I:518:GLN:CD	2.20	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
2:F:125:ASP:N	2:F:125:ASP:OD1	2.43	0.50
1:H:392:PRO:HG2	1:H:395:GLY:HA2	1.94	0.50
2:J:106:GLU:OE1	2:J:234:TYR:OH	2.30	0.50
2:J:145:GLN:HG3	2:J:351:LEU:HD12	1.94	0.50
1:H:209:MET:HE2	1:H:249:SER:HB3	1.94	0.50
1:I:251:VAL:HG11	1:I:325:ALA:HB2	1.93	0.50
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:J:235:LEU:HB3	2:J:241:MET:HE2	1.93	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:44:VAL:HG22	2:J:54:VAL:HG12	1.94	0.49
2:J:121:ARG:NH1	2:J:288:ALA:O	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:27:MET:HE3	1:I:71:LEU:HD13	1.95	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
2:D:7:THR:OG1	2:D:19:GLU:O	2.28	0.49
1:G:513:THR:HG23	1:G:517:LYS:HD3	1.95	0.49
1:B:582:GLN:H	1:B:582:GLN:CD	2.19	0.48
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
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
1:B:414:GLY:H	1:B:433:SER:HB3	1.78	0.48
2:L:326:GLN:O	2:L:347:SER:OG	2.25	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:OE1	2:J:159:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:GLN:CD	2:D:35:GLN:H	2.15	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:OE1	1:B:582:GLN:N	2.33	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:OD1	1:H:351:ASP:N	2.47	0.47
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:84:PHE:HB2	1:B:88:GLN:HA	1.95	0.47
1:B:212:GLY:N	1:B:217:ASP:OD2	2.48	0.47
1:C:329:ASP:HA	1:C:330:SER:HA	1.61	0.47
2:J:36:ASN:N	2:J:36:ASN:OD1	2.46	0.47
2:K:249:ASP:OD1	2:K:304:LEU:HA	2.14	0.47
1:A:453:TRP:HA	1:A:456:MET:HE2	1.97	0.47
2:D:362:ARG:NH2	2:D:428:ASP:OD1	2.47	0.47
2:E:29:LEU:HD21	2:E:41:ARG:HH21	1.79	0.47
2:E:143:ARG:HH12	2:E:242:HIS:CD2	2.33	0.47
2:E:352:LYS:O	2:E:356:THR:HG23	2.15	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
1:B:209:MET:HE2	1:B:249:SER:HB3	1.97	0.47
1:H:204:ASN:O	1:H:371:ARG:NH2	2.43	0.47
1:H:264:ASN:ND2	2:K:324:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:531:GLU:HB3	1:H:581:ILE:HD12	1.97	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
1:C:8:LYS:HD3	1:C:15:MET:HE2	1.97	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
1:B:258:GLY:HA3	1:B:266:MET:HE1	1.97	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
1:G:455:ASP:N	1:G:455:ASP:OD1	2.46	0.46
1:I:118:TRP:HB2	1:I:187:MET:HE1	1.98	0.46
2:L:73:LEU:HB3	2:L:75:HIS:CD2	2.50	0.46
2:L:136:ASP:O	2:L:140:THR:OG1	2.33	0.46
1:A:156:LYS:NZ	4:A:701:HOH:O	2.49	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:E:436:MET:HE2	2:E:436:MET:HB2	1.69	0.46
2:F:374:ALA:HB2	2:F:444:ARG:HH12	1.81	0.46
2:J:34:MET:HE2	2:J:63:ILE:HG12	1.96	0.46
2:K:221:ARG:HD2	2:K:256:ALA:HB2	1.98	0.46
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
1:C:261:GLU:CD	1:C:330:SER:N	2.70	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:OD1	2:E:309:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:454:LEU:HD12	2:J:455:PRO:HD2	1.96	0.46
2:L:34:MET:HE2	2:L:63:ILE:HG12	1.98	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:D:225:PRO:HA	2:D:247:MET:HE1	1.98	0.46
2:E:307:PRO:HG2	2:E:313:HIS:CE1	2.51	0.46
1:H:302:ALA:O	1:H:306:SER:OG	2.33	0.46
2:E:91:ASP:OD1	2:E:95:ARG:N	2.49	0.46
2:E:148:PRO:HD3	2:E:323:THR:HB	1.97	0.46
2:K:33:ARG:HE	2:K:71:ARG:NH1	2.14	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:80:ILE:HA	1:I:290:VAL:HG22	1.98	0.46
1:I:570:ILE:HD13	1:I:570:ILE:H	1.81	0.46
2:L:410:ASN:O	2:L:414:ASN:HB3	2.16	0.46
1:B:534:LYS:O	1:B:537:SER:OG	2.32	0.45
2:E:3:LYS:H	2:E:3:LYS:HG3	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
1:B:320:MET:HE2	1:B:322:TYR:HE2	1.79	0.45
1:C:298:MET:HG3	2:F:115:VAL:HG11	1.98	0.45
2:E:127:PHE:CE1	2:E:171:LEU:HD11	2.50	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
1:I:131:SER:N	1:I:134:ASP:OD2	2.49	0.45
2:J:137:HIS:ND1	2:J:412:TYR:OH	2.49	0.45
2:K:45:LEU:HD11	2:K:55:GLN:HB2	1.98	0.45
2:K:152:GLY:H	2:K:155:LEU:HD12	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:C:91:LEU:HD13	2:F:118:PRO:HG2	1.99	0.45
2:D:29:LEU:HD11	2:D:77:LEU:HD23	1.98	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:G:320:MET:HE2	1:G:322:TYR:CE2	2.47	0.45
1:A:81:SER:OG	1:A:286:MET:O	2.33	0.44
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:75:LEU:HD13	1:C:316:TYR:HB2	1.98	0.44
1:C:261:GLU:OE2	1:C:330:SER:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:6:ARG:HD3	2:K:69:SER:HB3	2.00	0.44
2:K:439:ARG:HH22	2:K:451:ASP:CG	2.26	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
1:C:445:MET:HE3	1:C:515:ARG:HG3	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:B:483:SER:OG	1:B:486:ASP:OD1	2.27	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:77:PRO:HA	1:H:78:GLY:HA2	1.50	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:I:467:GLU:CD	1:I:471:ASN:HD21	2.26	0.44
1:I:518:GLN:HE21	1:I:518:GLN:C	2.25	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
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: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:L:8:ILE:HG21	2:L:16:MET:HE2	2.00	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:135:ILE:HD13	1:I:148:LYS:HD3	2.00	0.43
1:I:219:PHE:C	1:I:221:PRO:HD3	2.43	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:OE1	2:J:83:GLU:N	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:133:SER:O	2:L:412:TYR:OH	2.24	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
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:HD3	2:K:446:LYS:HA	1.81	0.43
2:F:363:GLU:H	2:F:363:GLU:HG3	1.41	0.43
1:H:87:ILE:HG13	1:H:89:ARG:HG3	2.01	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
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:OD1	1:B:486:ASP:N	2.50	0.43
2:D:227:MET:HE3	2:D:227:MET:HB3	1.85	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:HB3	1:A:5:LYS:HE3	1.81	0.42
1:B:141:GLU:HG3	1:B:142:THR:HG23	2.01	0.42
2:D:57:PHE:CE1	2:D:219:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:ARG:H	2:F:95:ARG:HG2	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:H	1:C:105:ARG:HG2	1.61	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
1:H:41:GLU:HB2	1:H:48:SER:HB2	2.00	0.42
1:H:329:ASP:HA	1:H:330:SER:HA	1.52	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: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:A:521:MET:HE3	1:A:521:MET:HB2	1.91	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: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:I:437:TYR:OH	2:J:189:GLU:OE1	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:H:543:ASN:N	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:85:ASP:HB3	1:C:91:LEU:HD21	2.02	0.41
1:C:259:CYS:O	1:C:333:ARG:HB2	2.21	0.41
2:D:371:GLN:OE1	2:D:444:ARG:HG2	2.20	0.41
2:E:159:GLU:OE1	2:E:159:GLU:N	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
1:C:546:MET:HE3	1:C:546:MET:HB2	1.90	0.41
2:F:290:ARG:HG2	2:F:297:SER:HB3	2.01	0.41
1:G:73:VAL:HG23	1:G:88:GLN:CD	2.45	0.41
2:K:145:GLN:HG3	2:K:351:LEU:HD12	2.01	0.41
2:L:433:LEU:HD22	2:L:433:LEU:O	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:H:150:MET:HE1	1:H:319:ASP:HB2	2.02	0.41
1:I:518:GLN:HE21	1:I:518:GLN:CA	2.33	0.41
2:L:92:GLY:O	2:L:227:MET:HG3	2.19	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:H	1:I:3:ILE:HD13	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
2:F:136:ASP:OD1	2:F:136:ASP:N	2.53	0.41
1:H:125:GLU:O	1:H:128:THR:OG1	2.37	0.41
1:I:150:MET:HE2	1:I:150:MET:HB3	1.89	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
1:A:391:SER:OG	2:D:321:TYR:OH	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:ARG:HD3	2:D:69:SER:OG	2.20	0.41
2:D:307:PRO:HG2	2:D:313:HIS:CE1	2.55	0.41
2:E:431:TRP:O	2:E:435:ALA:N	2.54	0.41
2:F:135:ILE:H	2:F:135:ILE:HG12	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:HD12	2:F:219:ILE:H	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:B:90:PRO:HG2	1:B:93:THR:HB	2.02	0.41
1:B:242:GLN:HB2	1:B:327:MET:HE1	2.03	0.41
1:C:77:PRO:HG2	1:C:169:ILE:HG22	2.03	0.41
1:C:346:GLU:O	2:D:265:ARG:NH1	2.42	0.41
2:D:150:PHE:HB2	2:D:328:ILE:HD13	2.03	0.41
2:D:162:ALA:O	2:D:166:ARG:HG3	2.21	0.41
2:E:144:GLY:HA2	2:E:298:VAL:O	2.21	0.41
1:G:261:GLU:HB2	1:G:266:MET:HE2	2.02	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
1:I:27:MET:HE3	1:I:71:LEU:HB2	2.01	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:134:ALA:HB2	2:L:413:VAL:HB	2.02	0.41
2:L:397:ILE:HD12	2:L:398:ASP:N	2.36	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:HZ2	2:E:403:LYS:HG3	1.77	0.40
2:F:34:MET:HE3	2:F:38:GLU:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:254:VAL:O	1:I:289:THR:HA	2.21	0.40
1:I:500:TYR:HD2	1:I:500:TYR:HA	1.61	0.40
2:J:386:ALA:HB1	2:J:391:GLU:HA	2.02	0.40
2:J:397:ILE:H	2:J:397:ILE:HG13	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:H	1:C:173:ILE:HD13	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:A:565:GLU:H	1:A:565:GLU:CD	2.28	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
2:E:306:MET:HE1	2:E:311:LYS:HG2	2.02	0.40
1:I:8:LYS:HB3	1:I:15:MET:HB2	2.04	0.40
1:I:150:MET:HE1	1:I:320:MET:HA	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
1	C	582/594 (98%)	564 (97%)	18 (3%)	0	100	100
1	G	585/594 (98%)	563 (96%)	21 (4%)	1 (0%)	43	70
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%)	43	70
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%)	473 (94%)	30 (6%)	17	43
1	B	466/507 (92%)	433 (93%)	33 (7%)	13	39
1	C	482/507 (95%)	455 (94%)	27 (6%)	19	46
1	G	490/507 (97%)	468 (96%)	22 (4%)	24	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	476/507 (94%)	452 (95%)	24 (5%)	22	48
1	I	465/507 (92%)	427 (92%)	38 (8%)	10	36
2	D	367/385 (95%)	346 (94%)	21 (6%)	18	45
2	E	344/385 (89%)	312 (91%)	32 (9%)	8	29
2	F	340/385 (88%)	297 (87%)	43 (13%)	4	18
2	J	364/385 (94%)	339 (93%)	25 (7%)	14	40
2	K	360/385 (94%)	343 (95%)	17 (5%)	23	50
2	L	343/385 (89%)	316 (92%)	27 (8%)	11	37
All	All	5000/5352 (93%)	4661 (93%)	339 (7%)	14	40

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	3	ILE
1	A	19	MET
1	A	33	LEU
1	A	43	ARG
1	A	73	VAL
1	A	150	MET
1	A	222	VAL
1	A	259	CYS
1	A	261	GLU
1	A	273	PHE
1	A	297	ASN
1	A	327	MET
1	A	339	ARG
1	A	348	MET
1	A	375	LEU
1	A	396	ASP
1	A	399	GLU
1	A	401	VAL
1	A	449	LEU
1	A	463	ILE
1	A	465	GLN
1	A	479	ILE
1	A	480	ASP
1	A	485	ASN
1	A	533	ARG

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Mol	Chain	Res	Type
1	A	543	ASN
1	A	552	VAL
1	A	573	ILE
1	A	575	GLU
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
1	B	188	MET
1	B	230	VAL
1	B	257	VAL
1	B	259	CYS
1	B	273	PHE
1	B	275	GLU
1	B	277	ILE
1	B	297	ASN
1	B	348	MET
1	B	401	VAL
1	B	455	ASP
1	B	461	MET
1	B	465	GLN
1	B	470	LEU
1	B	480	ASP
1	B	482	LEU
1	B	487	ARG
1	B	500	TYR
1	B	511	THR
1	B	536	LEU
1	B	541	TYR
1	B	585	VAL
1	C	3	ILE
1	C	19	MET
1	C	25	GLN
1	C	69	GLU
1	C	87	ILE

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Mol	Chain	Res	Type
1	C	99	GLN
1	C	105	ARG
1	C	135	ILE
1	C	143	LYS
1	C	173	ILE
1	C	179	GLU
1	C	185	LEU
1	C	188	MET
1	C	204	ASN
1	C	215	VAL
1	C	222	VAL
1	C	250	ASP
1	C	253	LEU
1	C	273	PHE
1	C	277	ILE
1	C	292	ILE
1	C	295	THR
1	C	307	ILE
1	C	445	MET
1	C	476	LEU
1	C	482	LEU
1	C	562	ILE
2	D	6	ARG
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	93	LEU
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

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Mol	Chain	Res	Type
2	D	450	LEU
2	E	3	LYS
2	E	4	GLU
2	E	6	ARG
2	E	15	LEU
2	E	71	ARG
2	E	103	ILE
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	332	GLU
2	E	362	ARG
2	E	363	GLU
2	E	365	HIS
2	E	370	ASN
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	436	MET
2	E	450	LEU
2	F	6	ARG
2	F	21	VAL
2	F	41	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

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Mol	Chain	Res	Type
2	F	135	ILE
2	F	137	HIS
2	F	141	LEU
2	F	143	ARG
2	F	186	ILE
2	F	196	GLU
2	F	204	ILE
2	F	205	ASP
2	F	215	ASN
2	F	216	ASP
2	F	247	MET
2	F	267	VAL
2	F	276	TYR
2	F	294	LEU
2	F	311	LYS
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
2	F	422	THR
2	F	424	THR
2	F	427	LEU
2	F	429	LEU
2	F	434	LEU
2	F	437	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	73	VAL
1	G	88	GLN
1	G	161	LYS
1	G	222	VAL
1	G	230	VAL
1	G	268	ASP
1	G	273	PHE
1	G	297	ASN

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Mol	Chain	Res	Type
1	G	378	ASP
1	G	408	VAL
1	G	455	ASP
1	G	477	VAL
1	G	479	ILE
1	G	534	LYS
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	155	ILE
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	285	LEU
1	H	291	LEU
1	H	401	VAL
1	H	407	ARG
1	H	488	LEU
1	H	511	THR
1	H	534	LYS
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	87	ILE
1	I	89	ARG

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Mol	Chain	Res	Type
1	I	158	THR
1	I	159	VAL
1	I	182	LEU
1	I	216	ILE
1	I	250	ASP
1	I	262	ARG
1	I	275	GLU
1	I	288	ARG
1	I	291	LEU
1	I	338	LEU
1	I	339	ARG
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	500	TYR
1	I	509	VAL
1	I	518	GLN
1	I	525	ILE
1	I	534	LYS
1	I	538	LEU
1	I	545	ILE
1	I	554	GLU
1	I	555	ARG
1	I	560	LYS
1	I	566	GLU
1	I	570	ILE
1	I	583	LEU
2	J	15	LEU
2	J	36	ASN
2	J	39	ILE
2	J	47	VAL
2	J	79	LEU
2	J	115	VAL
2	J	116	ILE
2	J	123	TYR

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Mol	Chain	Res	Type
2	J	155	LEU
2	J	172	ASP
2	J	206	ARG
2	J	250	MET
2	J	352	LYS
2	J	360	LYS
2	J	361	THR
2	J	362	ARG
2	J	371	GLN
2	J	397	ILE
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	97	LYS
2	K	104	LEU
2	K	119	ILE
2	K	123	TYR
2	K	129	GLN
2	K	241	MET
2	K	247	MET
2	K	257	LEU
2	K	294	LEU
2	K	360	LYS
2	K	370	ASN
2	K	397	ILE
2	K	401	TYR
2	K	429	LEU
2	K	442	LEU
2	K	444	ARG
2	L	39	ILE
2	L	48	GLN
2	L	79	LEU
2	L	90	PHE
2	L	97	LYS
2	L	146	LYS
2	L	149	VAL
2	L	174	SER

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Mol	Chain	Res	Type
2	L	204	ILE
2	L	244	LEU
2	L	373	PHE
2	L	388	VAL
2	L	391	GLU
2	L	397	ILE
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	434	LEU
2	L	440	THR
2	L	443	LYS
2	L	444	ARG
2	L	447	ASP
2	L	449	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	146	GLN
1	A	403	GLN
1	A	485	ASN
1	B	146	GLN
1	B	160	GLN
1	B	264	ASN
1	C	50	GLN
1	C	204	ASN
2	D	129	GLN
2	D	139	ASN
2	D	163	GLN
2	D	167	GLN
2	E	67	ASN
2	E	139	ASN
2	E	371	GLN
2	E	381	GLN
1	G	88	GLN
1	G	146	GLN

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Mol	Chain	Res	Type
1	G	213	GLN
1	H	117	GLN
1	H	146	GLN
1	H	485	ASN
1	H	574	ASN
1	I	108	GLN
1	I	244	GLN
1	I	264	ASN
1	I	403	GLN
1	I	471	ASN
1	I	518	GLN
2	J	67	ASN
2	J	139	ASN
2	J	167	GLN
2	J	371	GLN
2	J	410	ASN
2	J	414	ASN
2	K	212	ASN
2	L	48	GLN
2	L	163	GLN
2	L	415	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	601	-	5,5,5	0.97	0	5,5,5	1.04	0
3	GOL	A	606	-	5,5,5	0.93	0	5,5,5	1.12	0
3	GOL	K	501	-	5,5,5	0.94	0	5,5,5	1.06	0
3	GOL	A	602	-	5,5,5	0.97	0	5,5,5	1.06	0
3	GOL	D	503	-	5,5,5	0.94	0	5,5,5	1.08	0
3	GOL	A	603	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	D	505	-	5,5,5	0.92	0	5,5,5	1.10	0
3	GOL	G	601	-	5,5,5	0.95	0	5,5,5	1.09	0
3	GOL	H	601	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	A	605	-	5,5,5	0.96	0	5,5,5	1.07	0
3	GOL	A	604	-	5,5,5	0.94	0	5,5,5	1.08	0
3	GOL	G	602	-	5,5,5	0.95	0	5,5,5	1.05	0
3	GOL	G	603	-	5,5,5	0.93	0	5,5,5	1.10	0
3	GOL	A	601	-	5,5,5	0.83	0	5,5,5	1.22	1 (20%)
3	GOL	D	501	-	5,5,5	0.93	0	5,5,5	1.11	0
3	GOL	D	502	-	5,5,5	0.96	0	5,5,5	1.04	0
3	GOL	D	504	-	5,5,5	0.96	0	5,5,5	1.05	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	C	601	-	-	2/4/4/4	-
3	GOL	A	606	-	-	4/4/4/4	-
3	GOL	K	501	-	-	0/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	D	505	-	-	0/4/4/4	-
3	GOL	G	601	-	-	2/4/4/4	-
3	GOL	H	601	-	-	0/4/4/4	-
3	GOL	A	605	-	-	0/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	G	602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	603	-	-	2/4/4/4	-
3	GOL	A	601	-	-	4/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	D	504	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	GOL	C3-C2-C1	-2.04	104.30	111.80

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	A	606	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-C3
3	D	503	GOL	O1-C1-C2-C3
3	G	601	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	602	GOL	O1-C1-C2-C3
3	A	604	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	G	603	GOL	O1-C1-C2-C3
3	A	601	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2
3	A	606	GOL	O1-C1-C2-O2
3	D	502	GOL	O1-C1-C2-O2
3	G	601	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	587/594 (98%)	-0.35	3 (0%) 87 77	42, 67, 119, 162	0
1	B	586/594 (98%)	-0.10	0 100 100	51, 126, 183, 248	0
1	C	584/594 (98%)	-0.10	1 (0%) 91 87	68, 110, 169, 252	0
1	G	587/594 (98%)	-0.24	1 (0%) 91 87	45, 85, 165, 251	0
1	H	586/594 (98%)	-0.18	1 (0%) 91 87	62, 101, 165, 225	0
1	I	584/594 (98%)	0.05	3 (0%) 87 77	73, 119, 212, 238	0
2	D	454/462 (98%)	-0.30	0 100 100	43, 76, 124, 161	0
2	E	452/462 (97%)	-0.18	1 (0%) 91 87	56, 93, 186, 266	0
2	F	451/462 (97%)	0.04	3 (0%) 84 72	73, 136, 232, 279	0
2	J	455/462 (98%)	-0.13	1 (0%) 91 87	58, 93, 152, 229	0
2	K	454/462 (98%)	-0.23	1 (0%) 91 87	54, 88, 139, 202	0
2	L	455/462 (98%)	0.04	6 (1%) 75 60	68, 123, 213, 305	0
All	All	6235/6336 (98%)	-0.14	21 (0%) 90 83	42, 101, 188, 305	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	CYS	3.5
1	G	260	GLY	3.4
1	A	260	GLY	3.1
2	F	130	THR	3.0
2	L	428	ASP	2.9
1	A	397	ILE	2.8
1	I	85	ASP	2.7
2	E	358	ALA	2.4
2	L	368	THR	2.4
1	I	500	TYR	2.4
2	L	435	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	93	LEU	2.2
2	J	171	LEU	2.2
2	F	445	ILE	2.1
1	H	52	TYR	2.1
1	A	297	ASN	2.1
2	L	449	LEU	2.1
1	I	501	LEU	2.0
2	F	134	ALA	2.0
2	L	434	LEU	2.0
2	K	103	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
3	GOL	A	602	6/6	0.59	0.13	102,103,104,105	0
3	GOL	K	501	6/6	0.61	0.13	104,105,105,105	0
3	GOL	A	605	6/6	0.64	0.14	94,96,96,97	0
3	GOL	G	602	6/6	0.67	0.11	91,92,93,95	0
3	GOL	C	601	6/6	0.67	0.11	116,118,119,120	0
3	GOL	D	505	6/6	0.71	0.17	116,117,117,118	0
3	GOL	D	504	6/6	0.76	0.17	114,115,116,116	0
3	GOL	G	601	6/6	0.77	0.09	95,95,95,96	0
3	GOL	D	503	6/6	0.80	0.16	137,137,138,138	0
3	GOL	G	603	6/6	0.81	0.09	92,94,94,94	0
3	GOL	A	601	6/6	0.81	0.11	108,110,110,112	0
3	GOL	D	502	6/6	0.84	0.10	84,86,86,86	0
3	GOL	A	603	6/6	0.85	0.12	93,95,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	501	6/6	0.85	0.11	74,76,77,77	0
3	GOL	A	604	6/6	0.86	0.12	77,79,80,80	0
3	GOL	A	606	6/6	0.89	0.14	110,110,111,111	0
3	GOL	H	601	6/6	0.92	0.10	89,90,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.