



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:15 PM UTC

PDB ID : 3JQO / pdb_00003jqo
Title : Crystal structure of the outer membrane complex of a type IV secretion system
Authors : Chandran, V.; Fronzes, R.; Duquerroy, S.; Cronin, N.; Navaza, J.; Waksman, G.
Deposited on : 2009-09-07
Resolution : 2.60 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

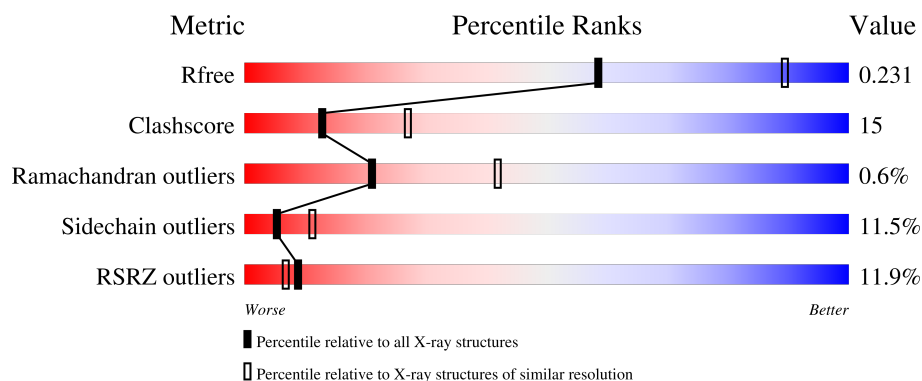
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	227	9% 59% 23% • • 14%
1	D	227	9% 59% 22% • 14%
1	G	227	8% 59% 22% • • 15%
1	J	227	11% 57% 26% • 13%
1	M	227	11% 59% 22% 5% • 13%

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Mol	Chain	Length	Quality of chain
1	P	227	
1	S	227	
1	V	227	
1	Y	227	
1	b	227	
1	e	227	
1	h	227	
1	k	227	
1	n	227	
2	B	135	
2	E	135	
2	H	135	
2	K	135	
2	N	135	
2	Q	135	
2	T	135	
2	W	135	
2	Z	135	
2	c	135	
2	f	135	
2	i	135	
2	l	135	
2	o	135	
3	C	34	
3	F	34	

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Mol	Chain	Length	Quality of chain
3	I	34	
3	L	34	
3	O	34	
3	R	34	
3	U	34	
3	X	34	
3	a	34	
3	d	34	
3	g	34	
3	j	34	
3	m	34	
3	p	34	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	LDA	J	1	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38842 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 TraF protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1448	898	253	290	2	5			
1	D	195	Total	C	N	O	S	Se	0	0	0
			1448	898	253	290	2	5			
1	G	193	Total	C	N	O	S	Se	0	0	0
			1437	890	252	288	2	5			
1	J	197	Total	C	N	O	S	Se	0	0	0
			1457	903	256	291	2	5			
1	M	197	Total	C	N	O	S	Se	0	0	0
			1461	905	256	293	2	5			
1	P	197	Total	C	N	O	S	Se	0	0	0
			1461	905	256	293	2	5			
1	S	197	Total	C	N	O	S	Se	0	0	0
			1461	905	256	293	2	5			
1	V	196	Total	C	N	O	S	Se	0	0	0
			1457	903	255	292	2	5			
1	Y	195	Total	C	N	O	S	Se	0	0	0
			1448	898	253	290	2	5			
1	b	195	Total	C	N	O	S	Se	0	0	0
			1449	898	254	290	2	5			
1	e	196	Total	C	N	O	S	Se	0	0	0
			1457	903	255	292	2	5			
1	h	195	Total	C	N	O	S	Se	0	0	0
			1439	893	250	289	2	5			
1	k	196	Total	C	N	O	S	Se	0	0	0
			1457	903	255	292	2	5			
1	n	196	Total	C	N	O	S	Se	0	0	0
			1457	900	256	294	2	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ARG	ALA	SEE REMARK 999	UNP Q46705

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Chain	Residue	Modelled	Actual	Comment	Reference
D	308	ARG	ALA	SEE REMARK 999	UNP Q46705
G	308	ARG	ALA	SEE REMARK 999	UNP Q46705
J	308	ARG	ALA	SEE REMARK 999	UNP Q46705
M	308	ARG	ALA	SEE REMARK 999	UNP Q46705
P	308	ARG	ALA	SEE REMARK 999	UNP Q46705
S	308	ARG	ALA	SEE REMARK 999	UNP Q46705
V	308	ARG	ALA	SEE REMARK 999	UNP Q46705
Y	308	ARG	ALA	SEE REMARK 999	UNP Q46705
b	308	ARG	ALA	SEE REMARK 999	UNP Q46705
e	308	ARG	ALA	SEE REMARK 999	UNP Q46705
h	308	ARG	ALA	SEE REMARK 999	UNP Q46705
k	308	ARG	ALA	SEE REMARK 999	UNP Q46705
n	308	ARG	ALA	SEE REMARK 999	UNP Q46705

- Molecule 2 is a protein called TraO protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	E	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	H	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	K	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	N	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	Q	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	T	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	W	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	Z	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	c	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	f	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	i	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	l	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	o	130	Total	C	N	O	Se	0	0	0
			1032	647	193	189	3			

- Molecule 3 is a protein called TraN protein.

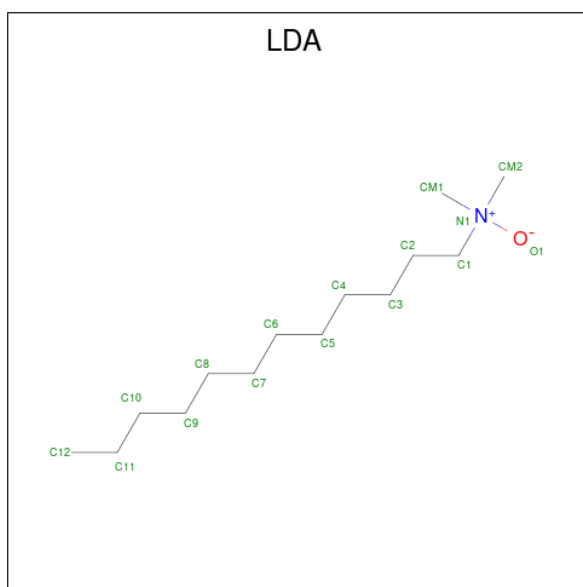
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O		0	0	0
			200	126	34	40				
3	F	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	I	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	L	28	Total	C	N	O	S	0	0	0
			212	132	36	43	1			
3	O	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	R	24	Total	C	N	O		0	0	0
			185	118	31	36				
3	U	27	Total	C	N	O		0	0	0
			206	129	35	42				
3	X	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	a	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	d	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	g	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	j	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	m	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	p	23	Total	C	N	O		0	0	0
			181	116	30	35				

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		
4	h	1	Total	C	O	0	0
			8	6	2		
4	k	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	65	Total O 65 65	0	0
6	B	31	Total O 31 31	0	0
6	C	7	Total O 7 7	0	0
6	D	65	Total O 65 65	0	0
6	E	28	Total O 28 28	0	0
6	F	9	Total O 9 9	0	0
6	G	50	Total O 50 50	0	0
6	H	22	Total O 22 22	0	0
6	I	9	Total O 9 9	0	0
6	J	49	Total O 49 49	0	0
6	K	30	Total O 30 30	0	0
6	L	12	Total O 12 12	0	0
6	M	48	Total O 48 48	0	0
6	N	35	Total O 35 35	0	0
6	O	11	Total O 11 11	0	0
6	P	58	Total O 58 58	0	0
6	Q	27	Total O 27 27	0	0
6	R	7	Total O 7 7	0	0
6	S	57	Total O 57 57	0	0
6	T	21	Total O 21 21	0	0
6	U	10	Total O 10 10	0	0

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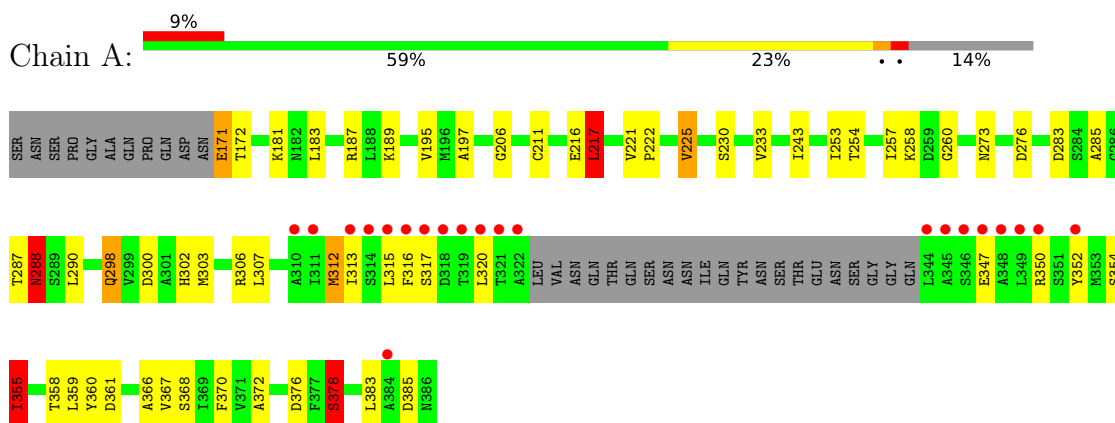
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	V	63	Total O 63 63	0	0
6	W	26	Total O 26 26	0	0
6	X	7	Total O 7 7	0	0
6	Y	57	Total O 57 57	0	0
6	Z	21	Total O 21 21	0	0
6	a	8	Total O 8 8	0	0
6	b	59	Total O 59 59	0	0
6	c	31	Total O 31 31	0	0
6	d	3	Total O 3 3	0	0
6	e	52	Total O 52 52	0	0
6	f	28	Total O 28 28	0	0
6	g	4	Total O 4 4	0	0
6	h	50	Total O 50 50	0	0
6	i	21	Total O 21 21	0	0
6	j	11	Total O 11 11	0	0
6	k	56	Total O 56 56	0	0
6	l	37	Total O 37 37	0	0
6	m	8	Total O 8 8	0	0
6	n	50	Total O 50 50	0	0
6	o	35	Total O 35 35	0	0
6	p	12	Total O 12 12	0	0

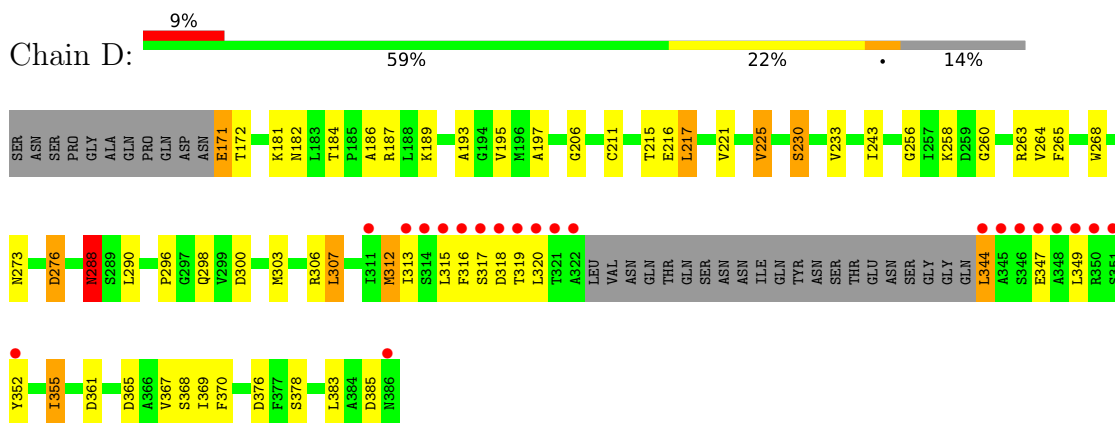
3 Residue-property plots [i](#)

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.

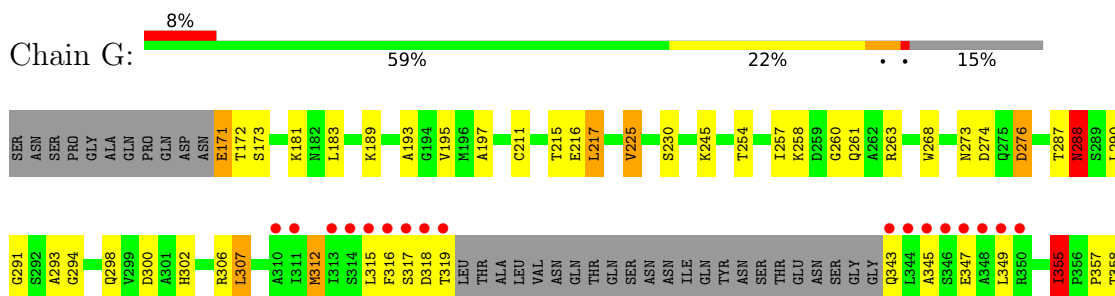
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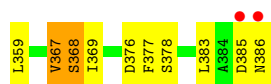


• Molecule 1: TraF protein

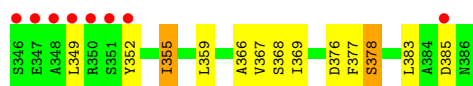


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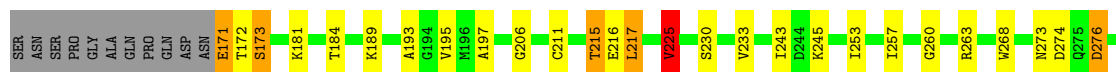




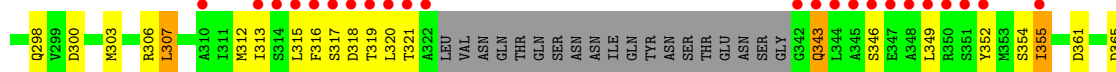
- Molecule 1: TraF protein



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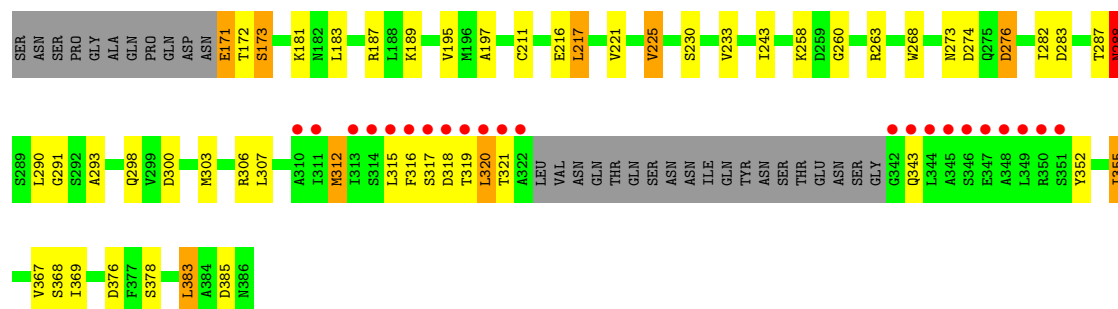


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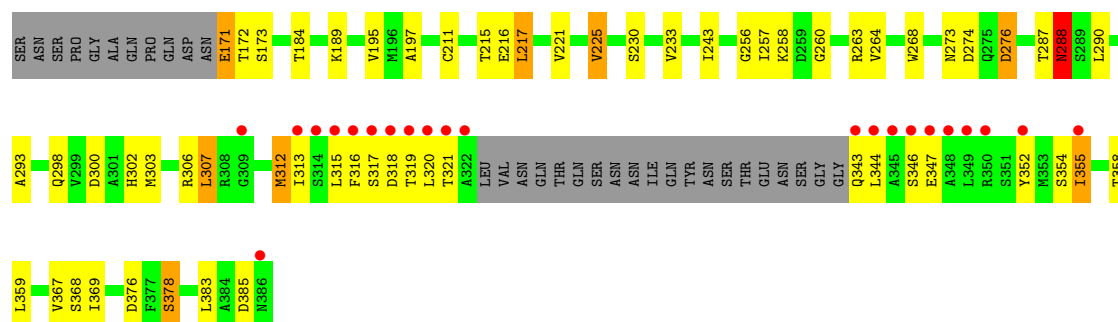


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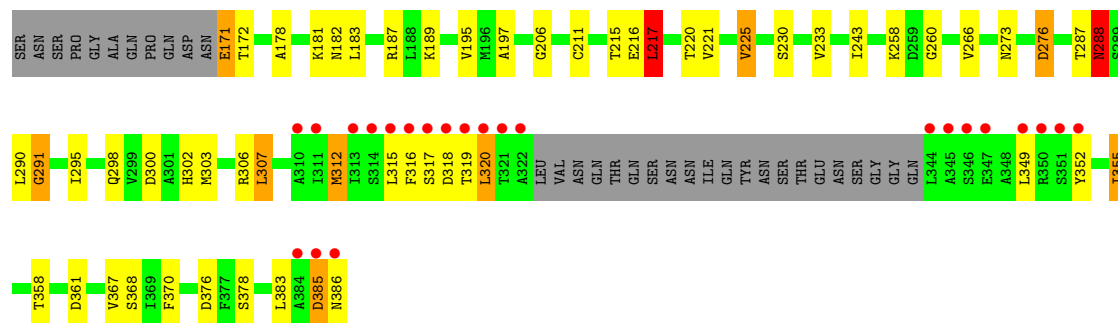




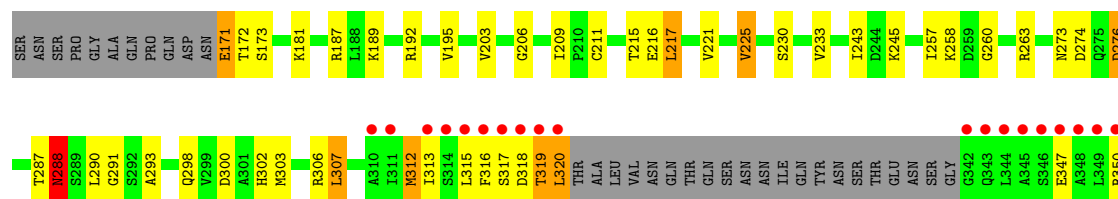
• Molecule 1: TraF protein



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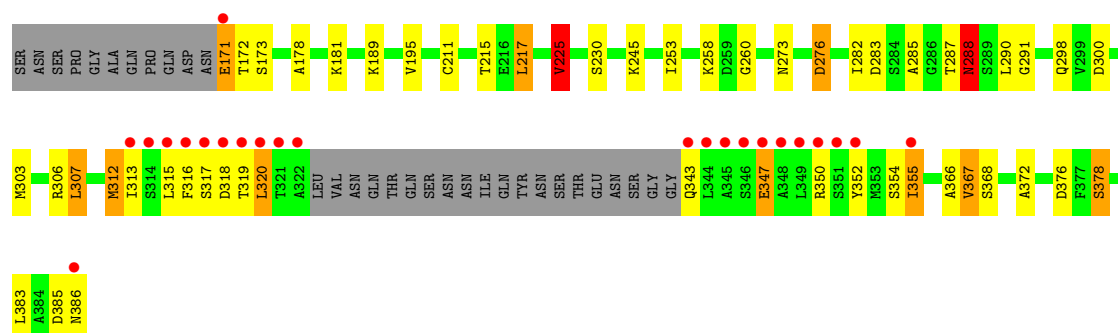


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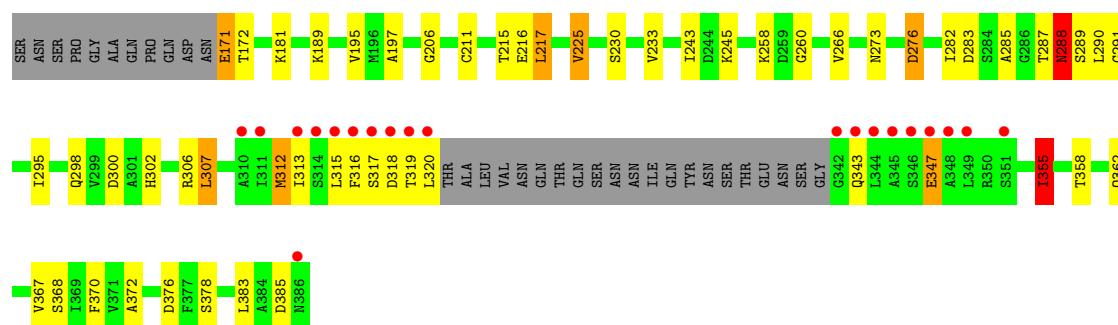




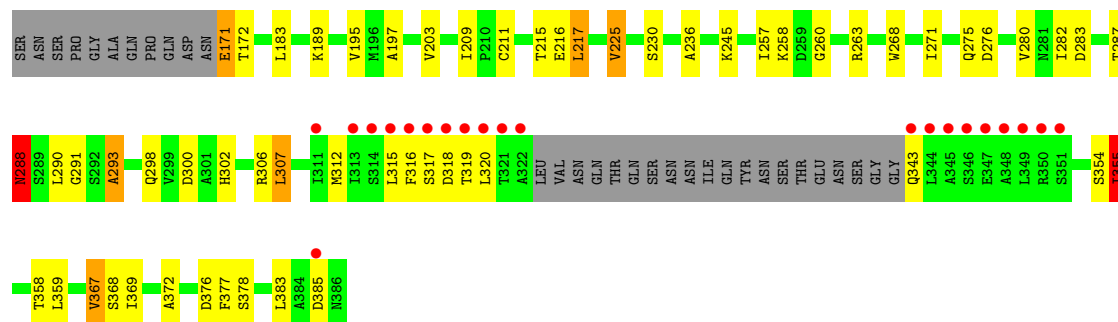
• Molecule 1: TraF protein



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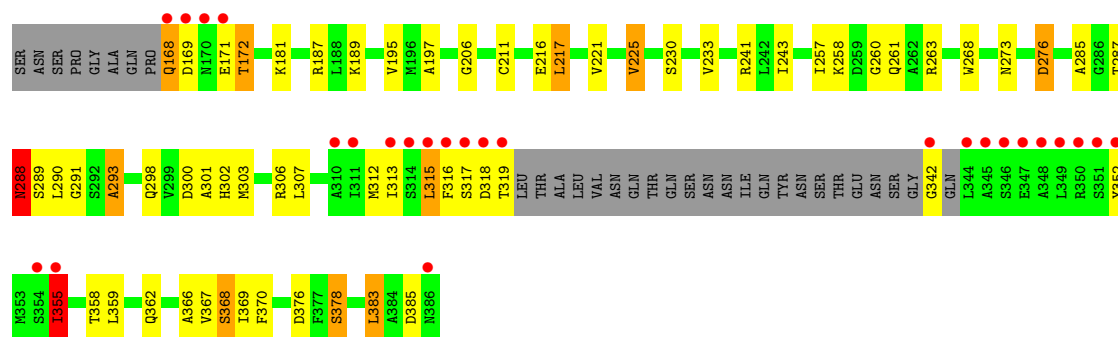


• Molecule 1: TraF protein

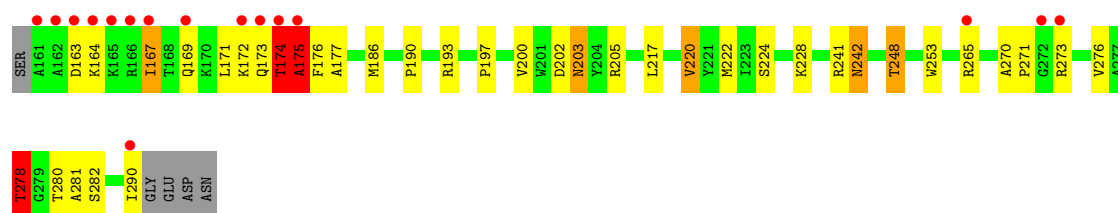


• Molecule 1: TraF protein

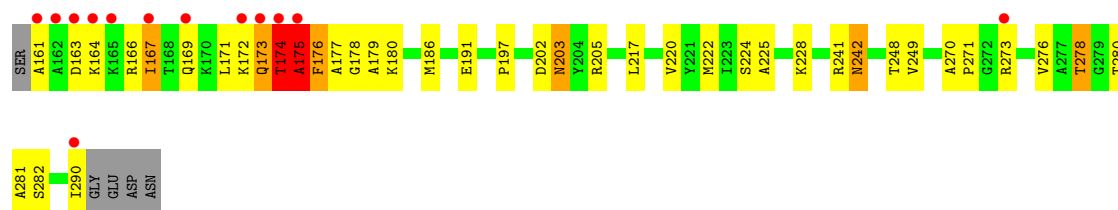




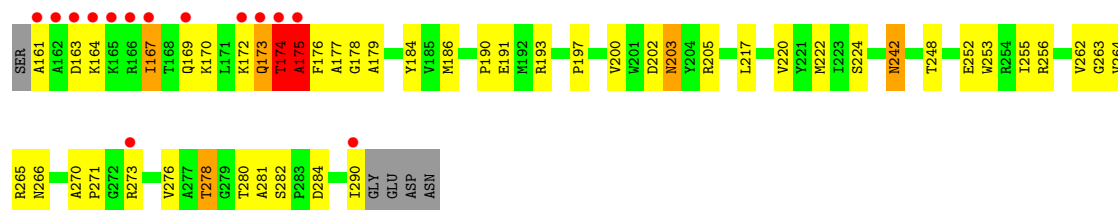
- Molecule 2: TraO protein



- Molecule 2: TraO protein

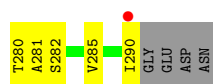


- Molecule 2: TraO protein



- Molecule 2: TraO protein





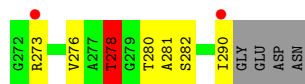
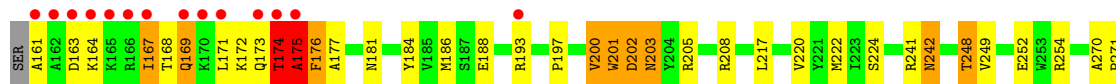
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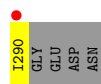
• Molecule 2: TraO protein



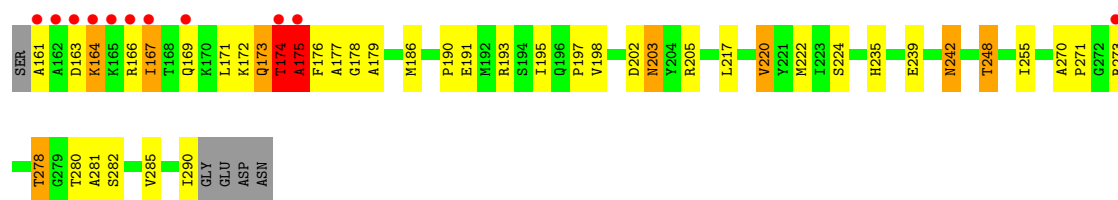
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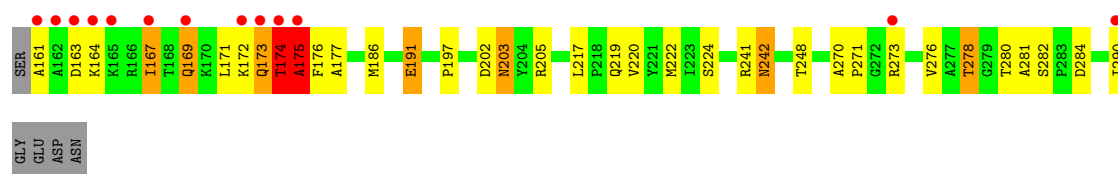
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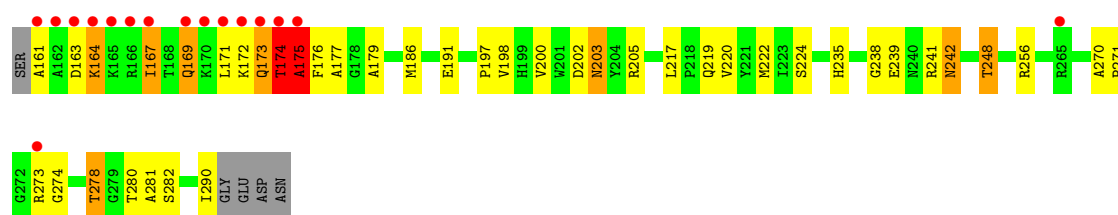
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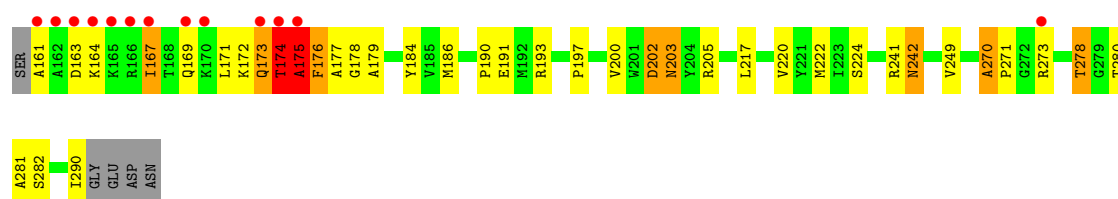
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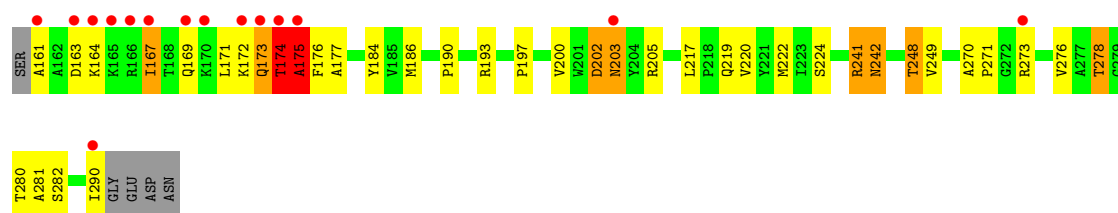
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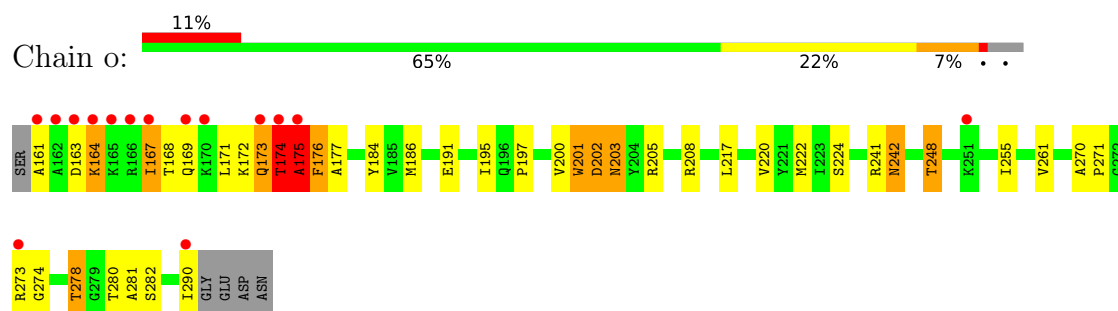
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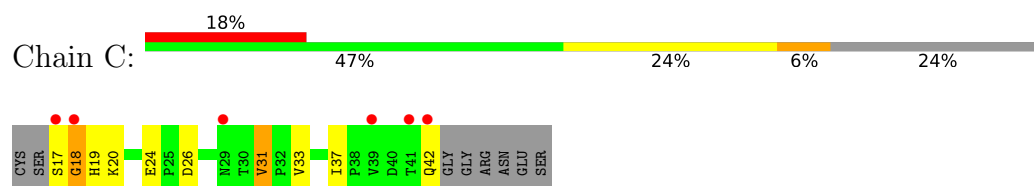
• Molecule 2: TraO protein



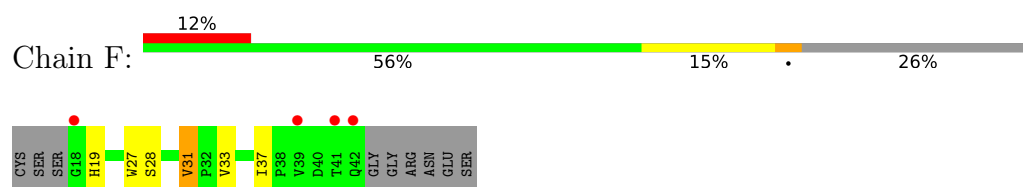
- Molecule 2: TraO protein



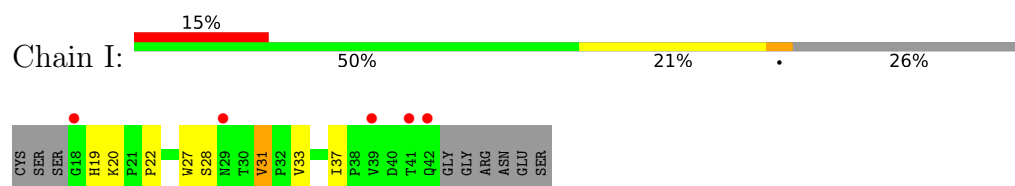
- Molecule 3: TraN protein



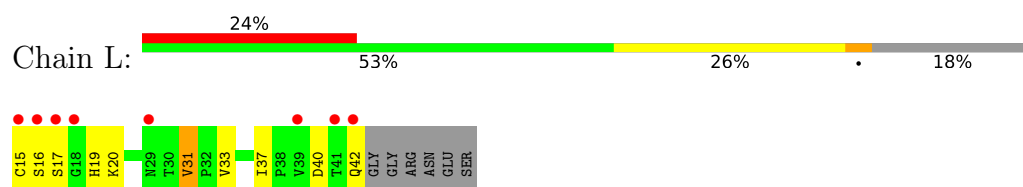
- Molecule 3: TraN protein



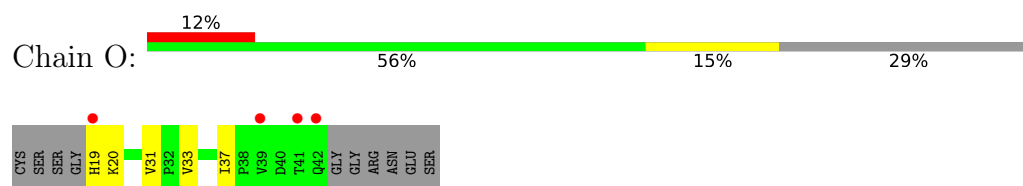
- Molecule 3: TraN protein



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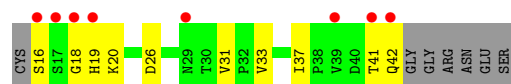
- Molecule 3: TraN protein



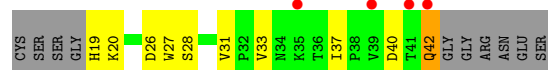
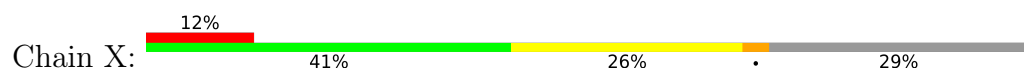
- Molecule 3: TraN protein



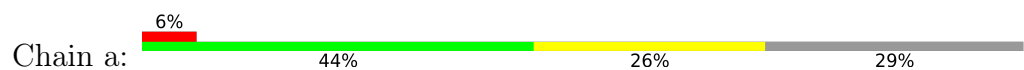
• Molecule 3: TraN protein



• Molecule 3: TraN protein



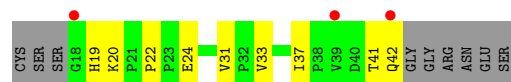
• Molecule 3: TraN protein



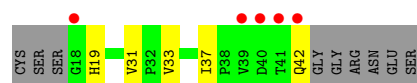
• Molecule 3: TraN protein



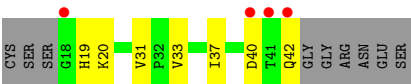
• Molecule 3: TraN protein



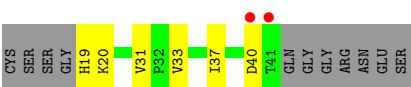
• Molecule 3: TraN protein



● Molecule 3: TraN protein



● Molecule 3: TraN protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	202.40Å 211.63Å 203.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.91 – 2.60 52.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (52.91-2.60) 97.2 (52.91-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.227 , 0.259 0.206 , 0.231	Depositor DCC
R_{free} test set	12939 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k 0.010 for -k,-h,l 0.011 for l,-k,h 0.003 for l,h,k 0.003 for k,l,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	38842	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.20	4/1464 (0.3%)	1.25	7/1978 (0.4%)
1	D	1.21	3/1464 (0.2%)	1.27	10/1978 (0.5%)
1	G	1.18	4/1453 (0.3%)	1.23	7/1962 (0.4%)
1	J	1.20	5/1473 (0.3%)	1.24	9/1990 (0.5%)
1	M	1.17	2/1477 (0.1%)	1.25	11/1995 (0.6%)
1	P	1.14	1/1477 (0.1%)	1.24	8/1995 (0.4%)
1	S	1.16	1/1477 (0.1%)	1.24	7/1995 (0.4%)
1	V	1.17	3/1473 (0.2%)	1.22	9/1990 (0.5%)
1	Y	1.20	4/1464 (0.3%)	1.26	9/1978 (0.5%)
1	b	1.22	3/1465 (0.2%)	1.26	7/1978 (0.4%)
1	e	1.19	5/1473 (0.3%)	1.24	8/1990 (0.4%)
1	h	1.21	4/1455 (0.3%)	1.28	8/1966 (0.4%)
1	k	1.20	6/1473 (0.4%)	1.24	11/1990 (0.6%)
1	n	1.22	7/1472 (0.5%)	1.27	11/1986 (0.6%)
2	B	1.17	1/1051 (0.1%)	1.27	10/1417 (0.7%)
2	E	1.14	1/1051 (0.1%)	1.27	10/1417 (0.7%)
2	H	1.30	2/1051 (0.2%)	1.29	10/1417 (0.7%)
2	K	1.13	0/1051	1.29	10/1417 (0.7%)
2	N	1.08	0/1051	1.28	13/1417 (0.9%)
2	Q	1.11	0/1051	1.30	12/1417 (0.8%)
2	T	1.15	2/1051 (0.2%)	1.27	8/1417 (0.6%)
2	W	1.13	0/1051	1.24	9/1417 (0.6%)
2	Z	1.09	0/1051	1.27	11/1417 (0.8%)
2	c	1.11	0/1051	1.30	10/1417 (0.7%)
2	f	1.20	1/1051 (0.1%)	1.28	14/1417 (1.0%)
2	i	1.21	2/1051 (0.2%)	1.25	10/1417 (0.7%)
2	l	1.14	0/1051	1.28	11/1417 (0.8%)
2	o	1.19	1/1050 (0.1%)	1.28	10/1415 (0.7%)
3	C	1.21	0/208	1.23	4/289 (1.4%)
3	F	1.02	0/202	1.06	1/281 (0.4%)
3	I	1.03	0/202	1.05	2/281 (0.7%)
3	L	0.98	0/220	1.26	2/305 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	O	0.88	0/198	1.09	0/276
3	R	1.04	0/193	1.15	2/269 (0.7%)
3	U	1.09	0/214	1.24	0/297
3	X	0.96	0/198	1.08	0/276
3	a	0.93	0/198	1.06	0/276
3	d	1.06	0/198	1.11	1/276 (0.4%)
3	g	1.10	0/202	1.18	2/281 (0.7%)
3	j	1.09	0/202	1.07	0/281
3	m	1.10	0/202	1.09	0/281
3	p	1.04	0/189	1.17	0/264
All	All	1.17	62/38099 (0.2%)	1.25	284/51540 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	J	0	1
1	M	0	1
1	P	0	2
1	S	0	1
1	V	0	1
1	Y	0	1
1	b	0	1
1	e	0	1
1	h	0	1
1	k	0	1
1	n	0	1
2	B	0	2
2	E	0	2
2	H	0	2
2	K	0	2
2	N	0	2
2	Q	0	2
2	T	0	2
2	W	0	2
2	Z	0	2
2	c	0	2
2	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	i	0	2
2	l	0	2
2	o	0	2
3	U	0	1
All	All	0	43

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	298	GLN	CD-NE2	-9.94	1.12	1.33
1	e	298	GLN	CD-OE1	-9.17	1.06	1.23
1	A	298	GLN	CD-OE1	-9.16	1.06	1.23
1	A	298	GLN	CD-NE2	-7.77	1.17	1.33
1	b	221	VAL	CA-CB	-7.67	1.48	1.54
1	n	221	VAL	CA-CB	-7.62	1.48	1.54
1	J	285	ALA	CA-CB	-7.56	1.42	1.53
1	J	221	VAL	CA-CB	-7.45	1.48	1.54
1	n	285	ALA	CA-CB	-7.41	1.42	1.53
1	h	285	ALA	CA-CB	-7.36	1.42	1.53
1	e	285	ALA	CA-CB	-7.17	1.42	1.53
1	S	221	VAL	CA-CB	-6.33	1.49	1.54
1	h	288	ASN	CB-CG	-6.32	1.36	1.52
1	A	221	VAL	CA-CB	-6.28	1.49	1.54
1	k	377	PHE	CA-C	6.21	1.61	1.52
2	E	225	ALA	CA-CB	-6.16	1.42	1.53
1	J	276	ASP	CB-CG	-6.13	1.36	1.52
1	k	276	ASP	CB-CG	-6.05	1.36	1.52
2	T	249	VAL	C-O	-6.00	1.18	1.24
1	A	285	ALA	CA-CB	-5.97	1.44	1.53
1	Y	178	ALA	CA-CB	-5.94	1.44	1.53
1	M	276	ASP	CB-CG	-5.88	1.37	1.52
2	f	179	ALA	CA-CB	-5.88	1.43	1.53
1	n	293	ALA	C-O	5.79	1.31	1.23
1	M	193	ALA	CA-CB	-5.75	1.43	1.53
1	k	203	VAL	CA-CB	5.71	1.59	1.53
1	J	366	ALA	CA-CB	-5.66	1.45	1.53
2	H	264	VAL	C-O	-5.63	1.18	1.24
1	n	241	ARG	C-O	-5.55	1.17	1.24
1	V	221	VAL	CA-CB	-5.49	1.50	1.54
2	H	263	GLY	C-O	-5.46	1.18	1.23
1	e	366	ALA	CA-CB	-5.43	1.46	1.53
1	D	276	ASP	CB-CG	-5.43	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	221	VAL	CA-C	-5.40	1.48	1.52
1	b	203	VAL	C-O	-5.39	1.18	1.24
1	n	366	ALA	CA-CB	-5.37	1.46	1.53
1	P	288	ASN	CB-CG	-5.33	1.38	1.52
1	h	276	ASP	CB-CG	-5.29	1.38	1.52
1	J	377	PHE	CA-C	5.29	1.60	1.52
2	i	270	ALA	CA-CB	-5.26	1.47	1.53
1	k	280	VAL	C-O	-5.25	1.18	1.24
1	D	186	ALA	CA-CB	-5.25	1.46	1.53
2	B	220	VAL	CA-CB	5.24	1.61	1.54
2	T	200	VAL	C-O	-5.22	1.18	1.24
1	n	362	GLN	CA-C	5.22	1.59	1.52
1	k	275	GLN	C-O	-5.20	1.17	1.24
1	V	256	GLY	C-O	-5.19	1.19	1.24
1	G	261	GLN	C-O	-5.17	1.17	1.23
1	G	377	PHE	CA-C	5.16	1.59	1.52
1	Y	276	ASP	CB-CG	-5.15	1.39	1.52
1	h	362	GLN	CA-C	5.13	1.59	1.52
2	o	261	VAL	CA-CB	5.13	1.61	1.54
1	n	261	GLN	C-O	-5.11	1.17	1.24
1	G	193	ALA	CA-CB	-5.09	1.44	1.53
1	D	193	ALA	CA-CB	-5.06	1.44	1.53
1	V	264	VAL	CA-C	5.05	1.58	1.52
1	G	276	ASP	CB-CG	-5.04	1.39	1.52
1	k	236	ALA	CA-CB	-5.04	1.44	1.53
1	e	276	ASP	CB-CG	-5.03	1.39	1.52
2	i	249	VAL	C-O	-5.01	1.19	1.24
1	Y	221	VAL	N-CA	5.00	1.50	1.46
1	b	209	ILE	CA-CB	5.00	1.59	1.53

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	176	PHE	N-CA-C	-11.18	97.50	112.26
2	Q	176	PHE	N-CA-C	-10.75	98.07	112.26
2	H	176	PHE	N-CA-C	-10.20	98.80	112.26
2	c	176	PHE	N-CA-C	-10.09	98.94	112.26
2	f	176	PHE	N-CA-C	-9.87	99.24	112.26
2	E	174	THR	N-CA-C	9.45	122.53	109.11
2	K	174	THR	N-CA-C	9.28	122.29	109.11
2	N	174	THR	N-CA-C	9.25	122.25	109.11
2	i	176	PHE	N-CA-C	-9.13	97.75	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	176	PHE	N-CA-C	-9.08	100.27	112.26
2	T	176	PHE	N-CA-C	-9.02	100.36	112.26
2	o	176	PHE	N-CA-C	-8.77	100.68	112.26
2	f	174	THR	N-CA-C	8.75	121.54	109.11
2	T	174	THR	N-CA-C	8.64	121.38	109.11
2	N	176	PHE	N-CA-C	-8.60	100.91	112.26
2	W	176	PHE	N-CA-C	-8.51	101.03	112.26
2	Z	176	PHE	N-CA-C	-8.33	101.26	112.26
2	l	174	THR	N-CA-C	8.32	120.92	109.11
2	B	176	PHE	N-CA-C	-7.97	99.53	111.81
2	W	174	THR	N-CA-C	7.94	120.39	109.11
2	N	175	ALA	N-CA-C	7.94	120.49	107.23
1	S	288	ASN	CB-CA-C	-7.88	94.74	110.42
2	i	174	THR	N-CA-C	7.71	121.61	107.73
2	Q	174	THR	N-CA-C	7.56	121.34	107.73
2	T	175	ALA	N-CA-C	7.55	119.84	107.23
2	H	174	THR	N-CA-C	7.35	120.97	107.73
1	V	225	VAL	CB-CA-C	-7.35	99.38	110.55
2	K	176	PHE	N-CA-C	-7.30	100.57	111.81
2	c	174	THR	N-CA-C	7.23	120.75	107.73
1	n	288	ASN	CB-CA-C	-7.14	96.22	110.42
2	W	202	ASP	CA-C-N	7.10	133.49	122.49
2	W	202	ASP	C-N-CA	7.10	133.49	122.49
2	Q	175	ALA	N-CA-C	7.08	119.93	107.61
1	D	288	ASN	CB-CA-C	-7.04	96.41	110.42
2	H	175	ALA	N-CA-C	6.98	119.75	107.61
2	B	202	ASP	CA-C-N	6.97	133.30	122.49
2	B	202	ASP	C-N-CA	6.97	133.30	122.49
1	Y	288	ASN	CB-CA-C	-6.97	96.56	110.42
1	h	225	VAL	CB-CA-C	-6.96	99.97	110.55
1	h	276	ASP	N-CA-CB	-6.94	100.54	110.81
2	B	174	THR	N-CA-C	6.88	120.11	107.73
1	J	225	VAL	CB-CA-C	-6.87	98.69	110.30
1	S	197	ALA	N-CA-C	6.87	118.42	111.07
2	H	203	ASN	CB-CA-C	-6.85	98.59	110.17
1	A	288	ASN	CB-CA-C	-6.83	96.82	110.42
2	W	203	ASN	CB-CA-C	-6.83	98.63	110.17
2	T	203	ASN	N-CA-CB	-6.82	99.73	110.98
1	b	276	ASP	N-CA-CB	-6.81	101.84	110.90
2	W	175	ALA	N-CA-C	6.81	118.60	107.23
1	k	288	ASN	CB-CA-C	-6.80	96.88	110.42
2	K	202	ASP	CA-C-N	6.80	134.03	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	202	ASP	C-N-CA	6.80	134.03	122.26
1	h	288	ASN	CB-CA-C	-6.80	96.89	110.42
1	V	288	ASN	CB-CA-C	-6.77	96.94	110.42
2	f	175	ALA	N-CA-C	6.77	118.53	107.23
2	B	271	PRO	CA-C-N	-6.76	108.16	121.41
2	B	271	PRO	C-N-CA	-6.76	108.16	121.41
2	Z	202	ASP	CA-C-N	6.71	132.89	122.49
2	Z	202	ASP	C-N-CA	6.71	132.89	122.49
2	Z	174	THR	N-CA-C	6.71	120.46	107.71
2	c	202	ASP	CA-C-N	6.68	132.85	122.49
2	c	202	ASP	C-N-CA	6.68	132.85	122.49
2	f	202	ASP	CA-C-N	6.68	132.88	122.26
2	f	202	ASP	C-N-CA	6.68	132.88	122.26
2	l	175	ALA	N-CA-C	6.63	119.15	107.61
1	M	225	VAL	CB-CA-C	-6.62	99.11	110.30
2	l	203	ASN	N-CA-CB	-6.60	100.72	110.49
1	D	225	VAL	CB-CA-C	-6.59	99.16	110.30
2	E	203	ASN	N-CA-CB	-6.59	100.74	110.49
1	J	288	ASN	CB-CA-C	-6.58	97.32	110.42
2	Z	203	ASN	CB-CA-C	-6.56	99.08	110.17
2	E	202	ASP	CA-C-N	6.54	133.33	122.54
2	E	202	ASP	C-N-CA	6.54	133.33	122.54
1	P	288	ASN	CB-CA-C	-6.53	97.42	110.42
1	V	354	SER	CA-C-N	-6.53	116.25	123.43
1	V	354	SER	C-N-CA	-6.53	116.25	123.43
1	G	288	ASN	CB-CA-C	-6.53	97.44	110.42
1	b	288	ASN	CB-CA-C	-6.51	97.46	110.42
1	b	276	ASP	CB-CA-C	-6.49	98.13	109.02
1	k	197	ALA	N-CA-C	6.46	117.99	111.07
2	i	271	PRO	N-CA-C	-6.45	100.96	111.21
2	l	203	ASN	CB-CA-C	-6.44	99.33	110.09
1	G	355	ILE	N-CA-C	6.43	114.90	107.89
1	n	187	ARG	CG-CD-NE	-6.43	97.85	112.00
2	c	203	ASN	CB-CA-C	-6.43	99.30	110.17
1	P	197	ALA	N-CA-C	6.43	117.95	111.07
2	l	271	PRO	N-CA-C	-6.38	101.06	111.21
1	M	288	ASN	CB-CA-C	-6.38	97.73	110.42
2	c	271	PRO	CA-C-N	-6.38	108.91	121.41
2	c	271	PRO	C-N-CA	-6.38	108.91	121.41
2	c	175	ALA	N-CA-C	6.37	118.69	107.61
1	G	217	LEU	CA-CB-CG	6.36	138.54	116.30
2	l	202	ASP	CA-C-N	6.33	132.99	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	202	ASP	C-N-CA	6.33	132.99	122.54
1	h	289	SER	N-CA-C	6.32	119.84	111.75
1	n	355	ILE	N-CA-C	6.32	114.78	107.89
2	N	271	PRO	CA-C-N	-6.30	109.05	121.41
2	N	271	PRO	C-N-CA	-6.30	109.05	121.41
2	E	203	ASN	CB-CA-C	-6.30	99.56	110.09
2	B	203	ASN	CB-CA-C	-6.29	99.53	110.17
1	G	225	VAL	CB-CA-C	-6.29	99.67	110.30
1	A	355	ILE	N-CA-C	6.23	114.69	107.89
2	c	203	ASN	N-CA-CB	-6.23	101.20	110.61
2	i	175	ALA	N-CA-C	6.23	118.45	107.61
2	Z	198	VAL	N-CA-C	-6.21	105.00	111.58
1	D	187	ARG	CG-CD-NE	-6.21	98.34	112.00
2	E	175	ALA	N-CA-C	6.21	118.41	107.61
1	b	225	VAL	CB-CA-C	-6.20	101.12	110.55
2	W	271	PRO	CA-C-N	-6.20	109.26	121.41
2	W	271	PRO	C-N-CA	-6.20	109.26	121.41
1	h	355	ILE	N-CA-C	6.17	114.62	107.89
2	K	271	PRO	CA-C-N	-6.15	109.35	121.41
2	K	271	PRO	C-N-CA	-6.15	109.35	121.41
2	Q	271	PRO	CA-C-N	-6.15	109.36	121.41
2	Q	271	PRO	C-N-CA	-6.15	109.36	121.41
1	M	276	ASP	CB-CA-C	-6.15	98.21	109.15
1	e	225	VAL	CB-CA-C	-6.14	101.22	110.55
2	Z	175	ALA	N-CA-C	6.14	118.29	107.61
2	N	202	ASP	CA-C-N	6.13	131.99	122.49
2	N	202	ASP	C-N-CA	6.13	131.99	122.49
2	Q	203	ASN	CB-CA-C	-6.12	99.83	110.17
2	o	175	ALA	N-CA-C	6.10	118.22	107.61
2	E	271	PRO	CA-C-N	-6.09	109.46	121.41
2	E	271	PRO	C-N-CA	-6.09	109.46	121.41
1	e	367	VAL	N-CA-CB	-6.08	103.28	112.35
1	n	225	VAL	CB-CA-C	-6.06	100.07	110.30
1	k	225	VAL	CB-CA-C	-6.04	100.09	110.30
2	B	175	ALA	N-CA-C	6.04	118.11	107.61
2	H	202	ASP	CA-C-N	6.03	131.84	122.49
2	H	202	ASP	C-N-CA	6.03	131.84	122.49
2	o	174	THR	N-CA-C	6.02	119.15	107.71
1	A	354	SER	CA-C-N	-6.01	116.81	123.43
1	A	354	SER	C-N-CA	-6.01	116.81	123.43
1	k	354	SER	CA-C-N	-6.01	116.82	123.43
1	k	354	SER	C-N-CA	-6.01	116.82	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	271	PRO	N-CA-C	-6.00	101.66	111.21
2	T	271	PRO	CA-C-N	-5.99	109.68	121.41
2	T	271	PRO	C-N-CA	-5.99	109.68	121.41
1	k	217	LEU	CA-CB-CG	5.98	137.23	116.30
1	e	288	ASN	CB-CA-C	-5.98	98.53	110.42
1	n	197	ALA	N-CA-C	5.97	117.46	111.07
2	f	203	ASN	CB-CA-C	-5.97	99.52	109.55
2	o	203	ASN	N-CA-C	-5.96	104.47	113.89
2	Z	220	VAL	N-CA-C	5.94	117.04	108.48
1	A	187	ARG	CG-CD-NE	-5.94	98.94	112.00
2	K	175	ALA	N-CA-C	5.94	117.94	107.61
1	h	197	ALA	N-CA-C	5.92	117.41	111.07
2	Q	202	ASP	CA-C-N	5.92	131.66	122.49
2	Q	202	ASP	C-N-CA	5.92	131.66	122.49
2	Q	203	ASN	N-CA-CB	-5.91	101.69	110.61
1	Y	225	VAL	CB-CA-C	-5.89	100.34	110.30
1	S	217	LEU	CA-CB-CG	5.89	136.90	116.30
1	A	217	LEU	CA-CB-CG	5.88	136.89	116.30
1	n	276	ASP	CB-CA-C	-5.88	98.69	109.15
1	e	217	LEU	CA-CB-CG	5.87	136.85	116.30
1	Y	291	GLY	N-CA-C	5.86	122.53	114.92
2	H	271	PRO	CA-C-N	-5.85	109.95	121.41
2	H	271	PRO	C-N-CA	-5.85	109.95	121.41
2	i	203	ASN	N-CA-C	-5.85	104.65	113.89
1	k	276	ASP	N-CA-CB	-5.84	102.16	110.81
1	D	184	THR	CB-CA-C	-5.83	104.39	110.33
1	k	293	ALA	N-CA-C	5.80	118.66	109.96
1	P	225	VAL	CB-CA-C	-5.80	100.50	110.30
2	T	278	THR	N-CA-CB	-5.80	102.01	110.53
1	b	187	ARG	CG-CD-NE	-5.79	99.27	112.00
1	M	217	LEU	CA-CB-CG	5.79	136.55	116.30
2	l	271	PRO	CA-C-N	-5.78	110.09	121.41
2	l	271	PRO	C-N-CA	-5.78	110.09	121.41
2	K	219	GLN	CB-CA-C	5.75	119.90	109.37
1	n	217	LEU	CA-CB-CG	5.75	136.42	116.30
1	S	276	ASP	CB-CA-C	-5.74	98.93	109.15
3	C	18	GLY	N-CA-C	5.72	119.10	110.18
1	k	276	ASP	CB-CA-C	-5.72	98.97	109.15
1	D	217	LEU	CA-CB-CG	5.72	136.31	116.30
3	g	24	GLU	CA-C-N	-5.71	114.08	119.85
3	g	24	GLU	C-N-CA	-5.71	114.08	119.85
1	J	276	ASP	N-CA-CB	-5.69	102.39	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	320	LEU	N-CA-C	-5.69	104.72	111.03
1	V	184	THR	CB-CA-C	-5.67	104.54	110.33
1	Y	276	ASP	N-CA-CB	-5.65	102.44	110.81
2	o	202	ASP	CA-C-N	5.65	130.81	121.99
2	o	202	ASP	C-N-CA	5.65	130.81	121.99
1	G	197	ALA	N-CA-C	5.65	117.11	111.07
1	Y	220	THR	CB-CA-C	-5.65	101.41	110.79
1	D	197	ALA	N-CA-C	5.63	117.10	111.07
1	M	320	LEU	N-CA-C	-5.63	102.32	111.04
1	J	276	ASP	CB-CA-C	-5.60	99.18	109.15
2	o	271	PRO	N-CA-C	-5.60	102.31	111.21
1	P	354	SER	CA-C-N	-5.58	117.29	123.43
1	P	354	SER	C-N-CA	-5.58	117.29	123.43
2	K	203	ASN	CB-CA-C	-5.56	99.97	109.65
1	M	197	ALA	N-CA-C	5.56	117.02	111.07
1	b	355	ILE	N-CA-C	5.56	114.07	107.73
2	N	203	ASN	CB-CA-C	-5.54	100.80	110.17
2	Q	239	GLU	CB-CA-C	-5.54	100.37	110.63
1	G	294	GLY	CA-C-N	-5.53	118.61	122.59
1	G	294	GLY	C-N-CA	-5.53	118.61	122.59
2	W	239	GLU	CB-CA-C	-5.53	100.41	110.63
1	k	355	ILE	N-CA-C	5.53	113.91	107.89
2	T	202	ASP	N-CA-C	5.51	116.34	108.74
2	B	203	ASN	N-CA-CB	-5.50	102.30	110.61
1	J	217	LEU	CA-CB-CG	5.49	135.53	116.30
1	D	230	SER	N-CA-CB	-5.49	101.85	110.30
1	Y	187	ARG	CG-CD-NE	-5.48	99.94	112.00
1	J	187	ARG	CG-CD-NE	-5.48	99.94	112.00
2	i	271	PRO	CA-C-N	-5.48	110.67	121.41
2	i	271	PRO	C-N-CA	-5.48	110.67	121.41
2	i	202	ASP	CA-C-N	5.46	130.51	121.99
2	i	202	ASP	C-N-CA	5.46	130.51	121.99
1	Y	197	ALA	N-CA-C	5.46	116.92	110.97
1	M	184	THR	CB-CA-C	-5.46	105.53	110.44
1	J	289	SER	N-CA-C	5.45	117.98	111.71
1	S	225	VAL	CB-CA-C	-5.45	100.95	110.71
1	P	217	LEU	CA-CB-CG	5.45	135.37	116.30
3	L	16	SER	N-CA-C	5.45	117.50	108.13
2	f	203	ASN	N-CA-CB	-5.44	102.65	110.65
2	f	198	VAL	N-CA-C	-5.43	105.82	111.58
1	A	197	ALA	N-CA-C	5.42	116.87	111.07
2	B	278	THR	N-CA-CB	-5.42	102.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	276	ASP	CB-CA-C	-5.41	99.53	109.15
2	f	271	PRO	CA-C-N	-5.41	110.81	121.41
2	f	271	PRO	C-N-CA	-5.41	110.81	121.41
1	n	289	SER	N-CA-C	5.40	118.97	112.38
1	J	197	ALA	N-CA-C	5.39	116.84	111.07
2	f	238	GLY	CA-C-N	5.38	128.23	120.38
2	f	238	GLY	C-N-CA	5.38	128.23	120.38
1	P	293	ALA	N-CA-C	5.37	118.02	109.96
1	V	217	LEU	CA-CB-CG	5.37	135.08	116.30
1	M	368	SER	N-CA-C	5.35	117.11	109.14
2	l	241	ARG	CG-CD-NE	-5.34	100.24	112.00
1	e	178	ALA	N-CA-C	-5.33	105.47	111.28
1	k	367	VAL	N-CA-CB	-5.33	103.53	112.06
1	P	276	ASP	CB-CA-C	-5.32	99.68	109.15
1	h	343	GLN	N-CA-C	-5.31	105.61	111.71
2	H	203	ASN	N-CA-CB	-5.30	102.60	110.61
1	e	354	SER	CA-C-N	-5.30	117.59	123.43
1	e	354	SER	C-N-CA	-5.30	117.59	123.43
3	I	31	VAL	CA-C-N	-5.29	114.50	119.85
3	I	31	VAL	C-N-CA	-5.29	114.50	119.85
2	f	239	GLU	CB-CA-C	-5.28	100.22	110.46
1	V	276	ASP	CB-CA-C	-5.27	99.77	109.15
1	b	217	LEU	CA-CB-CG	5.26	134.72	116.30
2	c	271	PRO	N-CA-C	-5.26	102.85	111.21
2	i	202	ASP	N-CA-C	5.25	115.98	108.74
2	N	220	VAL	N-CA-C	5.24	116.02	108.48
2	N	219	GLN	N-CA-CB	-5.23	102.49	110.85
3	C	24	GLU	CA-C-N	-5.22	114.61	120.14
3	C	24	GLU	C-N-CA	-5.22	114.61	120.14
1	n	378	SER	CB-CA-C	-5.21	101.82	110.68
1	J	220	THR	CB-CA-C	-5.21	102.15	110.79
1	S	187	ARG	CG-CD-NE	-5.19	100.58	112.00
1	D	221	VAL	CA-C-N	-5.17	114.58	119.76
1	D	221	VAL	C-N-CA	-5.17	114.58	119.76
1	h	217	LEU	CA-CB-CG	5.16	134.37	116.30
2	o	274	GLY	N-CA-C	5.16	122.84	114.90
2	Z	203	ASN	N-CA-CB	-5.16	102.82	110.61
2	N	238	GLY	CA-C-N	5.14	127.68	120.28
2	N	238	GLY	C-N-CA	5.14	127.68	120.28
2	Z	271	PRO	CA-C-N	-5.14	111.34	121.41
2	Z	271	PRO	C-N-CA	-5.14	111.34	121.41
1	S	276	ASP	N-CA-CB	-5.13	103.22	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	203	ASN	N-CA-CB	-5.13	102.86	110.61
3	R	31	VAL	CA-C-N	-5.13	114.67	119.85
3	R	31	VAL	C-N-CA	-5.13	114.67	119.85
1	n	172	THR	N-CA-C	-5.12	102.48	110.42
1	V	197	ALA	N-CA-C	5.11	116.53	111.07
2	E	271	PRO	N-CA-C	-5.09	103.12	111.21
2	Q	271	PRO	N-CA-C	-5.08	103.13	111.21
1	V	276	ASP	N-CA-CB	-5.08	103.29	110.81
2	K	203	ASN	N-CA-CB	-5.08	102.97	110.53
1	Y	217	LEU	CA-CB-CG	5.07	134.03	116.30
2	o	271	PRO	CA-C-N	-5.06	111.48	121.41
2	o	271	PRO	C-N-CA	-5.06	111.48	121.41
3	C	31	VAL	N-CA-CB	-5.05	104.13	111.21
3	L	31	VAL	N-CA-CB	-5.05	104.13	111.21
3	F	31	VAL	N-CA-CB	-5.04	104.15	111.21
1	M	215	THR	CB-CA-C	-5.04	101.83	109.89
1	M	355	ILE	N-CA-C	5.04	113.38	107.89
2	Q	236	VAL	N-CA-C	5.02	116.51	108.87
1	e	276	ASP	CB-CA-C	-5.01	100.22	109.15
2	f	274	GLY	N-CA-C	5.01	122.52	115.30
1	n	368	SER	N-CA-C	5.01	116.60	109.14
1	M	276	ASP	N-CA-CB	-5.00	103.40	110.81
3	d	31	VAL	N-CA-CB	-5.00	104.21	111.21

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	THR	Peptide
2	B	174	THR	Peptide
2	B	175	ALA	Peptide
2	E	174	THR	Peptide
2	E	175	ALA	Peptide
1	G	287	THR	Peptide
2	H	174	THR	Peptide
2	H	175	ALA	Peptide
1	J	287	THR	Peptide
2	K	174	THR	Peptide
2	K	175	ALA	Peptide
1	M	287	THR	Peptide
2	N	174	THR	Peptide
2	N	175	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	P	275	GLN	Peptide
1	P	287	THR	Peptide
2	Q	174	THR	Peptide
2	Q	175	ALA	Peptide
1	S	287	THR	Peptide
2	T	174	THR	Peptide
2	T	175	ALA	Peptide
3	U	18	GLY	Peptide
1	V	287	THR	Peptide
2	W	174	THR	Peptide
2	W	175	ALA	Peptide
1	Y	287	THR	Peptide
2	Z	174	THR	Peptide
2	Z	175	ALA	Peptide
1	b	287	THR	Peptide
2	c	174	THR	Peptide
2	c	175	ALA	Peptide
1	e	287	THR	Peptide
2	f	174	THR	Peptide
2	f	175	ALA	Peptide
1	h	287	THR	Peptide
2	i	174	THR	Peptide
2	i	175	ALA	Peptide
1	k	287	THR	Peptide
2	l	174	THR	Peptide
2	l	175	ALA	Peptide
1	n	287	THR	Peptide
2	o	174	THR	Peptide
2	o	175	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1448	0	1434	58	0
1	D	1448	0	1434	59	0
1	G	1437	0	1419	51	0
1	J	1457	0	1441	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1461	0	1445	59	0
1	P	1461	0	1445	57	0
1	S	1461	0	1445	51	0
1	V	1457	0	1442	51	0
1	Y	1448	0	1434	49	0
1	b	1449	0	1433	58	0
1	e	1457	0	1442	50	0
1	h	1439	0	1416	48	0
1	k	1457	0	1442	47	0
1	n	1457	0	1431	49	0
2	B	1033	0	1032	32	0
2	E	1033	0	1032	34	0
2	H	1033	0	1032	40	0
2	K	1033	0	1032	37	0
2	N	1033	0	1032	36	0
2	Q	1033	0	1032	33	0
2	T	1033	0	1032	38	1
2	W	1033	0	1032	36	0
2	Z	1033	0	1032	37	0
2	c	1033	0	1032	34	0
2	f	1033	0	1032	34	0
2	i	1033	0	1032	35	0
2	l	1033	0	1032	35	0
2	o	1032	0	1028	42	0
3	C	200	0	190	15	0
3	F	194	0	185	7	0
3	I	194	0	185	12	1
3	L	212	0	200	11	0
3	O	190	0	182	9	0
3	R	185	0	177	11	0
3	U	206	0	195	15	0
3	X	190	0	182	13	0
3	a	190	0	182	11	0
3	d	190	0	182	12	0
3	g	194	0	185	15	0
3	j	194	0	185	9	0
3	m	194	0	185	12	0
3	p	181	0	174	10	0
4	D	8	0	14	5	0
4	h	8	0	14	1	0
4	k	8	0	14	1	0
5	J	16	0	31	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	65	0	0	5	0
6	B	31	0	0	1	0
6	C	7	0	0	1	0
6	D	65	0	0	2	0
6	E	28	0	0	2	0
6	F	9	0	0	0	0
6	G	50	0	0	1	0
6	H	22	0	0	2	0
6	I	9	0	0	0	0
6	J	49	0	0	0	0
6	K	30	0	0	3	0
6	L	12	0	0	0	0
6	M	48	0	0	1	0
6	N	35	0	0	3	0
6	O	11	0	0	0	0
6	P	58	0	0	3	0
6	Q	27	0	0	2	0
6	R	7	0	0	0	0
6	S	57	0	0	0	0
6	T	21	0	0	0	0
6	U	10	0	0	1	0
6	V	63	0	0	1	0
6	W	26	0	0	1	0
6	X	7	0	0	1	0
6	Y	57	0	0	2	0
6	Z	21	0	0	2	0
6	a	8	0	0	0	0
6	b	59	0	0	2	0
6	c	31	0	0	2	0
6	d	3	0	0	0	0
6	e	52	0	0	4	0
6	f	28	0	0	2	0
6	g	4	0	0	1	0
6	h	50	0	0	3	0
6	i	21	0	0	1	0
6	j	11	0	0	0	0
6	k	56	0	0	3	0
6	l	37	0	0	2	0
6	m	8	0	0	0	0
6	n	50	0	0	5	0
6	o	35	0	0	3	0
6	p	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	38842	0	37209	1128	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HD3	6:A:1064:HOH:O	1.43	1.16
1:M:347:GLU:HG3	1:P:349:LEU:HD23	1.24	1.12
1:J:178:ALA:HB3	5:J:1:LDA:HM11	1.12	1.11
1:J:175:GLY:O	5:J:1:LDA:CM1	1.99	1.10
1:A:347:GLU:HG3	1:D:349:LEU:HD23	1.11	1.06
1:h:347:GLU:HA	1:h:347:GLU:OE2	1.54	1.05
1:J:175:GLY:O	5:J:1:LDA:HM13	1.55	1.05
6:A:685:HOH:O	2:B:167:ILE:HD13	1.59	1.02
1:D:298:GLN:HE22	3:I:20:LYS:H	1.04	1.01
1:V:298:GLN:HE22	3:a:20:LYS:H	1.06	1.00
1:e:347:GLU:OE2	1:e:347:GLU:HA	1.60	1.00
1:b:298:GLN:HE22	3:g:20:LYS:H	1.04	1.00
1:G:298:GLN:HE22	3:L:20:LYS:H	1.09	0.99
1:Y:298:GLN:HE22	3:d:20:LYS:H	1.05	0.98
1:h:317:SER:HA	1:h:320:LEU:HG	1.45	0.97
2:o:201:TRP:H	2:o:201:TRP:CD1	1.60	0.97
2:N:260:LYS:HE2	6:N:807:HOH:O	1.63	0.97
1:J:178:ALA:HB3	5:J:1:LDA:CM1	1.94	0.96
1:Y:317:SER:HA	1:Y:320:LEU:HG	1.44	0.96
2:o:201:TRP:CD1	2:o:201:TRP:N	2.29	0.95
2:W:278:THR:HG22	2:W:280:THR:H	1.32	0.95
1:h:298:GLN:HE22	3:m:20:LYS:H	1.02	0.95
1:M:298:GLN:HE22	3:R:20:LYS:H	1.13	0.94
2:Z:278:THR:HG22	2:Z:280:THR:H	1.29	0.94
1:A:347:GLU:HG3	1:D:349:LEU:CD2	1.98	0.93
1:A:316:PHE:C	1:A:320:LEU:HG	1.93	0.93
2:i:278:THR:HG22	2:i:280:THR:H	1.33	0.92
1:h:316:PHE:HB3	6:k:1248:HOH:O	1.69	0.92
2:T:186:MSE:HE3	3:U:33:VAL:HG22	1.49	0.92
1:P:298:GLN:HE22	3:U:20:LYS:H	0.94	0.92
2:Q:278:THR:HG22	2:Q:280:THR:H	1.36	0.91
1:k:298:GLN:HE22	3:p:20:LYS:H	0.93	0.90
1:J:178:ALA:CB	5:J:1:LDA:HM11	1.98	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:GLN:HE22	3:O:20:LYS:H	1.17	0.90
2:N:186:MSE:HE3	3:O:33:VAL:HG22	1.51	0.89
2:o:174:THR:O	6:o:1223:HOH:O	1.91	0.89
1:D:320:LEU:HD22	1:G:318:ASP:OD2	1.72	0.88
2:Z:205:ARG:NH1	2:Z:281:ALA:O	2.06	0.88
1:S:298:GLN:HE22	3:X:20:LYS:H	1.18	0.88
2:K:278:THR:HG22	2:K:280:THR:H	1.40	0.86
1:P:298:GLN:NE2	3:U:20:LYS:H	1.72	0.86
2:H:186:MSE:HE3	3:I:33:VAL:HG22	1.55	0.86
1:P:298:GLN:HE22	3:U:20:LYS:N	1.73	0.86
2:f:278:THR:HG22	2:f:280:THR:H	1.37	0.86
2:c:278:THR:HG22	2:c:280:THR:H	1.39	0.85
2:o:278:THR:HG22	2:o:280:THR:H	1.38	0.85
3:C:17:SER:HB2	6:C:1003:HOH:O	1.76	0.85
2:i:186:MSE:HE3	3:j:33:VAL:HG22	1.58	0.85
1:M:317:SER:HA	1:M:320:LEU:HG	1.56	0.85
1:P:355:ILE:CD1	1:S:260:GLY:HA3	2.06	0.85
1:k:298:GLN:NE2	3:p:20:LYS:H	1.73	0.85
2:W:205:ARG:NH1	2:W:281:ALA:O	2.10	0.85
2:B:278:THR:HG22	2:B:280:THR:H	1.42	0.84
2:Q:186:MSE:HE3	3:R:33:VAL:HG22	1.59	0.84
2:o:201:TRP:H	2:o:201:TRP:HD1	0.94	0.84
1:A:347:GLU:CG	1:D:349:LEU:HD23	2.04	0.83
2:Z:242:ASN:H	2:Z:242:ASN:HD22	1.25	0.83
1:J:316:PHE:C	1:J:320:LEU:HG	2.03	0.83
2:H:278:THR:HG22	2:H:280:THR:H	1.43	0.83
2:N:278:THR:HG22	2:N:280:THR:H	1.44	0.83
2:H:205:ARG:NH1	2:H:281:ALA:O	2.11	0.83
2:B:186:MSE:HE3	3:C:33:VAL:HG22	1.61	0.82
2:Q:241:ARG:NH2	6:Q:367:HOH:O	2.08	0.82
2:f:219:GLN:NE2	6:f:599:HOH:O	2.10	0.82
2:B:205:ARG:NH1	2:B:281:ALA:O	2.12	0.82
2:E:278:THR:HG22	2:E:280:THR:H	1.45	0.82
2:E:205:ARG:NH1	2:E:281:ALA:O	2.13	0.82
2:T:186:MSE:CE	3:U:33:VAL:HG22	2.09	0.81
2:N:186:MSE:CE	3:O:33:VAL:HG22	2.09	0.81
2:f:186:MSE:CE	3:g:33:VAL:HG22	2.10	0.81
2:o:201:TRP:N	2:o:201:TRP:HD1	1.70	0.81
2:T:184:TYR:OH	2:T:202:ASP:OD2	1.96	0.81
2:T:278:THR:HG22	2:T:280:THR:H	1.43	0.81
2:l:278:THR:HG21	2:l:282:SER:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:186:MSE:CE	3:R:33:VAL:HG22	2.10	0.81
3:C:20:LYS:H	1:n:298:GLN:HE22	1.29	0.80
2:l:205:ARG:NH1	2:l:281:ALA:O	2.14	0.80
2:H:186:MSE:CE	3:I:33:VAL:HG22	2.11	0.80
1:J:175:GLY:HA2	5:J:1:LDA:HM12	1.62	0.80
1:Y:317:SER:CA	1:Y:320:LEU:HG	2.11	0.80
2:T:205:ARG:NH1	2:T:281:ALA:O	2.15	0.80
2:Z:186:MSE:HE3	3:a:33:VAL:HG22	1.62	0.80
1:e:171:GLU:HB2	6:e:798:HOH:O	1.80	0.80
1:Y:355:ILE:CD1	1:b:260:GLY:HA3	2.12	0.80
1:e:317:SER:O	1:e:320:LEU:HB2	1.81	0.80
1:A:260:GLY:HA3	1:n:355:ILE:CD1	2.12	0.79
2:c:242:ASN:H	2:c:242:ASN:HD22	1.31	0.79
2:i:186:MSE:CE	3:j:33:VAL:HG22	2.12	0.78
2:K:205:ARG:NH1	2:K:281:ALA:O	2.16	0.78
1:D:264:VAL:HG23	5:J:1:LDA:H112	1.64	0.78
2:H:278:THR:HG21	2:H:282:SER:O	1.83	0.78
2:K:174:THR:O	6:K:899:HOH:O	2.02	0.78
1:M:288:ASN:HB3	1:M:290:LEU:H	1.47	0.78
1:S:317:SER:HA	1:S:320:LEU:HG	1.65	0.78
2:B:242:ASN:H	2:B:242:ASN:HD22	1.28	0.78
2:N:174:THR:O	6:N:1020:HOH:O	1.99	0.78
1:A:355:ILE:CD1	1:D:260:GLY:HA3	2.15	0.77
2:E:186:MSE:HE3	3:F:33:VAL:HG22	1.66	0.77
1:A:320:LEU:HA	1:D:318:ASP:OD2	1.84	0.77
1:b:355:ILE:CD1	1:e:260:GLY:HA3	2.15	0.77
1:k:316:PHE:C	1:k:320:LEU:HG	2.10	0.77
1:k:355:ILE:CD1	1:n:260:GLY:HA3	2.15	0.77
2:Q:278:THR:HG21	2:Q:282:SER:O	1.85	0.77
2:f:186:MSE:HE3	3:g:33:VAL:HG22	1.67	0.77
2:W:186:MSE:HE3	3:X:33:VAL:HG22	1.66	0.76
1:e:347:GLU:OE2	1:e:350:ARG:NE	2.14	0.76
2:i:205:ARG:NH1	2:i:281:ALA:O	2.18	0.76
2:E:278:THR:HG21	2:E:282:SER:O	1.84	0.76
1:S:355:ILE:CD1	1:V:260:GLY:HA3	2.16	0.76
2:H:170:LYS:HD2	6:H:296:HOH:O	1.84	0.76
1:M:355:ILE:CD1	1:P:260:GLY:HA3	2.15	0.76
2:o:278:THR:CG2	2:o:280:THR:H	1.99	0.76
1:P:288:ASN:HB3	1:P:290:LEU:H	1.50	0.76
1:Y:298:GLN:NE2	3:d:20:LYS:H	1.84	0.76
2:f:278:THR:HG21	2:f:282:SER:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:288:ASN:HB3	1:n:290:LEU:H	1.50	0.75
2:Z:278:THR:CG2	2:Z:280:THR:H	1.98	0.75
1:k:298:GLN:HE22	3:p:20:LYS:N	1.77	0.75
1:V:343:GLN:CG	1:V:344:LEU:H	2.00	0.75
2:c:186:MSE:CE	3:d:33:VAL:HG22	2.16	0.75
1:D:298:GLN:NE2	3:I:20:LYS:H	1.82	0.75
2:E:186:MSE:CE	3:F:33:VAL:HG22	2.17	0.75
2:Q:205:ARG:NH1	2:Q:281:ALA:O	2.18	0.75
2:Q:242:ASN:HD22	2:Q:242:ASN:H	1.34	0.75
1:Y:320:LEU:HA	1:b:318:ASP:OD2	1.87	0.75
1:b:298:GLN:NE2	3:g:20:LYS:H	1.81	0.75
2:o:242:ASN:HD22	2:o:242:ASN:H	1.35	0.75
2:f:205:ARG:NH1	2:f:281:ALA:O	2.19	0.75
1:V:288:ASN:HB3	1:V:290:LEU:H	1.51	0.75
2:W:186:MSE:CE	3:X:33:VAL:HG22	2.17	0.75
1:A:254:THR:O	5:J:1:LDA:O1	2.05	0.74
1:h:355:ILE:CD1	1:k:260:GLY:HA3	2.18	0.74
1:M:343:GLN:HG2	1:P:346:SER:OG	1.87	0.74
1:D:288:ASN:HB3	1:D:290:LEU:H	1.51	0.74
6:D:398:HOH:O	5:J:1:LDA:H102	1.85	0.74
2:o:205:ARG:NH1	2:o:281:ALA:O	2.19	0.74
2:K:186:MSE:CE	3:L:33:VAL:HG22	2.17	0.74
2:Z:186:MSE:CE	3:a:33:VAL:HG22	2.17	0.74
2:K:278:THR:HG21	2:K:282:SER:O	1.88	0.74
2:N:278:THR:HG21	2:N:282:SER:O	1.87	0.74
1:h:298:GLN:NE2	3:m:20:LYS:H	1.83	0.74
2:c:205:ARG:NH1	2:c:281:ALA:O	2.21	0.74
1:e:355:ILE:CD1	1:h:260:GLY:HA3	2.18	0.74
2:c:278:THR:HG21	2:c:282:SER:O	1.87	0.73
2:i:241:ARG:NH2	6:i:607:HOH:O	2.22	0.73
2:l:186:MSE:HE3	3:m:33:VAL:HG22	1.69	0.73
2:l:186:MSE:CE	3:m:33:VAL:HG22	2.18	0.73
1:G:288:ASN:HB3	1:G:290:LEU:H	1.52	0.73
1:h:317:SER:CA	1:h:320:LEU:HG	2.18	0.73
2:B:186:MSE:CE	3:C:33:VAL:HG22	2.19	0.73
2:N:205:ARG:NH1	2:N:281:ALA:O	2.20	0.73
2:W:242:ASN:H	2:W:242:ASN:HD22	1.36	0.73
2:K:270:ALA:HB1	2:K:273:ARG:HG2	1.71	0.72
2:W:203:ASN:HB3	2:W:205:ARG:H	1.52	0.72
2:B:278:THR:HG21	2:B:282:SER:O	1.89	0.72
2:T:278:THR:HG21	2:T:282:SER:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:1308:HOH:O	2:Z:167:ILE:HD13	1.89	0.72
1:e:171:GLU:CG	6:e:798:HOH:O	2.38	0.72
4:D:1:MPD:O2	4:D:1:MPD:H52	1.89	0.72
2:f:278:THR:CG2	2:f:280:THR:H	2.03	0.72
1:D:256:GLY:O	5:J:1:LDA:H122	1.91	0.71
1:G:298:GLN:NE2	3:L:20:LYS:H	1.86	0.71
1:Y:288:ASN:HB3	1:Y:290:LEU:H	1.54	0.71
2:W:278:THR:HG21	2:W:282:SER:O	1.91	0.71
1:V:355:ILE:CD1	1:Y:260:GLY:HA3	2.20	0.71
1:D:355:ILE:CD1	1:G:260:GLY:HA3	2.20	0.71
1:D:306:ARG:HG3	1:D:355:ILE:HG12	1.73	0.71
1:D:317:SER:HA	1:D:320:LEU:HG	1.71	0.71
2:T:278:THR:CG2	2:T:280:THR:H	2.04	0.70
1:G:355:ILE:CD1	1:J:260:GLY:HA3	2.21	0.70
2:l:278:THR:HG22	2:l:280:THR:H	1.56	0.70
2:K:242:ASN:H	2:K:242:ASN:HD22	1.39	0.70
2:Z:278:THR:HG21	2:Z:282:SER:O	1.91	0.70
1:S:288:ASN:HB3	1:S:290:LEU:H	1.56	0.70
1:V:317:SER:HA	1:V:320:LEU:HG	1.72	0.70
2:K:186:MSE:HE3	3:L:33:VAL:HG22	1.73	0.70
1:b:288:ASN:HB3	1:b:290:LEU:H	1.55	0.70
2:B:241:ARG:NH2	6:B:91:HOH:O	2.21	0.70
1:V:343:GLN:HG2	1:V:344:LEU:H	1.56	0.70
2:c:186:MSE:HE3	3:d:33:VAL:HG22	1.73	0.70
1:k:316:PHE:O	1:k:320:LEU:N	2.25	0.70
2:H:203:ASN:HB3	2:H:205:ARG:H	1.58	0.69
1:S:318:ASP:O	1:S:321:THR:N	2.22	0.69
1:Y:317:SER:HA	1:Y:320:LEU:CG	2.20	0.69
1:A:222:PRO:HB2	5:J:1:LDA:H12	1.75	0.69
1:A:316:PHE:O	1:A:320:LEU:N	2.26	0.69
1:V:320:LEU:HA	1:Y:318:ASP:OD2	1.92	0.69
2:E:242:ASN:HD22	2:E:242:ASN:H	1.41	0.69
1:J:355:ILE:CD1	1:M:260:GLY:HA3	2.23	0.69
2:o:270:ALA:HB1	2:o:273:ARG:HG2	1.74	0.69
1:D:306:ARG:CG	1:D:355:ILE:HG12	2.23	0.68
2:Q:278:THR:CG2	2:Q:280:THR:H	2.07	0.68
1:e:343:GLN:O	1:e:347:GLU:HB2	1.93	0.68
1:G:347:GLU:HG3	1:J:349:LEU:HD23	1.76	0.68
2:N:161:ALA:HA	6:N:605:HOH:O	1.92	0.68
2:f:203:ASN:HB3	2:f:205:ARG:H	1.59	0.67
1:S:320:LEU:HD22	1:V:318:ASP:OD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:298:GLN:NE2	3:a:20:LYS:H	1.85	0.67
1:P:306:ARG:CG	1:P:355:ILE:HG12	2.24	0.67
1:V:376:ASP:OD1	1:V:378:SER:HB2	1.95	0.67
2:o:278:THR:HG21	2:o:282:SER:O	1.94	0.67
1:Y:298:GLN:HE22	3:d:20:LYS:N	1.87	0.67
1:P:320:LEU:HD22	1:S:318:ASP:OD2	1.94	0.67
3:X:40:ASP:OD1	3:X:42:GLN:NE2	2.28	0.67
2:i:278:THR:CG2	2:i:280:THR:H	2.07	0.67
1:n:306:ARG:CG	1:n:355:ILE:HG12	2.25	0.67
2:K:278:THR:CG2	2:K:280:THR:H	2.08	0.66
2:W:278:THR:CG2	2:W:280:THR:H	2.06	0.66
2:Z:270:ALA:HB1	2:Z:273:ARG:HG2	1.76	0.66
2:l:278:THR:CG2	2:l:280:THR:H	2.08	0.66
1:D:182:ASN:ND2	6:D:717:HOH:O	2.27	0.66
2:i:172:LYS:NZ	2:i:172:LYS:HB3	2.09	0.66
2:c:203:ASN:HB3	2:c:205:ARG:H	1.59	0.66
1:D:298:GLN:HE22	3:I:20:LYS:N	1.86	0.66
1:A:306:ARG:CG	1:A:355:ILE:HG12	2.25	0.66
2:c:172:LYS:NZ	2:c:172:LYS:HB3	2.11	0.66
2:o:184:TYR:OH	2:o:202:ASP:OD2	2.14	0.66
1:A:222:PRO:HB2	5:J:1:LDA:H42	1.77	0.66
1:S:343:GLN:HG2	1:V:346:SER:OG	1.95	0.66
1:A:222:PRO:HG2	5:J:1:LDA:H42	1.76	0.66
1:V:298:GLN:HE22	3:a:20:LYS:N	1.86	0.65
1:e:306:ARG:CG	1:e:355:ILE:HG12	2.26	0.65
2:H:222:MSE:HE3	2:H:224:SER:HA	1.77	0.65
1:M:317:SER:CA	1:M:320:LEU:HG	2.25	0.65
1:n:316:PHE:CD1	6:n:1022:HOH:O	2.50	0.65
1:A:222:PRO:CB	5:J:1:LDA:H12	2.26	0.65
1:A:257:ILE:HD13	1:A:359:LEU:HB2	1.78	0.65
1:J:179:LEU:HB2	5:J:1:LDA:H11	1.78	0.65
2:T:172:LYS:NZ	2:T:172:LYS:HB3	2.11	0.65
2:W:270:ALA:HB1	2:W:273:ARG:HG2	1.78	0.65
1:b:320:LEU:HD13	1:e:318:ASP:OD1	1.97	0.65
1:J:175:GLY:CA	5:J:1:LDA:HM12	2.26	0.65
2:N:172:LYS:HB3	2:N:172:LYS:NZ	2.11	0.65
2:N:203:ASN:HB3	2:N:205:ARG:H	1.62	0.65
1:k:343:GLN:HB2	1:n:342:GLY:N	2.12	0.65
1:G:273:ASN:OD1	1:G:276:ASP:HB2	1.97	0.65
1:D:320:LEU:HD22	1:G:318:ASP:CG	2.21	0.65
2:E:222:MSE:HE3	2:E:224:SER:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:242:ASN:HD22	2:l:242:ASN:H	1.44	0.64
2:c:270:ALA:HB1	2:c:273:ARG:HG2	1.78	0.64
1:M:347:GLU:CG	1:P:349:LEU:HD23	2.16	0.64
1:P:355:ILE:HD12	1:S:260:GLY:HA3	1.77	0.64
2:i:174:THR:HG23	3:j:42:GLN:HB3	1.79	0.64
1:G:306:ARG:CG	1:G:355:ILE:HG12	2.26	0.64
2:E:172:LYS:NZ	2:E:172:LYS:HB3	2.12	0.64
1:h:288:ASN:HB3	1:h:290:LEU:H	1.63	0.64
2:o:172:LYS:C	2:o:174:THR:N	2.53	0.64
2:K:203:ASN:HB3	2:K:205:ARG:H	1.62	0.64
2:N:278:THR:CG2	2:N:280:THR:H	2.10	0.64
2:H:172:LYS:NZ	2:H:172:LYS:HB3	2.13	0.64
2:Q:172:LYS:NZ	2:Q:172:LYS:HB3	2.11	0.64
2:Q:203:ASN:HB3	2:Q:205:ARG:H	1.63	0.64
2:c:278:THR:CG2	2:c:280:THR:H	2.08	0.64
1:J:320:LEU:HD22	1:M:318:ASP:OD2	1.97	0.64
1:A:222:PRO:CG	5:J:1:LDA:H42	2.28	0.63
1:G:254:THR:HB	6:G:910:HOH:O	1.98	0.63
2:K:222:MSE:HE3	2:K:224:SER:HA	1.80	0.63
2:E:203:ASN:HB3	2:E:205:ARG:H	1.62	0.63
1:n:268:TRP:CD1	1:n:369:ILE:HG12	2.33	0.63
1:M:376:ASP:OD1	1:M:378:SER:HB2	1.99	0.63
2:Z:172:LYS:C	2:Z:174:THR:N	2.54	0.63
1:n:189:LYS:HE2	6:n:622:HOH:O	1.98	0.63
1:S:298:GLN:NE2	3:X:20:LYS:H	1.93	0.63
2:W:172:LYS:C	2:W:174:THR:N	2.56	0.63
2:i:222:MSE:HE3	2:i:224:SER:HA	1.81	0.63
2:l:241:ARG:NH2	6:l:675:HOH:O	2.31	0.63
2:o:186:MSE:CE	3:p:33:VAL:HG22	2.29	0.63
2:o:186:MSE:HE3	3:p:33:VAL:HG22	1.81	0.63
2:N:186:MSE:HE1	2:N:197:PRO:HD2	1.80	0.62
1:J:182:ASN:OD1	5:J:1:LDA:H31	1.98	0.62
2:N:242:ASN:H	2:N:242:ASN:HD22	1.45	0.62
2:T:186:MSE:HE3	3:U:33:VAL:CG2	2.26	0.62
2:i:278:THR:HG21	2:i:282:SER:O	1.98	0.62
2:o:186:MSE:HE3	3:p:33:VAL:HG13	1.80	0.62
2:E:270:ALA:HB1	2:E:273:ARG:HG2	1.81	0.62
1:Y:181:LYS:HE3	1:b:171:GLU:HA	1.80	0.62
2:l:203:ASN:HB3	2:l:205:ARG:H	1.64	0.62
2:B:172:LYS:NZ	2:B:172:LYS:HB3	2.13	0.62
2:E:278:THR:CG2	2:E:280:THR:H	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:242:ASN:HD22	2:H:242:ASN:H	1.46	0.62
1:b:298:GLN:HE22	3:g:20:LYS:N	1.87	0.62
2:H:270:ALA:HB1	2:H:273:ARG:HG2	1.82	0.62
1:J:306:ARG:CG	1:J:355:ILE:HG12	2.30	0.62
2:T:270:ALA:HB1	2:T:273:ARG:HG2	1.80	0.62
1:e:355:ILE:HD12	1:h:260:GLY:HA3	1.82	0.62
1:P:317:SER:HA	1:P:320:LEU:HG	1.82	0.62
1:M:298:GLN:NE2	3:R:20:LYS:H	1.93	0.61
2:Q:222:MSE:HE3	2:Q:224:SER:HA	1.82	0.61
1:M:306:ARG:CG	1:M:355:ILE:HG12	2.30	0.61
2:W:172:LYS:NZ	2:W:172:LYS:HB3	2.15	0.61
2:o:172:LYS:HB3	2:o:172:LYS:NZ	2.16	0.61
2:f:242:ASN:H	2:f:242:ASN:HD22	1.47	0.61
2:H:186:MSE:HE1	2:H:197:PRO:HG2	1.83	0.61
1:S:298:GLN:HE22	3:X:20:LYS:N	1.94	0.61
2:c:172:LYS:C	2:c:174:THR:N	2.57	0.61
1:G:215:THR:HG22	1:J:291:GLY:HA3	1.81	0.61
2:H:172:LYS:C	2:H:174:THR:N	2.56	0.61
1:J:216:GLU:OE2	1:M:288:ASN:ND2	2.34	0.61
1:h:306:ARG:CG	1:h:355:ILE:HG12	2.31	0.61
1:J:179:LEU:HA	5:J:1:LDA:H32	1.83	0.60
1:J:288:ASN:HB3	1:J:290:LEU:H	1.66	0.60
1:J:316:PHE:O	1:J:320:LEU:HG	2.01	0.60
2:i:242:ASN:H	2:i:242:ASN:HD22	1.49	0.60
3:L:40:ASP:OD1	3:L:42:GLN:HB2	2.02	0.60
1:J:245:LYS:HE3	2:N:241:ARG:O	2.01	0.60
1:e:376:ASP:OD1	1:e:378:SER:HB2	2.00	0.60
2:l:172:LYS:C	2:l:174:THR:N	2.58	0.60
1:k:288:ASN:HB3	1:k:290:LEU:H	1.65	0.60
1:h:298:GLN:HE22	3:m:20:LYS:N	1.87	0.60
2:B:186:MSE:HE3	3:C:33:VAL:HG13	1.84	0.60
2:f:186:MSE:HE2	3:g:33:VAL:HG22	1.84	0.60
2:l:177:ALA:O	2:l:205:ARG:NH2	2.34	0.60
1:V:306:ARG:CG	1:V:355:ILE:HG12	2.32	0.59
1:Y:306:ARG:CG	1:Y:355:ILE:HG12	2.32	0.59
2:B:278:THR:CG2	2:B:280:THR:H	2.12	0.59
2:H:172:LYS:HB3	2:H:172:LYS:HZ1	1.67	0.59
1:J:175:GLY:O	5:J:1:LDA:HM12	1.96	0.59
1:S:306:ARG:CG	1:S:355:ILE:HG12	2.32	0.59
1:A:171:GLU:N	1:A:171:GLU:OE2	2.36	0.59
2:c:172:LYS:HB3	2:c:172:LYS:HZ1	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:186:MSE:CE	3:p:33:VAL:HG13	2.33	0.59
2:T:172:LYS:C	2:T:174:THR:N	2.54	0.59
2:l:172:LYS:NZ	2:l:172:LYS:HB3	2.17	0.59
1:A:355:ILE:HD12	1:D:260:GLY:HA3	1.84	0.59
2:Z:242:ASN:HD22	2:Z:242:ASN:N	2.00	0.59
1:b:376:ASP:OD1	1:b:378:SER:HB2	2.02	0.59
1:k:306:ARG:CG	1:k:355:ILE:HG12	2.33	0.59
1:A:376:ASP:OD1	1:A:378:SER:HB2	2.02	0.59
2:B:203:ASN:HB3	2:B:205:ARG:H	1.66	0.59
2:E:172:LYS:C	2:E:174:THR:N	2.60	0.59
2:Q:172:LYS:C	2:Q:174:THR:N	2.59	0.59
2:W:222:MSE:HE3	2:W:224:SER:HA	1.85	0.59
2:T:200:VAL:HG23	3:U:33:VAL:HG11	1.85	0.59
2:T:222:MSE:HE3	2:T:224:SER:HA	1.85	0.59
2:Z:172:LYS:NZ	2:Z:172:LYS:HB3	2.17	0.59
2:f:172:LYS:C	2:f:174:THR:N	2.58	0.59
2:f:172:LYS:NZ	2:f:172:LYS:HB3	2.18	0.59
1:Y:171:GLU:C	1:Y:171:GLU:OE2	2.46	0.58
1:n:168:GLN:O	1:n:169:ASP:CB	2.50	0.58
2:N:186:MSE:HE3	3:O:33:VAL:CG2	2.30	0.58
2:B:172:LYS:C	2:B:174:THR:N	2.57	0.58
4:D:1:MPD:HM3	2:E:228:LYS:NZ	2.17	0.58
2:f:270:ALA:HB1	2:f:273:ARG:HG2	1.85	0.58
2:Q:177:ALA:O	2:Q:205:ARG:NH2	2.36	0.58
1:k:317:SER:HA	1:k:320:LEU:HB2	1.85	0.58
1:n:273:ASN:OD1	1:n:276:ASP:HB2	2.03	0.58
1:A:288:ASN:HB3	1:A:290:LEU:H	1.68	0.58
1:e:320:LEU:HD13	1:h:318:ASP:OD1	2.03	0.58
1:V:343:GLN:OE1	1:V:344:LEU:HB3	2.04	0.58
2:i:175:ALA:HB3	2:i:282:SER:HA	1.86	0.58
1:e:386:ASN:HB3	6:f:490:HOH:O	2.04	0.58
1:n:306:ARG:HG3	1:n:355:ILE:HG12	1.86	0.58
1:J:320:LEU:HD22	1:M:318:ASP:CG	2.29	0.58
1:G:306:ARG:HG3	1:G:355:ILE:HG12	1.86	0.58
2:Z:203:ASN:HB3	2:Z:205:ARG:H	1.69	0.58
1:A:298:GLN:HE21	1:A:360:TYR:HD2	1.52	0.58
2:K:172:LYS:NZ	2:K:172:LYS:HB3	2.17	0.58
2:N:172:LYS:HB3	2:N:172:LYS:HZ1	1.67	0.58
1:b:306:ARG:CG	1:b:355:ILE:HG12	2.33	0.57
1:k:257:ILE:HD13	1:k:359:LEU:HB2	1.86	0.57
1:n:303:MSE:SE	1:n:352:TYR:OH	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:PHE:HB3	5:J:1:LDA:H111	1.85	0.57
1:D:317:SER:CA	1:D:320:LEU:HG	2.34	0.57
1:V:171:GLU:OE2	1:V:171:GLU:C	2.48	0.57
4:D:1:MPD:CM	2:E:228:LYS:NZ	2.67	0.57
2:E:172:LYS:HB3	2:E:172:LYS:HZ1	1.68	0.57
2:K:241:ARG:NH2	6:K:298:HOH:O	2.35	0.57
2:T:242:ASN:HD22	2:T:242:ASN:H	1.53	0.57
1:A:181:LYS:HE3	1:D:171:GLU:HA	1.86	0.57
2:H:256:ARG:NH1	6:H:60:HOH:O	2.27	0.57
1:J:273:ASN:OD1	1:J:276:ASP:HB2	2.03	0.57
1:M:320:LEU:HA	1:P:318:ASP:OD2	2.05	0.57
2:B:270:ALA:HB1	2:B:273:ARG:HG2	1.86	0.57
1:J:376:ASP:OD1	1:J:378:SER:HB2	2.05	0.57
1:D:303:MSE:SE	1:D:352:TYR:OH	2.73	0.57
1:S:320:LEU:HD22	1:V:318:ASP:CG	2.30	0.57
1:A:306:ARG:HG3	1:A:355:ILE:HG12	1.88	0.56
2:E:186:MSE:HE3	3:F:33:VAL:HG13	1.86	0.56
1:S:376:ASP:OD1	1:S:378:SER:HB2	2.05	0.56
1:V:317:SER:CA	1:V:320:LEU:HG	2.34	0.56
2:o:177:ALA:O	2:o:205:ARG:NH2	2.38	0.56
2:K:186:MSE:HE1	2:K:197:PRO:HG2	1.88	0.56
2:W:242:ASN:HD22	2:W:242:ASN:N	2.02	0.56
1:b:318:ASP:C	1:b:320:LEU:H	2.13	0.56
1:k:171:GLU:C	1:k:171:GLU:OE2	2.48	0.56
2:B:186:MSE:CE	3:C:33:VAL:HG13	2.34	0.56
2:H:278:THR:CG2	2:H:280:THR:H	2.16	0.56
2:c:222:MSE:HE3	2:c:224:SER:HA	1.88	0.56
1:D:376:ASP:OD1	1:D:378:SER:HB2	2.05	0.56
1:P:306:ARG:HG2	1:P:355:ILE:HG12	1.88	0.56
1:P:320:LEU:HD22	1:S:318:ASP:CG	2.31	0.56
1:P:171:GLU:HA	6:P:1052:HOH:O	2.06	0.56
2:Q:242:ASN:HD22	2:Q:242:ASN:N	2.03	0.56
1:n:316:PHE:HD1	6:n:1022:HOH:O	1.87	0.56
3:g:42:GLN:NE2	6:g:480:HOH:O	2.37	0.56
2:i:200:VAL:HG23	3:j:33:VAL:HG11	1.88	0.56
1:k:317:SER:HA	1:k:320:LEU:HD12	1.88	0.56
2:l:222:MSE:HE3	2:l:224:SER:HA	1.87	0.56
2:Q:175:ALA:HB3	2:Q:282:SER:HA	1.88	0.56
1:e:171:GLU:OE2	1:e:171:GLU:C	2.48	0.56
1:M:245:LYS:HE3	2:Q:241:ARG:O	2.06	0.55
2:f:177:ALA:O	2:f:205:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:171:GLU:C	1:h:171:GLU:OE2	2.49	0.55
2:B:186:MSE:HE3	3:C:33:VAL:CG2	2.35	0.55
2:c:241:ARG:NH2	6:c:1017:HOH:O	2.38	0.55
2:o:273:ARG:HG3	6:o:330:HOH:O	2.05	0.55
1:A:222:PRO:CB	5:J:1:LDA:H42	2.36	0.55
2:H:256:ARG:NH1	3:I:22:PRO:HB2	2.21	0.55
2:Q:163:ASP:O	2:Q:167:ILE:HG22	2.06	0.55
1:Y:291:GLY:O	6:Y:20:HOH:O	2.18	0.55
2:f:222:MSE:HE3	2:f:224:SER:HA	1.89	0.55
1:G:376:ASP:OD1	1:G:378:SER:HB2	2.07	0.55
2:H:175:ALA:HB3	2:H:282:SER:HA	1.87	0.55
2:i:270:ALA:HB1	2:i:273:ARG:HG2	1.89	0.55
2:K:175:ALA:HB3	2:K:282:SER:HA	1.88	0.55
1:P:171:GLU:CA	6:P:1052:HOH:O	2.55	0.55
1:S:171:GLU:OE2	1:S:171:GLU:C	2.50	0.55
1:S:273:ASN:OD1	1:S:276:ASP:HB2	2.07	0.55
2:T:174:THR:HG23	3:U:42:GLN:HB2	1.89	0.55
2:c:242:ASN:H	2:c:242:ASN:ND2	2.03	0.55
1:e:171:GLU:CD	6:e:798:HOH:O	2.49	0.55
2:o:176:PHE:CE1	2:o:203:ASN:HB2	2.42	0.55
1:M:171:GLU:C	1:M:171:GLU:OE2	2.50	0.55
1:k:171:GLU:OE2	1:k:171:GLU:N	2.40	0.55
1:n:168:GLN:CA	1:n:168:GLN:OE1	2.54	0.55
3:C:20:LYS:H	1:n:298:GLN:NE2	2.03	0.54
1:Y:316:PHE:O	1:Y:320:LEU:N	2.35	0.54
2:l:175:ALA:HB3	2:l:282:SER:HA	1.89	0.54
2:o:172:LYS:O	2:o:174:THR:N	2.40	0.54
2:B:172:LYS:HB3	2:B:172:LYS:HZ1	1.72	0.54
2:T:181:ASN:O	2:T:201:TRP:HB2	2.06	0.54
1:e:171:GLU:CB	6:e:798:HOH:O	2.41	0.54
2:W:172:LYS:HB3	2:W:172:LYS:HZ1	1.73	0.54
1:P:171:GLU:C	1:P:171:GLU:OE2	2.50	0.54
1:S:300:ASP:HB2	3:X:19:HIS:CE1	2.42	0.54
1:S:317:SER:CA	1:S:320:LEU:HG	2.36	0.54
1:h:181:LYS:HE3	1:k:171:GLU:HA	1.89	0.54
1:A:260:GLY:HA3	1:n:355:ILE:HD13	1.90	0.54
1:D:171:GLU:OE2	1:D:171:GLU:N	2.41	0.54
1:D:265:PHE:H	5:J:1:LDA:H101	1.73	0.54
1:P:245:LYS:HE3	2:T:241:ARG:O	2.07	0.54
2:i:203:ASN:HB3	2:i:205:ARG:H	1.72	0.54
1:J:306:ARG:HG3	1:J:355:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:200:VAL:HG23	3:p:33:VAL:HG11	1.90	0.54
2:o:242:ASN:HD22	2:o:242:ASN:N	2.03	0.54
1:e:181:LYS:HE3	1:h:171:GLU:HA	1.89	0.54
2:f:163:ASP:O	2:f:167:ILE:HG22	2.08	0.54
2:l:186:MSE:HE1	2:l:197:PRO:HD2	1.90	0.54
2:o:222:MSE:HE3	2:o:224:SER:HA	1.90	0.54
1:M:273:ASN:CG	1:M:276:ASP:HB2	2.33	0.54
1:V:215:THR:HG22	1:Y:291:GLY:HA3	1.90	0.54
2:c:186:MSE:HE1	2:c:197:PRO:HD2	1.90	0.54
2:Z:166:ARG:NH1	6:Z:464:HOH:O	2.41	0.54
2:c:186:MSE:HE2	3:d:33:VAL:HG22	1.90	0.54
2:l:200:VAL:HG23	3:m:33:VAL:HG11	1.90	0.54
2:W:172:LYS:O	2:W:174:THR:N	2.41	0.53
1:Y:215:THR:HG22	1:b:291:GLY:HA3	1.89	0.53
2:c:186:MSE:HE1	2:c:197:PRO:HG2	1.89	0.53
4:D:1:MPD:O2	4:D:1:MPD:C5	2.56	0.53
1:V:343:GLN:HG2	1:V:344:LEU:N	2.22	0.53
2:W:177:ALA:O	2:W:205:ARG:NH2	2.42	0.53
1:b:347:GLU:OE2	1:b:347:GLU:HA	2.08	0.53
2:c:186:MSE:CE	3:d:33:VAL:HG13	2.38	0.53
2:o:241:ARG:NH2	6:o:295:HOH:O	2.38	0.53
1:J:320:LEU:HA	1:M:318:ASP:OD2	2.08	0.53
2:W:186:MSE:HE1	2:W:197:PRO:HG2	1.89	0.53
2:E:241:ARG:NH2	6:E:859:HOH:O	2.40	0.53
2:K:172:LYS:C	2:K:174:THR:N	2.64	0.53
2:Q:270:ALA:HB1	2:Q:273:ARG:HG2	1.91	0.53
1:J:171:GLU:OE2	1:J:171:GLU:C	2.52	0.53
2:N:163:ASP:O	2:N:167:ILE:HG22	2.09	0.53
2:N:270:ALA:HB1	2:N:273:ARG:HG2	1.90	0.53
1:b:257:ILE:HD13	1:b:359:LEU:HB2	1.91	0.53
2:E:175:ALA:HB3	2:E:282:SER:HA	1.91	0.53
2:N:175:ALA:HB3	2:N:282:SER:HA	1.91	0.53
1:V:288:ASN:HB3	1:V:290:LEU:N	2.23	0.53
2:W:273:ARG:NE	6:W:1173:HOH:O	2.41	0.53
2:i:186:MSE:HE3	3:j:33:VAL:CG2	2.35	0.53
1:k:245:LYS:HE3	2:o:241:ARG:O	2.09	0.53
1:J:320:LEU:CD2	1:M:318:ASP:OD2	2.57	0.53
2:T:177:ALA:O	2:T:205:ARG:NH2	2.42	0.53
2:o:163:ASP:O	2:o:167:ILE:HG22	2.09	0.53
2:H:186:MSE:HE3	3:I:33:VAL:CG2	2.33	0.53
1:M:273:ASN:OD1	1:M:276:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:172:LYS:C	2:i:174:THR:N	2.62	0.53
1:A:254:THR:HB	5:J:1:LDA:O1	2.09	0.53
1:G:216:GLU:OE2	1:J:288:ASN:ND2	2.42	0.53
2:T:203:ASN:HB3	2:T:205:ARG:H	1.73	0.53
1:e:288:ASN:HB3	1:e:290:LEU:H	1.74	0.53
2:c:186:MSE:HE3	3:d:33:VAL:HG13	1.90	0.52
1:e:306:ARG:HG3	1:e:355:ILE:HG12	1.91	0.52
1:h:273:ASN:OD1	1:h:276:ASP:HB2	2.09	0.52
2:B:242:ASN:HD22	2:B:242:ASN:N	2.03	0.52
1:b:312:MSE:HG2	1:e:307:LEU:HD21	1.91	0.52
2:N:177:ALA:O	2:N:205:ARG:NH2	2.43	0.52
2:Z:175:ALA:HB3	2:Z:282:SER:HA	1.90	0.52
1:D:171:GLU:OE2	1:D:171:GLU:C	2.53	0.52
2:K:270:ALA:CB	2:K:273:ARG:HG2	2.38	0.52
1:Y:355:ILE:HD13	1:b:260:GLY:HA3	1.92	0.52
1:b:273:ASN:OD1	1:b:276:ASP:HB2	2.08	0.52
2:i:163:ASP:O	2:i:167:ILE:HG22	2.09	0.52
4:k:3:MPD:H11	6:k:903:HOH:O	2.08	0.52
2:B:222:MSE:HE3	2:B:224:SER:HA	1.91	0.52
2:W:186:MSE:HE1	2:W:197:PRO:HD2	1.91	0.52
1:J:319:THR:HA	1:J:322:ALA:HB3	1.92	0.52
1:V:273:ASN:OD1	1:V:276:ASP:HB2	2.10	0.52
1:k:306:ARG:HG3	1:k:355:ILE:HG12	1.92	0.52
2:B:175:ALA:HB3	2:B:282:SER:HA	1.90	0.52
1:J:298:GLN:NE2	3:O:20:LYS:H	1.96	0.52
1:J:300:ASP:HB2	3:O:19:HIS:CE1	2.45	0.52
1:P:182:ASN:ND2	6:P:735:HOH:O	2.42	0.52
1:V:171:GLU:N	6:V:396:HOH:O	2.43	0.52
1:D:264:VAL:CG2	5:J:1:LDA:H112	2.37	0.52
1:M:306:ARG:HG2	1:M:355:ILE:HG12	1.92	0.52
1:P:303:MSE:SE	1:P:352:TYR:OH	2.78	0.52
1:A:316:PHE:O	1:A:320:LEU:HG	2.10	0.52
1:P:376:ASP:OD1	1:P:378:SER:HB2	2.09	0.52
1:b:171:GLU:OE2	1:b:171:GLU:C	2.53	0.52
1:k:355:ILE:HD12	1:n:260:GLY:HA3	1.90	0.52
2:c:163:ASP:O	2:c:167:ILE:HG22	2.09	0.51
1:e:171:GLU:OE2	1:e:171:GLU:CA	2.59	0.51
2:o:200:VAL:HA	2:o:208:ARG:O	2.10	0.51
1:A:288:ASN:ND2	1:n:216:GLU:OE2	2.43	0.51
2:N:172:LYS:C	2:N:174:THR:N	2.63	0.51
2:T:163:ASP:O	2:T:167:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:216:GLU:OE2	1:e:288:ASN:ND2	2.43	0.51
2:E:177:ALA:O	2:E:205:ARG:NH2	2.44	0.51
1:P:317:SER:CA	1:P:320:LEU:HG	2.40	0.51
1:h:171:GLU:OE2	1:h:171:GLU:N	2.44	0.51
1:n:383:LEU:HB3	2:o:168:THR:HG21	1.92	0.51
1:P:273:ASN:OD1	1:P:276:ASP:HB2	2.09	0.51
1:S:274:ASP:OD1	2:W:235:HIS:HA	2.09	0.51
1:b:300:ASP:HB2	3:g:19:HIS:CE1	2.45	0.51
1:h:355:ILE:HD12	1:k:260:GLY:HA3	1.89	0.51
1:G:171:GLU:OE2	1:G:171:GLU:C	2.53	0.51
2:H:172:LYS:O	2:H:174:THR:N	2.43	0.51
1:M:316:PHE:O	1:M:320:LEU:N	2.43	0.51
2:c:175:ALA:HB3	2:c:282:SER:HA	1.92	0.51
2:B:163:ASP:O	2:B:167:ILE:HG22	2.10	0.51
1:M:257:ILE:HD13	1:M:359:LEU:HB2	1.92	0.51
2:c:270:ALA:CB	2:c:273:ARG:HG2	2.41	0.51
1:D:273:ASN:CG	1:D:276:ASP:HB2	2.36	0.51
1:D:344:LEU:HG	1:G:345:ALA:HB1	1.92	0.51
1:J:273:ASN:CG	1:J:276:ASP:HB2	2.35	0.51
1:Y:171:GLU:OE2	1:Y:171:GLU:CA	2.58	0.51
2:Q:172:LYS:HB3	2:Q:172:LYS:HZ1	1.75	0.51
2:o:172:LYS:C	2:o:174:THR:H	2.19	0.51
2:Q:190:PRO:O	2:Q:193:ARG:HG3	2.11	0.51
1:S:283:ASP:HB3	1:Y:183:LEU:O	2.10	0.51
1:Y:273:ASN:OD1	1:Y:276:ASP:HB2	2.10	0.51
2:c:242:ASN:HD22	2:c:242:ASN:N	2.05	0.51
1:n:168:GLN:OE1	1:n:168:GLN:HA	2.10	0.51
1:D:273:ASN:OD1	1:D:276:ASP:HB2	2.10	0.50
1:G:273:ASN:CG	1:G:276:ASP:HB2	2.37	0.50
2:N:222:MSE:SE	2:N:248:THR:HG21	2.60	0.50
1:S:171:GLU:OE2	1:S:171:GLU:CA	2.59	0.50
2:Z:172:LYS:O	2:Z:174:THR:N	2.44	0.50
2:Z:186:MSE:HE3	3:a:33:VAL:HG13	1.93	0.50
1:b:192:ARG:HD3	6:b:777:HOH:O	2.10	0.50
2:l:186:MSE:HE3	3:m:33:VAL:HG13	1.92	0.50
1:n:273:ASN:CG	1:n:276:ASP:HB2	2.36	0.50
1:P:216:GLU:OE2	1:S:288:ASN:ND2	2.45	0.50
2:Q:186:MSE:HE2	3:R:33:VAL:HG22	1.91	0.50
2:l:242:ASN:H	2:l:242:ASN:ND2	2.10	0.50
1:M:283:ASP:HB3	1:S:183:LEU:O	2.11	0.50
2:Q:186:MSE:HE3	3:R:33:VAL:CG2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:320:LEU:HB3	1:e:318:ASP:CG	2.37	0.50
1:k:171:GLU:OE2	1:k:171:GLU:CA	2.59	0.50
1:G:268:TRP:CD1	1:G:369:ILE:HG12	2.46	0.50
2:T:222:MSE:SE	2:T:248:THR:HG21	2.62	0.50
1:Y:171:GLU:OE2	1:Y:171:GLU:N	2.45	0.50
2:Q:186:MSE:HE1	2:Q:197:PRO:HG2	1.94	0.50
1:V:233:VAL:HB	1:V:243:ILE:HB	1.93	0.50
2:Z:242:ASN:H	2:Z:242:ASN:ND2	2.00	0.50
2:i:172:LYS:HB3	2:i:172:LYS:HZ1	1.77	0.50
1:A:216:GLU:OE2	1:D:288:ASN:ND2	2.45	0.50
1:M:298:GLN:HE22	3:R:20:LYS:N	1.94	0.50
1:G:298:GLN:HE22	3:L:20:LYS:N	1.93	0.50
2:K:200:VAL:HG23	3:L:33:VAL:HG11	1.92	0.50
1:k:300:ASP:HB2	3:p:19:HIS:CE1	2.47	0.50
2:l:222:MSE:SE	2:l:248:THR:HG21	2.62	0.50
2:N:222:MSE:HE3	2:N:224:SER:HA	1.93	0.49
2:T:172:LYS:O	2:T:174:THR:N	2.45	0.49
2:N:186:MSE:HE3	3:O:33:VAL:HG13	1.92	0.49
1:S:171:GLU:OE2	1:S:171:GLU:N	2.45	0.49
1:S:288:ASN:HB3	1:S:290:LEU:N	2.27	0.49
1:b:306:ARG:HG3	1:b:355:ILE:HG12	1.92	0.49
1:D:233:VAL:HB	1:D:243:ILE:HB	1.93	0.49
2:l:163:ASP:O	2:l:167:ILE:HG22	2.13	0.49
2:H:163:ASP:O	2:H:167:ILE:HG22	2.11	0.49
2:H:177:ALA:O	2:H:205:ARG:NH2	2.44	0.49
1:J:317:SER:N	1:J:320:LEU:HG	2.28	0.49
1:P:316:PHE:O	1:P:317:SER:C	2.56	0.49
1:Y:376:ASP:OD1	1:Y:378:SER:HB2	2.12	0.49
2:o:161:ALA:HB1	2:o:163:ASP:OD1	2.12	0.49
1:Y:216:GLU:OE2	1:b:288:ASN:ND2	2.46	0.49
1:J:181:LYS:HE3	1:M:171:GLU:HA	1.94	0.49
2:Q:242:ASN:H	2:Q:242:ASN:ND2	2.07	0.49
1:D:265:PHE:H	5:J:1:LDA:C11	2.25	0.49
1:b:215:THR:HG22	1:e:291:GLY:HA3	1.95	0.49
1:k:263:ARG:CD	1:k:293:ALA:O	2.61	0.49
1:n:302:HIS:HE1	1:n:358:THR:OG1	1.95	0.49
1:D:318:ASP:C	1:D:320:LEU:H	2.20	0.49
2:H:186:MSE:HE3	3:I:33:VAL:HG13	1.94	0.49
1:b:273:ASN:CG	1:b:276:ASP:HB2	2.38	0.49
2:f:222:MSE:SE	2:f:248:THR:HG21	2.63	0.49
1:h:171:GLU:OE2	1:h:171:GLU:CA	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HB	1:A:243:ILE:HB	1.95	0.49
1:A:273:ASN:CG	1:A:276:ASP:HB2	2.38	0.49
1:J:312:MSE:HG2	1:M:307:LEU:CD2	2.43	0.49
2:K:186:MSE:HE2	3:L:33:VAL:HG22	1.92	0.49
2:W:163:ASP:O	2:W:167:ILE:HG22	2.12	0.49
2:f:200:VAL:HG23	3:g:33:VAL:HG11	1.94	0.49
1:h:312:MSE:HG2	1:k:307:LEU:HD21	1.94	0.49
1:P:300:ASP:HB2	3:U:19:HIS:CE1	2.48	0.49
2:E:186:MSE:HE1	2:E:197:PRO:HD2	1.95	0.48
1:b:263:ARG:CD	1:b:293:ALA:O	2.61	0.48
2:f:256:ARG:NH1	3:g:22:PRO:HB2	2.28	0.48
2:o:175:ALA:HB3	2:o:282:SER:HA	1.94	0.48
2:E:163:ASP:O	2:E:167:ILE:HG22	2.12	0.48
1:V:312:MSE:HG2	1:Y:307:LEU:HD21	1.95	0.48
2:W:222:MSE:SE	2:W:248:THR:HG21	2.63	0.48
2:Z:222:MSE:HE3	2:Z:224:SER:HA	1.95	0.48
1:e:245:LYS:HE3	2:i:241:ARG:O	2.13	0.48
2:l:270:ALA:HB1	2:l:273:ARG:HG2	1.96	0.48
1:n:355:ILE:O	1:n:355:ILE:HG13	2.06	0.48
1:A:183:LEU:O	1:k:283:ASP:HB3	2.13	0.48
1:b:318:ASP:O	1:b:320:LEU:N	2.46	0.48
2:f:175:ALA:HB3	2:f:282:SER:HA	1.95	0.48
1:h:206:GLY:HA2	1:h:370:PHE:CZ	2.47	0.48
1:J:312:MSE:HG2	1:M:307:LEU:HD21	1.95	0.48
1:M:263:ARG:CD	1:M:293:ALA:O	2.62	0.48
2:Z:239:GLU:HG3	6:Z:297:HOH:O	2.12	0.48
1:h:320:LEU:HD22	1:k:318:ASP:OD1	2.13	0.48
1:G:316:PHE:O	1:G:317:SER:C	2.56	0.48
2:K:163:ASP:O	2:K:167:ILE:HG22	2.14	0.48
2:Z:163:ASP:O	2:Z:167:ILE:HG22	2.13	0.48
1:b:316:PHE:O	1:b:320:LEU:HD23	2.13	0.48
1:A:171:GLU:HA	1:n:181:LYS:HE3	1.94	0.48
1:A:189:LYS:HE2	6:A:442:HOH:O	2.12	0.48
1:A:372:ALA:HB2	6:A:67:HOH:O	2.13	0.48
2:E:186:MSE:CE	3:F:33:VAL:HG13	2.43	0.48
2:W:186:MSE:CE	2:W:197:PRO:HG2	2.44	0.48
1:Y:217:LEU:HD13	1:Y:361:ASP:HB3	1.94	0.48
1:e:312:MSE:HG2	1:h:307:LEU:HD21	1.96	0.48
1:P:320:LEU:CD2	1:S:318:ASP:OD2	2.61	0.48
3:U:16:SER:HA	6:U:891:HOH:O	2.14	0.48
1:V:171:GLU:OE2	1:V:171:GLU:CA	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:186:MSE:HE1	2:Z:197:PRO:HG2	1.94	0.48
2:H:186:MSE:CE	2:H:197:PRO:HG2	2.43	0.48
1:J:171:GLU:OE2	1:J:171:GLU:N	2.47	0.48
1:J:175:GLY:C	5:J:1:LDA:HM12	2.38	0.48
1:V:171:GLU:OE2	1:V:171:GLU:N	2.46	0.48
1:D:265:PHE:H	5:J:1:LDA:C10	2.27	0.48
1:J:257:ILE:HD13	1:J:359:LEU:HB2	1.94	0.48
2:N:161:ALA:HB1	2:N:163:ASP:OD1	2.14	0.48
1:Y:312:MSE:HG2	1:b:307:LEU:HD21	1.96	0.48
1:h:215:THR:HG22	1:k:291:GLY:HA3	1.95	0.48
1:A:317:SER:N	1:A:320:LEU:HG	2.26	0.47
1:D:216:GLU:OE2	1:G:288:ASN:ND2	2.47	0.47
1:G:355:ILE:HD12	1:J:260:GLY:HA3	1.96	0.47
2:H:242:ASN:H	2:H:242:ASN:ND2	2.12	0.47
2:T:175:ALA:HB3	2:T:282:SER:HA	1.95	0.47
1:Y:273:ASN:CG	1:Y:276:ASP:HB2	2.39	0.47
1:Y:355:ILE:HD12	1:b:260:GLY:HA3	1.95	0.47
1:b:347:GLU:OE2	1:b:350:ARG:NE	2.39	0.47
1:k:376:ASP:OD1	1:k:378:SER:HB2	2.13	0.47
2:H:200:VAL:HG23	3:I:33:VAL:HG11	1.96	0.47
2:H:252:GLU:HG3	2:H:265:ARG:HG2	1.96	0.47
1:M:171:GLU:OE2	1:M:171:GLU:N	2.47	0.47
2:N:186:MSE:CE	2:N:197:PRO:HD2	2.44	0.47
1:P:171:GLU:OE2	1:P:171:GLU:N	2.47	0.47
2:c:177:ALA:O	2:c:205:ARG:NH2	2.46	0.47
2:i:161:ALA:HB1	2:i:163:ASP:OD1	2.14	0.47
1:P:316:PHE:C	1:P:320:LEU:HG	2.39	0.47
1:V:268:TRP:CD1	1:V:369:ILE:HG12	2.49	0.47
1:V:347:GLU:HG3	1:Y:349:LEU:HD23	1.95	0.47
2:Z:186:MSE:HE3	3:a:33:VAL:CG2	2.38	0.47
1:h:282:ILE:O	1:h:283:ASP:C	2.57	0.47
1:J:175:GLY:C	5:J:1:LDA:CM1	2.84	0.47
1:M:171:GLU:OE2	1:M:171:GLU:CA	2.63	0.47
1:M:312:MSE:HG2	1:P:307:LEU:HD21	1.96	0.47
2:T:172:LYS:C	2:T:174:THR:H	2.21	0.47
2:Z:186:MSE:CE	3:a:33:VAL:HG13	2.45	0.47
1:G:245:LYS:HE3	2:K:241:ARG:O	2.15	0.47
1:J:215:THR:HG22	1:M:291:GLY:HA3	1.96	0.47
1:M:320:LEU:C	1:M:322:ALA:H	2.21	0.47
1:b:386:ASN:HA	2:c:284:ASP:O	2.15	0.47
1:h:216:GLU:OE2	1:k:288:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:263:ARG:HD2	1:k:293:ALA:O	2.15	0.47
1:D:171:GLU:OE2	1:D:171:GLU:CA	2.62	0.47
1:D:316:PHE:O	1:D:319:THR:N	2.47	0.47
1:V:355:ILE:HD12	1:Y:260:GLY:HA3	1.93	0.47
1:e:273:ASN:OD1	1:e:276:ASP:HB2	2.15	0.47
1:h:306:ARG:HG3	1:h:355:ILE:HG12	1.97	0.47
1:n:189:LYS:HE2	1:n:189:LYS:HB3	1.71	0.47
1:G:302:HIS:HE1	1:G:358:THR:OG1	1.98	0.47
1:G:343:GLN:OE1	1:J:342:GLY:N	2.48	0.47
2:H:161:ALA:HB1	2:H:163:ASP:OD1	2.14	0.47
2:H:222:MSE:HB3	2:H:253:TRP:CZ3	2.49	0.47
2:W:242:ASN:H	2:W:242:ASN:ND2	2.08	0.47
2:Z:172:LYS:C	2:Z:174:THR:H	2.22	0.47
2:Z:177:ALA:O	2:Z:205:ARG:NH2	2.48	0.47
1:b:318:ASP:C	1:b:320:LEU:N	2.72	0.47
1:e:303:MSE:SE	1:e:352:TYR:OH	2.82	0.47
1:h:181:LYS:NZ	6:h:691:HOH:O	2.43	0.47
1:h:245:LYS:HE3	2:l:241:ARG:O	2.15	0.47
1:h:302:HIS:HE1	1:h:358:THR:OG1	1.97	0.47
1:h:316:PHE:O	1:h:319:THR:N	2.48	0.47
1:k:302:HIS:HE1	1:k:358:THR:OG1	1.97	0.47
2:l:172:LYS:O	2:l:174:THR:N	2.48	0.47
2:o:201:TRP:HH2	3:p:40:ASP:N	2.13	0.47
1:J:274:ASP:OD1	2:N:235:HIS:HA	2.15	0.47
2:K:242:ASN:HD22	2:K:242:ASN:N	2.10	0.47
1:Y:316:PHE:O	1:Y:317:SER:C	2.58	0.47
2:c:172:LYS:O	2:c:174:THR:N	2.48	0.47
1:e:171:GLU:OE2	1:e:171:GLU:N	2.47	0.47
1:n:233:VAL:HB	1:n:243:ILE:HB	1.96	0.47
1:P:306:ARG:HG3	1:P:355:ILE:HG12	1.97	0.47
2:W:172:LYS:C	2:W:174:THR:H	2.22	0.47
2:W:175:ALA:HB3	2:W:282:SER:HA	1.96	0.47
2:l:186:MSE:CE	3:m:33:VAL:HG13	2.45	0.47
2:E:186:MSE:HE1	2:E:197:PRO:HG2	1.96	0.47
1:J:231:GLN:HG2	6:K:296:HOH:O	2.14	0.47
1:M:216:GLU:OE2	1:P:288:ASN:ND2	2.47	0.47
1:V:316:PHE:O	1:V:319:THR:N	2.48	0.47
1:Y:182:ASN:HA	1:b:173:SER:HB2	1.96	0.47
1:b:355:ILE:O	1:b:355:ILE:HG13	2.09	0.47
1:G:189:LYS:HE2	1:G:189:LYS:HB3	1.66	0.46
2:K:186:MSE:CE	2:K:197:PRO:HG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:316:PHE:O	1:e:317:SER:C	2.57	0.46
4:D:1:MPD:CM	2:E:228:LYS:HZ3	2.28	0.46
2:E:166:ARG:NH2	6:E:297:HOH:O	2.48	0.46
1:Y:316:PHE:O	1:Y:319:THR:N	2.47	0.46
2:l:186:MSE:HE3	3:m:33:VAL:CG2	2.43	0.46
2:B:186:MSE:HE1	2:B:197:PRO:HG2	1.98	0.46
3:C:19:HIS:CE1	1:n:300:ASP:HB2	2.51	0.46
1:D:355:ILE:HD12	1:G:260:GLY:HA3	1.97	0.46
3:R:27:TRP:O	3:R:28:SER:C	2.57	0.46
2:i:177:ALA:O	2:i:205:ARG:NH2	2.48	0.46
1:J:171:GLU:OE2	1:J:171:GLU:CA	2.63	0.46
1:M:302:HIS:HE1	1:M:358:THR:OG1	1.99	0.46
2:T:186:MSE:HE1	2:T:197:PRO:HG2	1.98	0.46
1:e:189:LYS:HB3	1:e:189:LYS:HE2	1.72	0.46
2:f:242:ASN:H	2:f:242:ASN:ND2	2.13	0.46
2:f:242:ASN:HD22	2:f:242:ASN:N	2.13	0.46
2:B:242:ASN:H	2:B:242:ASN:ND2	2.05	0.46
1:M:263:ARG:HD2	1:M:293:ALA:O	2.15	0.46
1:M:274:ASP:OD1	2:Q:235:HIS:HA	2.16	0.46
1:P:171:GLU:CA	1:P:171:GLU:OE2	2.63	0.46
1:P:181:LYS:HE3	1:S:171:GLU:HA	1.96	0.46
2:W:270:ALA:CB	2:W:273:ARG:HG2	2.45	0.46
2:H:190:PRO:O	2:H:193:ARG:HG3	2.16	0.46
1:S:181:LYS:HE3	1:V:171:GLU:HA	1.98	0.46
1:S:316:PHE:O	1:S:317:SER:C	2.58	0.46
1:S:316:PHE:O	1:S:319:THR:N	2.49	0.46
3:X:27:TRP:O	3:X:28:SER:C	2.57	0.46
1:M:317:SER:HA	1:M:320:LEU:CG	2.39	0.46
1:M:372:ALA:HB2	6:M:392:HOH:O	2.15	0.46
1:e:273:ASN:CG	1:e:276:ASP:HB2	2.41	0.46
2:i:242:ASN:HD22	2:i:242:ASN:N	2.13	0.46
1:k:316:PHE:O	1:k:317:SER:C	2.59	0.46
1:A:350:ARG:CD	6:A:1064:HOH:O	2.26	0.46
2:B:177:ALA:O	2:B:205:ARG:NH2	2.49	0.46
3:C:18:GLY:O	3:C:19:HIS:ND1	2.49	0.46
1:D:316:PHE:O	1:D:317:SER:C	2.59	0.46
2:K:190:PRO:O	2:K:193:ARG:HG3	2.16	0.46
2:c:161:ALA:HB1	2:c:163:ASP:OD1	2.16	0.46
1:e:283:ASP:HB3	1:k:183:LEU:O	2.16	0.46
1:k:320:LEU:HD23	1:n:318:ASP:OD2	2.16	0.46
1:M:181:LYS:HE3	1:P:171:GLU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:306:ARG:HG3	1:S:355:ILE:HG12	1.97	0.46
1:e:282:ILE:O	1:e:283:ASP:C	2.58	0.46
2:i:176:PHE:CE1	2:i:203:ASN:HB2	2.51	0.46
2:i:184:TYR:OH	2:i:202:ASP:OD2	2.30	0.46
2:i:190:PRO:O	2:i:193:ARG:HG3	2.16	0.46
2:o:172:LYS:HB3	2:o:172:LYS:HZ1	1.81	0.46
3:C:17:SER:HA	1:n:301:ALA:H	1.81	0.46
1:J:316:PHE:O	1:J:317:SER:C	2.59	0.46
1:M:233:VAL:HB	1:M:243:ILE:HB	1.96	0.46
2:N:186:MSE:HE1	2:N:197:PRO:HG2	1.97	0.46
1:S:320:LEU:HD22	1:V:318:ASP:OD1	2.16	0.46
2:T:270:ALA:CB	2:T:273:ARG:HG2	2.46	0.46
2:f:186:MSE:HE1	2:f:197:PRO:HG2	1.97	0.46
2:i:186:MSE:HE1	2:i:197:PRO:HD2	1.98	0.46
2:E:186:MSE:HE3	3:F:33:VAL:CG2	2.41	0.45
1:G:288:ASN:HB3	1:G:290:LEU:N	2.27	0.45
1:J:189:LYS:HE2	1:J:189:LYS:HB3	1.73	0.45
1:Y:312:MSE:HG2	1:b:307:LEU:CD2	2.46	0.45
1:S:318:ASP:C	1:S:320:LEU:N	2.73	0.45
2:f:186:MSE:HE3	3:g:33:VAL:CG2	2.42	0.45
2:l:186:MSE:HE1	2:l:197:PRO:HG2	1.99	0.45
1:A:300:ASP:HB2	3:F:19:HIS:CE1	2.51	0.45
2:K:270:ALA:O	2:K:271:PRO:C	2.60	0.45
1:M:189:LYS:HE2	1:M:189:LYS:HB3	1.73	0.45
1:P:189:LYS:HB3	1:P:189:LYS:HE2	1.75	0.45
2:i:186:MSE:HE2	3:j:33:VAL:HG22	1.97	0.45
2:o:270:ALA:CB	2:o:273:ARG:HG2	2.44	0.45
1:A:206:GLY:HA2	1:A:370:PHE:CZ	2.51	0.45
2:E:172:LYS:O	2:E:174:THR:N	2.49	0.45
2:W:186:MSE:HE3	3:X:33:VAL:HG13	1.99	0.45
1:J:316:PHE:O	1:J:320:LEU:N	2.50	0.45
1:S:216:GLU:OE2	1:V:288:ASN:ND2	2.50	0.45
2:Z:270:ALA:CB	2:Z:273:ARG:HG2	2.44	0.45
2:f:186:MSE:CE	3:g:33:VAL:HG13	2.46	0.45
1:h:300:ASP:HB2	3:m:19:HIS:CE1	2.51	0.45
1:k:268:TRP:CD1	1:k:369:ILE:HG12	2.52	0.45
1:n:316:PHE:O	1:n:319:THR:N	2.49	0.45
1:D:317:SER:O	1:D:320:LEU:HB2	2.16	0.45
2:E:161:ALA:HB1	2:E:163:ASP:OD1	2.16	0.45
1:G:171:GLU:OE2	1:G:171:GLU:N	2.49	0.45
1:M:316:PHE:O	1:M:317:SER:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:178:GLY:O	2:Z:179:ALA:C	2.60	0.45
2:c:169:GLN:HE21	2:c:169:GLN:HB3	1.48	0.45
2:l:186:MSE:CE	2:l:197:PRO:HD2	2.46	0.45
1:M:303:MSE:SE	1:M:352:TYR:OH	2.85	0.45
2:N:169:GLN:HE21	2:N:169:GLN:HB3	1.52	0.45
1:S:273:ASN:CG	1:S:276:ASP:HB2	2.42	0.45
1:b:263:ARG:HD2	1:b:293:ALA:O	2.16	0.45
2:i:186:MSE:CE	3:j:33:VAL:HG13	2.47	0.45
1:A:189:LYS:HE2	1:A:189:LYS:HB3	1.73	0.45
1:M:206:GLY:HA2	1:M:370:PHE:CZ	2.52	0.45
2:W:184:TYR:OH	2:W:202:ASP:OD2	2.29	0.45
1:b:303:MSE:SE	1:b:352:TYR:OH	2.85	0.45
1:b:312:MSE:HG2	1:e:307:LEU:CD2	2.46	0.45
1:A:303:MSE:SE	1:A:352:TYR:OH	2.85	0.45
1:D:268:TRP:CD1	1:D:369:ILE:HG12	2.52	0.45
2:E:242:ASN:H	2:E:242:ASN:ND2	2.13	0.45
1:J:233:VAL:HB	1:J:243:ILE:HB	1.99	0.45
1:P:215:THR:HG22	1:S:291:GLY:HA3	1.99	0.45
1:P:273:ASN:CG	1:P:276:ASP:HB2	2.42	0.45
2:Q:216:GLU:HG3	6:Q:1323:HOH:O	2.17	0.45
1:b:274:ASP:OD1	2:f:235:HIS:HA	2.16	0.45
1:e:313:ILE:HA	1:e:316:PHE:CE2	2.52	0.45
1:h:312:MSE:HG2	1:k:307:LEU:CD2	2.47	0.45
1:n:206:GLY:HA2	1:n:370:PHE:CZ	2.52	0.45
1:G:171:GLU:OE2	1:G:171:GLU:CA	2.65	0.44
1:S:282:ILE:O	1:S:283:ASP:C	2.61	0.44
1:S:355:ILE:HD12	1:V:260:GLY:HA3	1.96	0.44
1:V:263:ARG:HD2	1:V:293:ALA:O	2.17	0.44
2:W:200:VAL:HG23	3:X:33:VAL:HG11	1.99	0.44
1:k:189:LYS:HE2	1:k:189:LYS:HB3	1.74	0.44
1:D:189:LYS:HB3	1:D:189:LYS:HE2	1.72	0.44
1:M:316:PHE:O	1:M:319:THR:N	2.50	0.44
1:V:189:LYS:HB3	1:V:189:LYS:HE2	1.70	0.44
2:W:161:ALA:HB1	2:W:163:ASP:OD1	2.17	0.44
1:Y:273:ASN:OD1	1:Y:273:ASN:C	2.60	0.44
1:V:306:ARG:HG2	1:V:355:ILE:HG12	1.99	0.44
2:i:186:MSE:HE1	2:i:197:PRO:HG2	1.98	0.44
1:A:317:SER:HA	1:A:320:LEU:HB2	1.98	0.44
1:D:347:GLU:HG3	1:G:349:LEU:HD23	2.00	0.44
1:G:316:PHE:HA	1:G:319:THR:OG1	2.18	0.44
1:V:274:ASP:OD1	2:Z:235:HIS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:169:GLN:HE21	2:f:169:GLN:HB3	1.49	0.44
2:i:186:MSE:HE3	3:j:33:VAL:HG13	1.99	0.44
2:H:184:TYR:CE2	2:H:266:ASN:HB2	2.53	0.44
2:H:186:MSE:CE	3:I:33:VAL:HG13	2.47	0.44
2:K:172:LYS:HB3	2:K:172:LYS:HZ1	1.81	0.44
1:S:318:ASP:C	1:S:320:LEU:H	2.25	0.44
1:b:302:HIS:HE1	1:b:358:THR:OG1	2.00	0.44
3:d:27:TRP:O	3:d:28:SER:C	2.61	0.44
2:N:186:MSE:CE	3:O:33:VAL:HG13	2.47	0.44
1:n:288:ASN:HB3	1:n:290:LEU:N	2.27	0.44
1:G:263:ARG:HD2	1:G:293:ALA:O	2.17	0.44
2:K:222:MSE:SE	2:K:248:THR:HG21	2.68	0.44
2:Q:200:VAL:HG23	3:R:33:VAL:HG11	2.00	0.44
2:T:176:PHE:CE1	2:T:203:ASN:HB2	2.52	0.44
2:T:186:MSE:HE3	3:U:33:VAL:HG13	2.00	0.44
1:Y:320:LEU:HA	1:b:318:ASP:CG	2.41	0.44
2:f:172:LYS:O	2:f:174:THR:N	2.51	0.44
2:f:186:MSE:HE3	3:g:33:VAL:HA	1.99	0.44
2:l:270:ALA:O	2:l:273:ARG:HG2	2.18	0.44
1:D:355:ILE:HD13	1:G:260:GLY:HA3	2.00	0.44
2:K:186:MSE:HE3	3:L:33:VAL:HG13	1.98	0.44
2:T:169:GLN:HE21	2:T:169:GLN:HB3	1.49	0.44
1:Y:302:HIS:HE1	1:Y:358:THR:OG1	2.01	0.44
6:b:92:HOH:O	1:e:372:ALA:HB2	2.17	0.44
1:k:282:ILE:O	1:k:283:ASP:C	2.61	0.44
2:l:242:ASN:HD22	2:l:242:ASN:N	2.14	0.44
1:A:225:VAL:HG22	1:A:253:ILE:HG13	2.00	0.44
1:G:316:PHE:O	1:G:319:THR:N	2.51	0.44
1:V:316:PHE:O	1:V:320:LEU:N	2.51	0.44
1:b:316:PHE:O	1:b:317:SER:C	2.61	0.44
1:b:320:LEU:HD22	1:e:318:ASP:OD1	2.18	0.44
1:e:306:ARG:HG2	1:e:355:ILE:HG12	1.99	0.44
1:h:318:ASP:C	1:h:320:LEU:H	2.25	0.44
1:n:168:GLN:OE1	1:n:168:GLN:N	2.51	0.44
2:o:242:ASN:H	2:o:242:ASN:ND2	2.09	0.44
1:G:257:ILE:HG13	1:G:357:PRO:HG2	1.99	0.43
2:H:242:ASN:HD22	2:H:242:ASN:N	2.13	0.43
1:M:268:TRP:CD1	1:M:369:ILE:HG12	2.51	0.43
1:P:212:GLY:HA2	1:P:365:ASP:O	2.18	0.43
1:Y:306:ARG:HG3	1:Y:355:ILE:HG12	1.99	0.43
3:a:27:TRP:O	3:a:28:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:300:ASP:HB2	3:j:19:HIS:CE1	2.52	0.43
1:h:316:PHE:O	1:h:317:SER:C	2.60	0.43
1:V:317:SER:HA	1:V:320:LEU:CG	2.45	0.43
1:Y:189:LYS:HE2	1:Y:189:LYS:HB3	1.59	0.43
2:Z:161:ALA:HB1	2:Z:163:ASP:OD1	2.17	0.43
1:e:215:THR:HG22	1:h:291:GLY:HA3	2.00	0.43
1:k:355:ILE:HD13	1:n:260:GLY:HA3	1.97	0.43
1:A:312:MSE:HG2	1:D:307:LEU:HD21	2.00	0.43
2:E:270:ALA:CB	2:E:273:ARG:HG2	2.46	0.43
1:M:300:ASP:HB2	3:R:19:HIS:CE1	2.53	0.43
1:S:189:LYS:HE2	1:S:189:LYS:HB3	1.66	0.43
2:T:252:GLU:OE2	2:T:254:ARG:NH1	2.35	0.43
2:l:161:ALA:HB1	2:l:163:ASP:OD1	2.19	0.43
1:A:316:PHE:HB3	1:A:320:LEU:HD21	2.00	0.43
1:G:300:ASP:HB2	3:L:19:HIS:CE1	2.53	0.43
1:J:179:LEU:CB	5:J:1:LDA:H11	2.46	0.43
1:S:233:VAL:HB	1:S:243:ILE:HB	2.00	0.43
1:b:245:LYS:HE3	2:f:241:ARG:O	2.18	0.43
3:d:26:ASP:OD1	3:d:26:ASP:C	2.60	0.43
1:k:316:PHE:O	1:k:319:THR:N	2.51	0.43
2:H:161:ALA:CB	2:H:163:ASP:OD1	2.66	0.43
1:J:316:PHE:O	1:J:319:THR:N	2.52	0.43
2:Q:172:LYS:O	2:Q:174:THR:N	2.51	0.43
2:T:186:MSE:CE	3:U:33:VAL:HG13	2.49	0.43
1:Y:355:ILE:O	1:Y:355:ILE:HG13	2.09	0.43
1:b:233:VAL:HB	1:b:243:ILE:HB	1.99	0.43
1:b:316:PHE:HA	1:b:319:THR:OG1	2.18	0.43
1:e:320:LEU:CD1	1:h:318:ASP:OD1	2.67	0.43
1:h:376:ASP:OD1	1:h:378:SER:HB2	2.18	0.43
2:i:172:LYS:HB2	2:i:172:LYS:HE3	1.74	0.43
1:n:316:PHE:O	1:n:317:SER:C	2.61	0.43
2:B:222:MSE:HB3	2:B:253:TRP:CZ3	2.54	0.43
1:D:265:PHE:CD1	5:J:1:LDA:H51	2.54	0.43
1:J:224:GLN:HA	1:J:252:GLN:HA	2.00	0.43
1:M:355:ILE:HD12	1:P:260:GLY:HA3	1.97	0.43
1:S:268:TRP:CD1	1:S:369:ILE:HG12	2.54	0.43
1:V:316:PHE:O	1:V:317:SER:C	2.62	0.43
2:W:186:MSE:CE	2:W:197:PRO:HD2	2.48	0.43
1:b:171:GLU:OE2	1:b:171:GLU:CA	2.66	0.43
2:c:191:GLU:OE2	2:c:191:GLU:N	2.38	0.43
1:G:312:MSE:HG2	1:J:307:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:177:ALA:O	2:K:205:ARG:NH2	2.51	0.43
2:Q:172:LYS:HB2	2:Q:172:LYS:HE3	1.67	0.43
2:W:186:MSE:HE3	3:X:33:VAL:CG2	2.43	0.43
2:Z:186:MSE:CE	2:Z:197:PRO:HG2	2.49	0.43
1:e:317:SER:HA	1:e:320:LEU:HD23	1.99	0.43
2:o:161:ALA:HB3	2:o:164:LYS:HB2	2.00	0.43
1:D:300:ASP:HB2	3:I:19:HIS:CE1	2.53	0.43
2:H:270:ALA:CB	2:H:273:ARG:HG2	2.48	0.43
3:I:27:TRP:O	3:I:28:SER:C	2.61	0.43
2:K:186:MSE:CE	3:L:33:VAL:HG13	2.48	0.43
1:J:355:ILE:HD12	1:M:260:GLY:HA3	1.99	0.43
2:K:225:ALA:O	2:N:260:LYS:HD2	2.19	0.43
2:Z:222:MSE:SE	2:Z:248:THR:HG21	2.69	0.43
1:b:181:LYS:HE3	1:e:171:GLU:HA	2.01	0.43
2:f:161:ALA:HB1	2:f:163:ASP:OD1	2.18	0.43
1:D:181:LYS:HE3	1:G:171:GLU:HA	2.00	0.43
2:N:161:ALA:CB	2:N:163:ASP:OD1	2.66	0.43
1:b:355:ILE:HD13	1:e:260:GLY:HA3	1.96	0.43
2:l:184:TYR:OH	2:l:202:ASP:OD2	2.30	0.43
2:l:219:GLN:NE2	6:l:1260:HOH:O	2.51	0.43
2:o:161:ALA:CB	2:o:163:ASP:OD1	2.67	0.43
1:A:273:ASN:OD1	1:A:276:ASP:HB2	2.19	0.42
1:A:316:PHE:O	1:A:317:SER:C	2.62	0.42
1:D:182:ASN:HA	1:G:173:SER:HB2	2.01	0.42
1:D:312:MSE:HG2	1:G:307:LEU:HD21	2.00	0.42
1:J:303:MSE:SE	1:J:352:TYR:OH	2.87	0.42
1:Y:300:ASP:HB2	3:d:19:HIS:CE1	2.54	0.42
1:b:316:PHE:O	1:b:319:THR:N	2.52	0.42
1:e:318:ASP:C	1:e:320:LEU:N	2.76	0.42
1:h:189:LYS:HB3	1:h:189:LYS:HE2	1.67	0.42
2:i:242:ASN:H	2:i:242:ASN:ND2	2.15	0.42
1:A:171:GLU:OE2	1:A:171:GLU:CA	2.68	0.42
2:B:172:LYS:O	2:B:174:THR:N	2.53	0.42
2:Z:195:ILE:HD12	2:Z:255:ILE:HG22	2.00	0.42
2:i:161:ALA:CB	2:i:163:ASP:OD1	2.67	0.42
3:m:40:ASP:OD1	3:m:42:GLN:OE1	2.37	0.42
1:n:263:ARG:HD2	1:n:293:ALA:O	2.18	0.42
1:n:313:ILE:HA	1:n:316:PHE:CE2	2.54	0.42
2:o:222:MSE:SE	2:o:248:THR:HG21	2.68	0.42
1:P:361:ASP:OD2	1:P:365:ASP:OD2	2.37	0.42
1:S:316:PHE:HA	1:S:319:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:242:ASN:HD22	2:T:242:ASN:N	2.18	0.42
1:Y:303:MSE:SE	1:Y:352:TYR:OH	2.87	0.42
1:k:320:LEU:CD2	1:n:318:ASP:OD2	2.67	0.42
1:n:306:ARG:HG2	1:n:355:ILE:HG12	2.02	0.42
1:P:355:ILE:HD13	1:S:260:GLY:HA3	1.95	0.42
1:h:320:LEU:HD22	1:k:318:ASP:CG	2.45	0.42
2:l:161:ALA:CB	2:l:163:ASP:OD1	2.67	0.42
1:n:263:ARG:CD	1:n:293:ALA:O	2.68	0.42
1:n:376:ASP:OD1	1:n:378:SER:HB2	2.19	0.42
1:G:181:LYS:HE3	1:J:171:GLU:HA	2.01	0.42
1:M:225:VAL:HG22	1:M:253:ILE:HG13	2.01	0.42
1:P:385:ASP:HA	1:P:386:ASN:HA	1.93	0.42
2:T:172:LYS:HB3	2:T:172:LYS:HZ1	1.82	0.42
1:V:300:ASP:HB2	3:a:19:HIS:CE1	2.54	0.42
1:b:320:LEU:HB3	1:e:318:ASP:OD2	2.20	0.42
1:A:171:GLU:OE2	1:A:171:GLU:C	2.63	0.42
1:D:206:GLY:HA2	1:D:370:PHE:CZ	2.54	0.42
2:H:178:GLY:O	2:H:179:ALA:C	2.62	0.42
2:N:195:ILE:HD12	2:N:255:ILE:HG22	2.01	0.42
1:P:317:SER:O	1:P:321:THR:HG23	2.19	0.42
1:V:273:ASN:CG	1:V:276:ASP:HB2	2.44	0.42
1:V:306:ARG:HG3	1:V:355:ILE:HG12	1.99	0.42
2:W:175:ALA:HB3	2:W:282:SER:HB2	2.02	0.42
3:g:41:THR:C	3:g:42:GLN:CD	2.88	0.42
3:C:19:HIS:CD2	6:n:1195:HOH:O	2.73	0.42
1:D:215:THR:HG22	1:G:291:GLY:HA3	2.02	0.42
2:Q:169:GLN:HE21	2:Q:169:GLN:HB3	1.52	0.42
1:S:303:MSE:SE	1:S:352:TYR:OH	2.88	0.42
1:V:302:HIS:HE1	1:V:358:THR:OG1	2.02	0.42
2:E:161:ALA:CB	2:E:163:ASP:OD1	2.67	0.42
1:J:268:TRP:CD1	1:J:369:ILE:HG12	2.55	0.42
2:K:161:ALA:HB1	2:K:163:ASP:OD1	2.19	0.42
1:P:313:ILE:HA	1:P:316:PHE:CE2	2.55	0.42
3:U:41:THR:O	3:U:42:GLN:HG3	2.20	0.42
1:h:233:VAL:HB	1:h:243:ILE:HB	2.02	0.42
1:G:367:VAL:HG13	1:G:368:SER:N	2.35	0.42
1:M:282:ILE:O	1:M:283:ASP:C	2.62	0.42
2:T:200:VAL:HA	2:T:208:ARG:O	2.20	0.42
2:W:169:GLN:HE21	2:W:169:GLN:HB3	1.54	0.42
3:X:42:GLN:NE2	6:X:69:HOH:O	2.52	0.42
2:Z:278:THR:HG23	2:Z:285:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:186:MSE:HE3	3:g:33:VAL:HG13	2.02	0.42
1:h:317:SER:HA	1:h:320:LEU:CG	2.31	0.42
2:Q:252:GLU:HG2	2:Q:253:TRP:N	2.35	0.41
3:R:26:ASP:OD1	3:R:26:ASP:C	2.62	0.41
1:h:313:ILE:HA	1:h:316:PHE:CE2	2.55	0.41
2:K:161:ALA:HB3	2:K:164:LYS:HB2	2.02	0.41
2:T:186:MSE:HE3	3:U:33:VAL:CB	2.51	0.41
3:X:26:ASP:OD1	3:X:26:ASP:C	2.62	0.41
1:Y:233:VAL:HB	1:Y:243:ILE:HB	2.02	0.41
2:B:190:PRO:O	2:B:193:ARG:HG3	2.19	0.41
1:P:343:GLN:H	1:P:343:GLN:HG2	1.50	0.41
1:V:303:MSE:SE	1:V:352:TYR:OH	2.88	0.41
1:V:313:ILE:HA	1:V:316:PHE:CE2	2.56	0.41
1:Y:206:GLY:HA2	1:Y:370:PHE:CZ	2.55	0.41
2:c:161:ALA:CB	2:c:163:ASP:OD1	2.68	0.41
1:n:257:ILE:HD13	1:n:359:LEU:HB2	2.02	0.41
1:A:313:ILE:HA	1:A:316:PHE:CE2	2.55	0.41
2:E:178:GLY:O	2:E:179:ALA:C	2.63	0.41
1:G:312:MSE:HG2	1:J:307:LEU:CD2	2.49	0.41
1:J:179:LEU:CA	5:J:1:LDA:H11	2.50	0.41
1:M:319:THR:HA	1:M:322:ALA:HB2	2.01	0.41
1:P:182:ASN:HA	1:S:173:SER:HB2	2.03	0.41
1:P:268:TRP:CD1	1:P:369:ILE:HG12	2.55	0.41
1:e:225:VAL:HG22	1:e:253:ILE:HG13	2.02	0.41
1:D:313:ILE:HA	1:D:316:PHE:CE2	2.55	0.41
1:G:386:ASN:HA	2:H:284:ASP:O	2.19	0.41
1:S:383:LEU:HB3	2:T:168:THR:HG21	2.01	0.41
1:e:318:ASP:C	1:e:320:LEU:H	2.27	0.41
1:h:372:ALA:HB2	6:h:24:HOH:O	2.19	0.41
1:k:209:ILE:HD13	1:k:271:ILE:HD11	2.03	0.41
1:k:216:GLU:OE2	1:n:288:ASN:ND2	2.53	0.41
1:G:257:ILE:HD13	1:G:359:LEU:HB2	2.03	0.41
1:G:347:GLU:OE2	1:G:347:GLU:HA	2.21	0.41
2:W:172:LYS:HB2	2:W:172:LYS:HE3	1.72	0.41
2:f:172:LYS:HB2	2:f:172:LYS:HE3	1.80	0.41
2:o:186:MSE:HE1	2:o:197:PRO:HD2	2.02	0.41
1:A:306:ARG:HG2	1:A:355:ILE:HG12	2.01	0.41
1:A:366:ALA:HB3	2:B:228:LYS:HE2	2.02	0.41
1:D:265:PHE:HB2	5:J:1:LDA:H81	2.02	0.41
2:H:172:LYS:HE3	2:H:172:LYS:HB2	1.70	0.41
2:N:186:MSE:HE1	2:N:197:PRO:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:242:ASN:H	2:N:242:ASN:ND2	2.14	0.41
1:P:206:GLY:HA2	1:P:370:PHE:CZ	2.56	0.41
1:P:317:SER:HA	1:P:320:LEU:CG	2.49	0.41
1:V:216:GLU:OE2	1:Y:288:ASN:ND2	2.53	0.41
2:Z:161:ALA:HB3	2:Z:164:LYS:HB2	2.03	0.41
1:b:288:ASN:HB3	1:b:290:LEU:N	2.29	0.41
1:b:313:ILE:HA	1:b:316:PHE:CE2	2.55	0.41
1:D:263:ARG:HB3	1:D:296:PRO:HA	2.03	0.41
2:E:176:PHE:CE2	2:E:180:LYS:HE3	2.56	0.41
2:T:184:TYR:CE1	2:T:201:TRP:HA	2.56	0.41
1:Y:266:VAL:HG21	1:Y:295:ILE:HG13	2.03	0.41
1:h:316:PHE:HA	1:h:319:THR:OG1	2.21	0.41
1:k:215:THR:HG22	1:n:291:GLY:HA3	2.03	0.41
1:k:320:LEU:HD22	1:n:318:ASP:CG	2.46	0.41
1:D:318:ASP:C	1:D:320:LEU:N	2.79	0.41
1:D:361:ASP:OD2	1:D:365:ASP:OD2	2.38	0.41
3:F:27:TRP:O	3:F:28:SER:C	2.63	0.41
1:J:244:ASP:O	1:J:245:LYS:C	2.64	0.41
1:J:283:ASP:HB3	1:P:183:LEU:O	2.20	0.41
1:P:224:GLN:HA	1:P:252:GLN:HA	2.01	0.41
1:P:316:PHE:HA	1:P:319:THR:OG1	2.20	0.41
2:Q:184:TYR:OH	2:Q:202:ASP:OD2	2.34	0.41
1:S:312:MSE:HG2	1:V:307:LEU:HD21	2.03	0.41
1:b:206:GLY:HA2	1:b:370:PHE:CZ	2.56	0.41
1:h:266:VAL:HG21	1:h:295:ILE:HG13	2.02	0.41
2:i:178:GLY:O	2:i:179:ALA:C	2.63	0.41
2:l:190:PRO:O	2:l:193:ARG:HG3	2.21	0.41
2:B:265:ARG:HH11	2:B:265:ARG:HD2	1.73	0.41
3:C:17:SER:N	1:n:301:ALA:H	2.19	0.41
1:J:288:ASN:HB3	1:J:290:LEU:N	2.33	0.41
2:T:161:ALA:HB1	2:T:163:ASP:OD1	2.21	0.41
1:V:257:ILE:HD13	1:V:359:LEU:HB2	2.03	0.41
1:b:189:LYS:HB3	1:b:189:LYS:HE2	1.62	0.41
1:h:306:ARG:HG2	1:h:355:ILE:HG12	2.03	0.41
1:n:315:LEU:C	6:n:1022:HOH:O	2.63	0.41
1:A:260:GLY:HA3	1:n:355:ILE:HD12	1.96	0.40
1:A:302:HIS:HE1	1:A:358:THR:OG1	2.04	0.40
2:B:200:VAL:HG23	3:C:33:VAL:HG11	2.03	0.40
3:C:26:ASP:OD1	3:C:26:ASP:C	2.63	0.40
2:K:172:LYS:HE3	2:K:172:LYS:HB2	1.71	0.40
2:K:178:GLY:O	2:K:179:ALA:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:385:ASP:HA	1:Y:386:ASN:HA	1.95	0.40
3:a:40:ASP:C	3:a:42:GLN:H	2.30	0.40
2:c:186:MSE:HE3	3:d:33:VAL:CG2	2.45	0.40
2:B:222:MSE:SE	2:B:248:THR:HG21	2.71	0.40
2:E:186:MSE:CE	2:E:197:PRO:HG2	2.49	0.40
2:K:278:THR:HG23	2:K:285:VAL:O	2.21	0.40
1:M:215:THR:HG22	1:P:291:GLY:HA3	2.03	0.40
2:N:200:VAL:HG23	3:O:33:VAL:HG11	2.02	0.40
2:Q:266:ASN:OD1	2:Q:266:ASN:C	2.65	0.40
4:h:2:MPD:HM1	6:h:388:HOH:O	2.21	0.40
1:k:372:ALA:HB2	6:k:394:HOH:O	2.22	0.40
2:l:186:MSE:HE2	3:m:33:VAL:HG22	2.01	0.40
2:H:255:ILE:HB	2:H:262:VAL:HB	2.04	0.40
1:J:182:ASN:HA	1:M:173:SER:HB2	2.02	0.40
3:U:26:ASP:OD1	3:U:26:ASP:C	2.65	0.40
2:Z:190:PRO:O	2:Z:193:ARG:HG3	2.21	0.40
1:A:217:LEU:HD13	1:A:361:ASP:HB3	2.03	0.40
2:B:172:LYS:C	2:B:174:THR:H	2.29	0.40
1:G:274:ASP:OD1	2:K:235:HIS:HA	2.21	0.40
2:Z:161:ALA:CB	2:Z:163:ASP:OD1	2.69	0.40
2:o:195:ILE:HD12	2:o:255:ILE:HG22	2.03	0.40
1:A:222:PRO:HD2	5:J:1:LDA:H52	2.04	0.40
1:A:283:ASP:HB3	1:G:183:LEU:O	2.22	0.40
2:H:172:LYS:C	2:H:174:THR:H	2.27	0.40
1:M:312:MSE:HG2	1:P:307:LEU:CD2	2.51	0.40
1:S:263:ARG:HD2	1:S:293:ALA:O	2.22	0.40
2:c:186:MSE:CE	2:c:197:PRO:HG2	2.51	0.40
2:c:219:GLN:NE2	6:c:811:HOH:O	2.54	0.40
2:f:161:ALA:HB3	2:f:164:LYS:HB2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:27:TRP:CB	2:T:193:ARG:NH1[4_444]	1.66	0.54

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	191/227 (84%)	179 (94%)	10 (5%)	2 (1%)	12	28
1	D	191/227 (84%)	177 (93%)	13 (7%)	1 (0%)	24	46
1	G	189/227 (83%)	176 (93%)	12 (6%)	1 (0%)	24	46
1	J	193/227 (85%)	178 (92%)	14 (7%)	1 (0%)	24	46
1	M	193/227 (85%)	178 (92%)	13 (7%)	2 (1%)	12	28
1	P	193/227 (85%)	179 (93%)	13 (7%)	1 (0%)	24	46
1	S	193/227 (85%)	179 (93%)	13 (7%)	1 (0%)	24	46
1	V	192/227 (85%)	179 (93%)	12 (6%)	1 (0%)	24	46
1	Y	191/227 (84%)	179 (94%)	11 (6%)	1 (0%)	24	46
1	b	191/227 (84%)	176 (92%)	13 (7%)	2 (1%)	12	28
1	e	192/227 (85%)	180 (94%)	10 (5%)	2 (1%)	12	28
1	h	191/227 (84%)	179 (94%)	11 (6%)	1 (0%)	24	46
1	k	192/227 (85%)	180 (94%)	11 (6%)	1 (0%)	24	46
1	n	191/227 (84%)	178 (93%)	12 (6%)	1 (0%)	24	46
2	B	128/135 (95%)	118 (92%)	10 (8%)	0	100	100
2	E	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	16	34
2	H	128/135 (95%)	118 (92%)	9 (7%)	1 (1%)	16	34
2	K	128/135 (95%)	119 (93%)	9 (7%)	0	100	100
2	N	128/135 (95%)	121 (94%)	7 (6%)	0	100	100
2	Q	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	16	34
2	T	128/135 (95%)	120 (94%)	8 (6%)	0	100	100
2	W	128/135 (95%)	122 (95%)	5 (4%)	1 (1%)	16	34
2	Z	128/135 (95%)	118 (92%)	9 (7%)	1 (1%)	16	34
2	c	128/135 (95%)	119 (93%)	8 (6%)	1 (1%)	16	34
2	f	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	16	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	16	34
2	l	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	16	34
2	o	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	16	34
3	C	24/34 (71%)	23 (96%)	1 (4%)	0	100	100
3	F	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
3	I	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
3	L	26/34 (76%)	24 (92%)	1 (4%)	1 (4%)	2	3
3	O	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	R	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	U	25/34 (74%)	24 (96%)	1 (4%)	0	100	100
3	X	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	a	22/34 (65%)	20 (91%)	2 (9%)	0	100	100
3	d	22/34 (65%)	20 (91%)	2 (9%)	0	100	100
3	g	23/34 (68%)	21 (91%)	2 (9%)	0	100	100
3	j	23/34 (68%)	21 (91%)	2 (9%)	0	100	100
3	m	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
3	p	21/34 (62%)	21 (100%)	0	0	100	100
All	All	4796/5544 (86%)	4475 (93%)	292 (6%)	29 (1%)	21	42

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	D	288	ASN
1	G	288	ASN
3	L	17	SER
1	M	288	ASN
1	P	288	ASN
1	V	288	ASN
1	b	288	ASN
1	b	319	THR
1	e	288	ASN
1	h	288	ASN
1	k	288	ASN
1	n	288	ASN
1	J	288	ASN

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Mol	Chain	Res	Type
1	M	321	THR
1	S	288	ASN
1	Y	288	ASN
2	E	173	GLN
2	H	173	GLN
2	W	173	GLN
1	A	378	SER
2	i	173	GLN
2	l	173	GLN
2	o	173	GLN
2	Q	173	GLN
2	Z	173	GLN
1	e	319	THR
2	f	173	GLN
2	c	173	GLN

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	157/180 (87%)	140 (89%)	17 (11%)	6	13
1	D	157/180 (87%)	140 (89%)	17 (11%)	6	13
1	G	156/180 (87%)	140 (90%)	16 (10%)	7	15
1	J	157/180 (87%)	138 (88%)	19 (12%)	5	10
1	M	158/180 (88%)	140 (89%)	18 (11%)	5	11
1	P	158/180 (88%)	140 (89%)	18 (11%)	5	11
1	S	158/180 (88%)	140 (89%)	18 (11%)	5	11
1	V	158/180 (88%)	139 (88%)	19 (12%)	5	10
1	Y	157/180 (87%)	141 (90%)	16 (10%)	7	15
1	b	157/180 (87%)	140 (89%)	17 (11%)	6	13
1	e	158/180 (88%)	138 (87%)	20 (13%)	4	9
1	h	155/180 (86%)	138 (89%)	17 (11%)	6	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	158/180 (88%)	142 (90%)	16 (10%)	7	15
1	n	158/180 (88%)	141 (89%)	17 (11%)	6	13
2	B	109/110 (99%)	96 (88%)	13 (12%)	5	10
2	E	109/110 (99%)	94 (86%)	15 (14%)	3	7
2	H	109/110 (99%)	96 (88%)	13 (12%)	5	10
2	K	109/110 (99%)	97 (89%)	12 (11%)	6	13
2	N	109/110 (99%)	94 (86%)	15 (14%)	3	7
2	Q	109/110 (99%)	94 (86%)	15 (14%)	3	7
2	T	109/110 (99%)	94 (86%)	15 (14%)	3	7
2	W	109/110 (99%)	96 (88%)	13 (12%)	5	10
2	Z	109/110 (99%)	96 (88%)	13 (12%)	5	10
2	c	109/110 (99%)	95 (87%)	14 (13%)	4	8
2	f	109/110 (99%)	96 (88%)	13 (12%)	5	10
2	i	109/110 (99%)	97 (89%)	12 (11%)	6	13
2	l	109/110 (99%)	95 (87%)	14 (13%)	4	8
2	o	108/110 (98%)	94 (87%)	14 (13%)	4	8
3	C	25/31 (81%)	22 (88%)	3 (12%)	5	10
3	F	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	I	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	L	27/31 (87%)	24 (89%)	3 (11%)	6	12
3	O	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	R	23/31 (74%)	21 (91%)	2 (9%)	9	21
3	U	26/31 (84%)	24 (92%)	2 (8%)	12	27
3	X	24/31 (77%)	21 (88%)	3 (12%)	4	9
3	a	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	d	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	g	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	j	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	m	24/31 (77%)	22 (92%)	2 (8%)	10	23
3	p	23/31 (74%)	21 (91%)	2 (9%)	9	21
All	All	4067/4494 (90%)	3600 (88%)	467 (12%)	5	11

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	GLU
1	A	172	THR
1	A	195	VAL
1	A	211	CYS
1	A	217	LEU
1	A	225	VAL
1	A	230	SER
1	A	258	LYS
1	A	307	LEU
1	A	312	MSE
1	A	315	LEU
1	A	355	ILE
1	A	367	VAL
1	A	368	SER
1	A	378	SER
1	A	383	LEU
1	A	385	ASP
2	B	164	LYS
2	B	167	ILE
2	B	169	GLN
2	B	171	LEU
2	B	173	GLN
2	B	174	THR
2	B	217	LEU
2	B	220	VAL
2	B	242	ASN
2	B	248	THR
2	B	276	VAL
2	B	278	THR
2	B	290	ILE
3	C	31	VAL
3	C	37	ILE
3	C	42	GLN
1	D	171	GLU
1	D	172	THR
1	D	195	VAL
1	D	211	CYS
1	D	217	LEU
1	D	225	VAL
1	D	230	SER
1	D	258	LYS
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	312	MSE
1	D	315	LEU
1	D	344	LEU
1	D	355	ILE
1	D	367	VAL
1	D	368	SER
1	D	383	LEU
1	D	385	ASP
2	E	164	LYS
2	E	167	ILE
2	E	169	GLN
2	E	171	LEU
2	E	173	GLN
2	E	174	THR
2	E	191	GLU
2	E	217	LEU
2	E	220	VAL
2	E	242	ASN
2	E	248	THR
2	E	249	VAL
2	E	276	VAL
2	E	278	THR
2	E	290	ILE
3	F	31	VAL
3	F	37	ILE
1	G	171	GLU
1	G	172	THR
1	G	195	VAL
1	G	211	CYS
1	G	217	LEU
1	G	225	VAL
1	G	230	SER
1	G	258	LYS
1	G	307	LEU
1	G	312	MSE
1	G	315	LEU
1	G	355	ILE
1	G	367	VAL
1	G	368	SER
1	G	383	LEU
1	G	385	ASP
2	H	164	LYS

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Mol	Chain	Res	Type
2	H	167	ILE
2	H	169	GLN
2	H	173	GLN
2	H	174	THR
2	H	191	GLU
2	H	217	LEU
2	H	220	VAL
2	H	242	ASN
2	H	248	THR
2	H	276	VAL
2	H	278	THR
2	H	290	ILE
3	I	31	VAL
3	I	37	ILE
1	J	171	GLU
1	J	172	THR
1	J	195	VAL
1	J	211	CYS
1	J	217	LEU
1	J	225	VAL
1	J	230	SER
1	J	258	LYS
1	J	307	LEU
1	J	312	MSE
1	J	315	LEU
1	J	321	THR
1	J	343	GLN
1	J	355	ILE
1	J	367	VAL
1	J	368	SER
1	J	378	SER
1	J	383	LEU
1	J	385	ASP
2	K	164	LYS
2	K	167	ILE
2	K	169	GLN
2	K	171	LEU
2	K	173	GLN
2	K	174	THR
2	K	217	LEU
2	K	220	VAL
2	K	242	ASN

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Mol	Chain	Res	Type
2	K	248	THR
2	K	278	THR
2	K	290	ILE
3	L	15	CYS
3	L	31	VAL
3	L	37	ILE
1	M	171	GLU
1	M	172	THR
1	M	173	SER
1	M	195	VAL
1	M	211	CYS
1	M	217	LEU
1	M	225	VAL
1	M	230	SER
1	M	307	LEU
1	M	312	MSE
1	M	315	LEU
1	M	343	GLN
1	M	355	ILE
1	M	367	VAL
1	M	368	SER
1	M	378	SER
1	M	383	LEU
1	M	385	ASP
2	N	164	LYS
2	N	167	ILE
2	N	169	GLN
2	N	171	LEU
2	N	173	GLN
2	N	174	THR
2	N	191	GLU
2	N	217	LEU
2	N	220	VAL
2	N	232	PRO
2	N	242	ASN
2	N	248	THR
2	N	249	VAL
2	N	278	THR
2	N	290	ILE
3	O	31	VAL
3	O	37	ILE
1	P	171	GLU

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Mol	Chain	Res	Type
1	P	172	THR
1	P	195	VAL
1	P	211	CYS
1	P	217	LEU
1	P	225	VAL
1	P	230	SER
1	P	258	LYS
1	P	307	LEU
1	P	312	MSE
1	P	315	LEU
1	P	343	GLN
1	P	355	ILE
1	P	367	VAL
1	P	368	SER
1	P	378	SER
1	P	383	LEU
1	P	385	ASP
2	Q	164	LYS
2	Q	167	ILE
2	Q	169	GLN
2	Q	171	LEU
2	Q	173	GLN
2	Q	174	THR
2	Q	191	GLU
2	Q	217	LEU
2	Q	220	VAL
2	Q	242	ASN
2	Q	248	THR
2	Q	249	VAL
2	Q	276	VAL
2	Q	278	THR
2	Q	290	ILE
3	R	31	VAL
3	R	37	ILE
1	S	171	GLU
1	S	172	THR
1	S	173	SER
1	S	195	VAL
1	S	211	CYS
1	S	217	LEU
1	S	225	VAL
1	S	230	SER

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Mol	Chain	Res	Type
1	S	258	LYS
1	S	307	LEU
1	S	312	MSE
1	S	315	LEU
1	S	320	LEU
1	S	355	ILE
1	S	367	VAL
1	S	368	SER
1	S	383	LEU
1	S	385	ASP
2	T	164	LYS
2	T	167	ILE
2	T	169	GLN
2	T	171	LEU
2	T	173	GLN
2	T	174	THR
2	T	188	GLU
2	T	201	TRP
2	T	217	LEU
2	T	220	VAL
2	T	242	ASN
2	T	248	THR
2	T	276	VAL
2	T	278	THR
2	T	290	ILE
3	U	31	VAL
3	U	37	ILE
1	V	171	GLU
1	V	172	THR
1	V	173	SER
1	V	195	VAL
1	V	211	CYS
1	V	217	LEU
1	V	225	VAL
1	V	230	SER
1	V	258	LYS
1	V	307	LEU
1	V	312	MSE
1	V	315	LEU
1	V	321	THR
1	V	355	ILE
1	V	367	VAL

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Mol	Chain	Res	Type
1	V	368	SER
1	V	378	SER
1	V	383	LEU
1	V	385	ASP
2	W	164	LYS
2	W	167	ILE
2	W	169	GLN
2	W	171	LEU
2	W	173	GLN
2	W	174	THR
2	W	191	GLU
2	W	217	LEU
2	W	220	VAL
2	W	242	ASN
2	W	248	THR
2	W	278	THR
2	W	290	ILE
3	X	31	VAL
3	X	37	ILE
3	X	42	GLN
1	Y	171	GLU
1	Y	172	THR
1	Y	195	VAL
1	Y	211	CYS
1	Y	217	LEU
1	Y	225	VAL
1	Y	230	SER
1	Y	258	LYS
1	Y	307	LEU
1	Y	312	MSE
1	Y	315	LEU
1	Y	355	ILE
1	Y	367	VAL
1	Y	368	SER
1	Y	383	LEU
1	Y	385	ASP
2	Z	164	LYS
2	Z	167	ILE
2	Z	169	GLN
2	Z	171	LEU
2	Z	173	GLN
2	Z	174	THR

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Mol	Chain	Res	Type
2	Z	191	GLU
2	Z	217	LEU
2	Z	220	VAL
2	Z	242	ASN
2	Z	248	THR
2	Z	278	THR
2	Z	290	ILE
3	a	31	VAL
3	a	37	ILE
1	b	171	GLU
1	b	172	THR
1	b	195	VAL
1	b	211	CYS
1	b	217	LEU
1	b	225	VAL
1	b	230	SER
1	b	258	LYS
1	b	307	LEU
1	b	312	MSE
1	b	315	LEU
1	b	320	LEU
1	b	355	ILE
1	b	367	VAL
1	b	368	SER
1	b	383	LEU
1	b	385	ASP
2	c	164	LYS
2	c	167	ILE
2	c	169	GLN
2	c	171	LEU
2	c	173	GLN
2	c	174	THR
2	c	191	GLU
2	c	217	LEU
2	c	220	VAL
2	c	242	ASN
2	c	248	THR
2	c	276	VAL
2	c	278	THR
2	c	290	ILE
3	d	31	VAL
3	d	37	ILE

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Mol	Chain	Res	Type
1	e	171	GLU
1	e	172	THR
1	e	173	SER
1	e	195	VAL
1	e	211	CYS
1	e	217	LEU
1	e	225	VAL
1	e	230	SER
1	e	258	LYS
1	e	307	LEU
1	e	312	MSE
1	e	315	LEU
1	e	320	LEU
1	e	347	GLU
1	e	355	ILE
1	e	367	VAL
1	e	368	SER
1	e	378	SER
1	e	383	LEU
1	e	385	ASP
2	f	164	LYS
2	f	167	ILE
2	f	169	GLN
2	f	171	LEU
2	f	173	GLN
2	f	174	THR
2	f	191	GLU
2	f	217	LEU
2	f	220	VAL
2	f	242	ASN
2	f	248	THR
2	f	278	THR
2	f	290	ILE
3	g	31	VAL
3	g	37	ILE
1	h	171	GLU
1	h	172	THR
1	h	195	VAL
1	h	211	CYS
1	h	217	LEU
1	h	225	VAL
1	h	230	SER

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Mol	Chain	Res	Type
1	h	258	LYS
1	h	307	LEU
1	h	312	MSE
1	h	315	LEU
1	h	347	GLU
1	h	355	ILE
1	h	367	VAL
1	h	368	SER
1	h	383	LEU
1	h	385	ASP
2	i	164	LYS
2	i	167	ILE
2	i	169	GLN
2	i	171	LEU
2	i	173	GLN
2	i	174	THR
2	i	191	GLU
2	i	217	LEU
2	i	220	VAL
2	i	242	ASN
2	i	278	THR
2	i	290	ILE
3	j	31	VAL
3	j	37	ILE
1	k	171	GLU
1	k	172	THR
1	k	195	VAL
1	k	211	CYS
1	k	217	LEU
1	k	225	VAL
1	k	230	SER
1	k	258	LYS
1	k	307	LEU
1	k	312	MSE
1	k	315	LEU
1	k	355	ILE
1	k	367	VAL
1	k	368	SER
1	k	383	LEU
1	k	385	ASP
2	l	164	LYS
2	l	167	ILE

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Mol	Chain	Res	Type
2	l	169	GLN
2	l	171	LEU
2	l	173	GLN
2	l	174	THR
2	l	217	LEU
2	l	220	VAL
2	l	242	ASN
2	l	248	THR
2	l	249	VAL
2	l	276	VAL
2	l	278	THR
2	l	290	ILE
3	m	31	VAL
3	m	37	ILE
1	n	168	GLN
1	n	171	GLU
1	n	172	THR
1	n	195	VAL
1	n	211	CYS
1	n	217	LEU
1	n	225	VAL
1	n	230	SER
1	n	258	LYS
1	n	307	LEU
1	n	312	MSE
1	n	315	LEU
1	n	355	ILE
1	n	367	VAL
1	n	368	SER
1	n	383	LEU
1	n	385	ASP
2	o	164	LYS
2	o	167	ILE
2	o	169	GLN
2	o	171	LEU
2	o	173	GLN
2	o	174	THR
2	o	191	GLU
2	o	201	TRP
2	o	217	LEU
2	o	220	VAL
2	o	242	ASN

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Mol	Chain	Res	Type
2	o	248	THR
2	o	278	THR
2	o	290	ILE
3	p	31	VAL
3	p	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	302	HIS
2	B	169	GLN
2	B	173	GLN
2	B	199	HIS
2	B	242	ASN
2	B	268	ASN
3	C	29	ASN
1	D	182	ASN
1	D	298	GLN
1	D	302	HIS
2	E	169	GLN
2	E	173	GLN
2	E	219	GLN
2	E	242	ASN
2	E	268	ASN
1	G	182	ASN
1	G	252	GLN
1	G	298	GLN
1	G	302	HIS
2	H	219	GLN
2	H	242	ASN
2	H	268	ASN
1	J	298	GLN
1	J	302	HIS
2	K	169	GLN
2	K	219	GLN
2	K	242	ASN
2	K	268	ASN
1	M	182	ASN
1	M	298	GLN
1	M	302	HIS
2	N	219	GLN

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Mol	Chain	Res	Type
2	N	242	ASN
2	N	268	ASN
3	O	19	HIS
1	P	182	ASN
1	P	298	GLN
1	P	302	HIS
2	Q	169	GLN
2	Q	199	HIS
2	Q	242	ASN
2	Q	268	ASN
3	R	19	HIS
1	S	182	ASN
1	S	252	GLN
1	S	298	GLN
1	S	302	HIS
2	T	169	GLN
2	T	173	GLN
2	T	199	HIS
2	T	219	GLN
2	T	242	ASN
2	T	268	ASN
1	V	182	ASN
1	V	298	GLN
1	V	302	HIS
2	W	169	GLN
2	W	173	GLN
2	W	219	GLN
2	W	242	ASN
2	W	268	ASN
3	X	19	HIS
1	Y	182	ASN
1	Y	298	GLN
1	Y	302	HIS
2	Z	169	GLN
2	Z	173	GLN
2	Z	219	GLN
2	Z	242	ASN
2	Z	268	ASN
3	a	19	HIS
1	b	182	ASN
1	b	281	ASN
1	b	298	GLN

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Mol	Chain	Res	Type
1	b	302	HIS
2	c	169	GLN
2	c	173	GLN
2	c	219	GLN
2	c	242	ASN
2	c	268	ASN
3	d	19	HIS
1	e	182	ASN
1	e	302	HIS
2	f	169	GLN
2	f	173	GLN
2	f	242	ASN
2	f	268	ASN
3	g	19	HIS
1	h	182	ASN
1	h	298	GLN
1	h	302	HIS
2	i	169	GLN
2	i	173	GLN
2	i	199	HIS
2	i	242	ASN
2	i	268	ASN
3	j	34	ASN
1	k	182	ASN
1	k	298	GLN
1	k	302	HIS
1	k	343	GLN
2	l	169	GLN
2	l	173	GLN
2	l	219	GLN
2	l	242	ASN
1	n	170	ASN
1	n	182	ASN
1	n	298	GLN
1	n	302	HIS
2	o	169	GLN
2	o	219	GLN
2	o	242	ASN
2	o	268	ASN
3	p	19	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
5	LDA	J	1	-	13,15,15	2.50	2 (15%)	14,17,17	1.17	2 (14%)
4	MPD	k	3	-	7,7,7	0.32	0	9,10,10	0.95	0
4	MPD	h	2	-	7,7,7	0.20	0	9,10,10	0.81	0
4	MPD	D	1	-	7,7,7	0.25	0	9,10,10	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LDA	J	1	-	-	11/13/13/13	-
4	MPD	k	3	-	-	0/5/5/5	-
4	MPD	h	2	-	-	3/5/5/5	-
4	MPD	D	1	-	-	5/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	LDA	O1-N1	-7.70	1.23	1.42
5	J	1	LDA	C1-N1	-4.24	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1	LDA	CM2-N1-C1	3.17	116.89	110.23
5	J	1	LDA	C12-C11-C10	2.17	128.01	113.36

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	MPD	C2-C3-C4-O4
4	D	1	MPD	C2-C3-C4-C5
5	J	1	LDA	C2-C1-N1-O1
5	J	1	LDA	C2-C1-N1-CM1
5	J	1	LDA	C2-C1-N1-CM2
5	J	1	LDA	C5-C6-C7-C8
5	J	1	LDA	C2-C3-C4-C5
5	J	1	LDA	C11-C10-C9-C8
5	J	1	LDA	C4-C5-C6-C7
5	J	1	LDA	C9-C10-C11-C12
5	J	1	LDA	C6-C7-C8-C9
5	J	1	LDA	C3-C4-C5-C6
4	D	1	MPD	O2-C2-C3-C4
4	D	1	MPD	C1-C2-C3-C4
4	D	1	MPD	CM-C2-C3-C4
5	J	1	LDA	C7-C8-C9-C10
4	h	2	MPD	O2-C2-C3-C4
4	h	2	MPD	C1-C2-C3-C4
4	h	2	MPD	CM-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	LDA	34	0
4	k	3	MPD	1	0
4	h	2	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	MPD	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	190/227 (83%)	0.14	21 (11%) 10 8	19, 27, 76, 95	0
1	D	190/227 (83%)	0.20	21 (11%) 10 8	19, 27, 76, 96	0
1	G	188/227 (82%)	0.02	19 (10%) 12 9	19, 27, 74, 87	0
1	J	192/227 (84%)	0.20	24 (12%) 8 6	19, 27, 76, 97	0
1	M	192/227 (84%)	0.16	24 (12%) 8 6	19, 27, 77, 93	0
1	P	192/227 (84%)	0.20	25 (13%) 7 5	19, 27, 77, 97	0
1	S	192/227 (84%)	0.19	22 (11%) 9 7	19, 27, 77, 95	0
1	V	191/227 (84%)	0.13	22 (11%) 9 7	19, 27, 77, 95	0
1	Y	190/227 (83%)	0.12	23 (12%) 8 6	19, 27, 76, 95	0
1	b	190/227 (83%)	0.12	20 (10%) 11 9	19, 27, 76, 90	0
1	e	191/227 (84%)	0.19	23 (12%) 9 7	19, 27, 76, 97	0
1	h	190/227 (83%)	0.17	20 (10%) 11 9	19, 27, 76, 89	0
1	k	191/227 (84%)	0.17	21 (10%) 10 8	19, 27, 77, 98	0
1	n	191/227 (84%)	0.18	26 (13%) 7 5	19, 27, 75, 126	0
2	B	127/135 (94%)	0.25	16 (12%) 8 6	24, 33, 68, 93	0
2	E	127/135 (94%)	0.16	13 (10%) 12 9	24, 33, 68, 93	0
2	H	127/135 (94%)	0.19	14 (11%) 10 8	24, 33, 68, 93	0
2	K	127/135 (94%)	0.23	16 (12%) 8 6	24, 33, 68, 93	0
2	N	127/135 (94%)	0.11	13 (10%) 12 9	24, 33, 68, 93	0
2	Q	127/135 (94%)	0.18	14 (11%) 10 8	24, 33, 68, 93	0
2	T	127/135 (94%)	0.24	16 (12%) 8 6	24, 33, 68, 93	0
2	W	127/135 (94%)	0.12	13 (10%) 12 9	24, 33, 68, 93	0
2	Z	127/135 (94%)	0.16	11 (8%) 16 12	24, 33, 68, 93	0
2	c	127/135 (94%)	0.08	13 (10%) 12 9	24, 33, 68, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	f	127/135 (94%)	0.21	16 (12%) 8 6	24, 33, 68, 93	0
2	i	127/135 (94%)	0.15	13 (10%) 12 9	24, 33, 68, 93	0
2	l	127/135 (94%)	0.20	15 (11%) 9 7	24, 33, 68, 93	0
2	o	127/135 (94%)	0.31	15 (11%) 9 7	24, 33, 68, 93	0
3	C	26/34 (76%)	1.32	6 (23%) 2 1	30, 40, 76, 83	0
3	F	25/34 (73%)	0.65	4 (16%) 5 4	31, 37, 76, 84	0
3	I	25/34 (73%)	0.90	5 (20%) 3 2	30, 37, 76, 82	0
3	L	28/34 (82%)	0.93	8 (28%) 1 1	30, 41, 79, 82	0
3	O	24/34 (70%)	0.66	4 (16%) 4 3	30, 37, 76, 85	0
3	R	24/34 (70%)	0.50	3 (12%) 8 6	30, 37, 69, 81	0
3	U	27/34 (79%)	1.47	8 (29%) 1 1	30, 40, 76, 84	0
3	X	24/34 (70%)	0.59	4 (16%) 4 3	30, 37, 76, 84	0
3	a	24/34 (70%)	0.34	2 (8%) 17 13	31, 37, 76, 83	0
3	d	24/34 (70%)	0.65	5 (20%) 2 2	30, 37, 76, 85	0
3	g	25/34 (73%)	0.67	3 (12%) 9 7	30, 37, 76, 86	0
3	j	25/34 (73%)	0.64	5 (20%) 3 2	30, 37, 76, 84	0
3	m	25/34 (73%)	0.61	4 (16%) 5 4	30, 37, 76, 84	0
3	p	23/34 (67%)	0.79	2 (8%) 16 12	30, 37, 69, 81	0
All	All	4797/5544 (86%)	0.21	572 (11%) 9 7	19, 31, 77, 126	0

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	e	316	PHE	10.5
1	n	342	GLY	10.2
1	A	345	ALA	9.0
1	D	345	ALA	8.9
1	h	343	GLN	8.6
1	b	316	PHE	8.5
1	h	349	LEU	8.5
1	J	342	GLY	8.4
1	e	317	SER	8.4
1	D	322	ALA	8.3
1	k	345	ALA	8.3
1	h	345	ALA	8.3
1	P	322	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
1	b	345	ALA	8.2
1	S	344	LEU	8.1
1	S	345	ALA	8.1
1	D	316	PHE	7.9
1	A	316	PHE	7.9
1	h	344	LEU	7.8
1	h	342	GLY	7.7
1	P	345	ALA	7.7
1	Y	345	ALA	7.5
1	n	319	THR	7.5
1	e	344	LEU	7.4
1	D	320	LEU	7.4
1	V	316	PHE	7.4
1	V	345	ALA	7.4
1	h	316	PHE	7.4
1	P	342	GLY	7.3
1	S	316	PHE	7.3
1	Y	316	PHE	7.3
1	P	316	PHE	7.2
1	J	322	ALA	7.2
1	Y	344	LEU	7.2
1	k	316	PHE	7.1
1	h	317	SER	7.1
1	G	319	THR	7.0
1	Y	322	ALA	7.0
1	G	344	LEU	6.9
1	D	344	LEU	6.9
1	G	316	PHE	6.9
1	n	345	ALA	6.9
1	e	318	ASP	6.8
1	J	316	PHE	6.8
1	J	344	LEU	6.8
1	M	344	LEU	6.7
1	V	317	SER	6.7
1	Y	317	SER	6.7
1	k	320	LEU	6.7
1	M	342	GLY	6.7
1	b	317	SER	6.7
1	n	316	PHE	6.7
1	S	322	ALA	6.7
1	h	319	THR	6.6
1	Y	320	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	346	SER	6.6
1	G	349	LEU	6.6
1	M	316	PHE	6.5
1	M	322	ALA	6.5
1	h	318	ASP	6.5
1	h	320	LEU	6.5
1	b	344	LEU	6.4
1	b	342	GLY	6.4
3	U	18	GLY	6.4
1	V	322	ALA	6.4
1	Y	319	THR	6.3
1	b	319	THR	6.3
1	M	320	LEU	6.3
1	M	319	THR	6.3
1	S	342	GLY	6.2
1	P	320	LEU	6.1
1	e	349	LEU	6.1
1	S	317	SER	6.1
1	V	344	LEU	6.1
1	h	346	SER	6.0
1	b	318	ASP	6.0
1	A	344	LEU	6.0
1	k	321	THR	6.0
1	D	319	THR	5.9
1	Y	321	THR	5.9
3	m	42	GLN	5.9
1	M	318	ASP	5.9
1	n	344	LEU	5.8
1	A	317	SER	5.8
1	A	320	LEU	5.8
1	e	322	ALA	5.8
1	b	320	LEU	5.8
1	G	318	ASP	5.8
1	J	317	SER	5.7
1	V	319	THR	5.7
1	V	321	THR	5.7
1	G	345	ALA	5.7
1	S	314	SER	5.7
1	e	319	THR	5.7
1	k	318	ASP	5.6
1	D	317	SER	5.6
1	J	321	THR	5.6

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Mol	Chain	Res	Type	RSRZ
2	o	273	ARG	5.6
1	M	343	GLN	5.6
1	S	321	THR	5.6
1	e	345	ALA	5.5
1	P	344	LEU	5.4
1	b	349	LEU	5.4
1	b	343	GLN	5.4
1	k	349	LEU	5.4
1	J	320	LEU	5.4
1	M	317	SER	5.4
1	M	345	ALA	5.4
1	P	314	SER	5.4
1	k	317	SER	5.3
1	k	344	LEU	5.3
1	G	317	SER	5.3
1	A	318	ASP	5.3
3	C	18	GLY	5.3
1	J	318	ASP	5.2
1	G	346	SER	5.2
3	U	29	ASN	5.2
1	e	343	GLN	5.2
1	Y	318	ASP	5.2
1	V	349	LEU	5.1
1	G	314	SER	5.1
1	S	319	THR	5.1
1	e	321	THR	5.1
1	D	348	ALA	5.1
1	e	348	ALA	5.1
1	D	349	LEU	5.1
1	S	320	LEU	5.1
1	V	318	ASP	5.1
1	k	319	THR	5.1
1	A	319	THR	5.0
1	k	346	SER	5.0
1	M	321	THR	5.0
1	V	320	LEU	5.0
1	n	314	SER	4.9
2	W	163	ASP	4.9
2	f	273	ARG	4.9
1	n	170	ASN	4.9
2	l	166	ARG	4.8
1	J	345	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	e	347	GLU	4.8
3	p	41	THR	4.8
1	e	346	SER	4.7
1	M	314	SER	4.7
3	C	17	SER	4.7
2	Z	273	ARG	4.7
1	S	318	ASP	4.7
1	n	169	ASP	4.7
1	e	320	LEU	4.7
1	J	319	THR	4.7
3	U	17	SER	4.7
1	P	349	LEU	4.7
2	T	167	ILE	4.6
1	k	348	ALA	4.6
1	P	351	SER	4.6
1	n	317	SER	4.6
2	i	161	ALA	4.6
2	E	273	ARG	4.6
2	H	161	ALA	4.6
2	B	273	ARG	4.5
1	A	314	SER	4.5
1	J	346	SER	4.5
1	J	349	LEU	4.5
1	D	321	THR	4.5
1	J	343	GLN	4.5
1	G	311	ILE	4.5
1	J	350	ARG	4.5
2	T	273	ARG	4.5
1	P	319	THR	4.5
2	N	164	LYS	4.4
1	V	315	LEU	4.4
2	K	161	ALA	4.4
2	B	166	ARG	4.4
1	S	343	GLN	4.4
1	k	314	SER	4.4
3	U	16	SER	4.4
1	A	315	LEU	4.3
1	P	315	LEU	4.3
2	T	161	ALA	4.3
1	P	313	ILE	4.3
1	k	322	ALA	4.3
3	I	18	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	Y	315	LEU	4.3
1	P	348	ALA	4.3
1	V	350	ARG	4.2
2	N	273	ARG	4.2
1	h	348	ALA	4.2
2	E	161	ALA	4.2
3	O	41	THR	4.2
2	Q	273	ARG	4.2
1	D	318	ASP	4.2
2	f	163	ASP	4.2
3	I	42	GLN	4.2
3	j	18	GLY	4.2
2	E	169	GLN	4.2
1	J	347	GLU	4.2
3	L	15	CYS	4.2
2	K	164	LYS	4.2
2	o	167	ILE	4.2
2	i	273	ARG	4.2
1	Y	350	ARG	4.1
1	S	315	LEU	4.1
2	T	164	LYS	4.1
1	k	347	GLU	4.1
1	P	318	ASP	4.1
1	V	346	SER	4.1
1	b	314	SER	4.1
2	c	164	LYS	4.0
3	F	18	GLY	4.0
1	M	346	SER	4.0
3	R	41	THR	4.0
2	K	169	GLN	4.0
3	U	42	GLN	4.0
1	Y	349	LEU	4.0
1	h	314	SER	4.0
1	D	347	GLU	4.0
2	H	273	ARG	4.0
2	W	273	ARG	4.0
3	C	29	ASN	4.0
1	P	317	SER	3.9
1	n	351	SER	3.9
2	E	167	ILE	3.9
1	V	343	GLN	3.9
3	g	42	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	f	167	ILE	3.9
2	i	167	ILE	3.9
1	n	168	GLN	3.9
1	M	349	LEU	3.9
2	E	165	LYS	3.9
1	b	350	ARG	3.9
1	D	351	SER	3.9
2	Q	163	ASP	3.9
1	e	314	SER	3.8
1	S	349	LEU	3.8
2	Q	161	ALA	3.8
2	Q	164	LYS	3.8
2	o	164	LYS	3.8
1	n	349	LEU	3.8
2	l	175	ALA	3.8
3	F	42	GLN	3.8
3	d	41	THR	3.8
1	b	315	LEU	3.8
1	V	313	ILE	3.8
2	K	167	ILE	3.8
2	N	167	ILE	3.8
2	o	290	ILE	3.8
1	J	348	ALA	3.8
1	M	310	ALA	3.8
2	l	273	ARG	3.8
3	O	42	GLN	3.7
2	T	163	ASP	3.7
1	D	315	LEU	3.7
2	K	163	ASP	3.7
1	J	314	SER	3.7
2	c	161	ALA	3.7
2	f	161	ALA	3.7
3	d	42	GLN	3.7
1	J	315	LEU	3.7
1	Y	313	ILE	3.7
1	G	350	ARG	3.7
1	V	348	ALA	3.7
3	C	42	GLN	3.7
1	P	321	THR	3.7
2	l	167	ILE	3.7
1	P	310	ALA	3.7
1	S	347	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	Z	164	LYS	3.6
2	c	273	ARG	3.6
1	P	343	GLN	3.6
1	V	347	GLU	3.6
1	A	321	THR	3.6
2	o	165	LYS	3.6
1	A	350	ARG	3.6
3	j	41	THR	3.6
1	k	350	ARG	3.6
2	Q	175	ALA	3.6
2	N	169	GLN	3.6
2	l	169	GLN	3.6
1	b	313	ILE	3.5
2	c	163	ASP	3.5
2	l	161	ALA	3.5
2	o	173	GLN	3.5
1	k	315	LEU	3.5
1	D	346	SER	3.5
2	c	167	ILE	3.5
2	N	162	ALA	3.5
2	H	169	GLN	3.5
1	n	318	ASP	3.5
2	Z	162	ALA	3.5
2	f	164	LYS	3.5
1	h	347	GLU	3.5
2	Q	173	GLN	3.5
1	P	385	ASP	3.5
1	k	343	GLN	3.5
2	Z	165	LYS	3.4
1	G	348	ALA	3.4
2	B	175	ALA	3.4
2	H	162	ALA	3.4
2	B	169	GLN	3.4
1	M	313	ILE	3.4
1	k	313	ILE	3.4
1	J	351	SER	3.4
1	A	348	ALA	3.4
2	N	163	ASP	3.4
3	j	42	GLN	3.4
2	H	164	LYS	3.4
1	S	350	ARG	3.4
1	n	313	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	o	166	ARG	3.4
1	Y	347	GLU	3.3
2	T	169	GLN	3.3
2	Z	169	GLN	3.3
2	o	161	ALA	3.3
2	E	163	ASP	3.3
2	T	193	ARG	3.3
2	N	161	ALA	3.3
2	N	175	ALA	3.3
2	T	173	GLN	3.3
2	f	175	ALA	3.3
2	i	164	LYS	3.3
2	l	163	ASP	3.3
1	D	313	ILE	3.3
2	W	167	ILE	3.3
1	e	315	LEU	3.3
2	K	173	GLN	3.3
1	D	311	ILE	3.3
1	S	348	ALA	3.3
2	i	162	ALA	3.3
3	L	41	THR	3.2
2	E	290	ILE	3.2
2	Q	167	ILE	3.2
2	H	163	ASP	3.2
2	Z	163	ASP	3.2
1	M	350	ARG	3.2
2	E	174	THR	3.2
1	P	346	SER	3.2
1	b	346	SER	3.2
1	A	347	GLU	3.2
1	Y	314	SER	3.2
3	L	18	GLY	3.2
2	B	162	ALA	3.2
1	J	313	ILE	3.2
2	T	166	ARG	3.2
2	W	169	GLN	3.2
2	o	169	GLN	3.2
1	A	322	ALA	3.2
1	G	313	ILE	3.2
2	Q	290	ILE	3.2
3	L	29	ASN	3.1
3	L	42	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
3	a	42	GLN	3.1
1	S	313	ILE	3.1
1	h	313	ILE	3.1
2	f	174	THR	3.1
2	E	175	ALA	3.1
2	Z	161	ALA	3.1
1	P	352	TYR	3.1
2	B	173	GLN	3.1
2	W	161	ALA	3.1
2	c	290	ILE	3.1
1	G	386	ASN	3.0
3	O	19	HIS	3.0
2	B	163	ASP	3.0
2	B	161	ALA	3.0
1	k	351	SER	3.0
1	P	347	GLU	3.0
2	i	173	GLN	3.0
2	Q	174	THR	3.0
1	n	348	ALA	3.0
2	c	175	ALA	3.0
1	A	349	LEU	3.0
1	e	351	SER	3.0
1	Y	352	TYR	3.0
1	k	385	ASP	3.0
2	l	164	LYS	3.0
1	e	350	ARG	3.0
2	E	162	ALA	3.0
2	W	162	ALA	3.0
1	V	314	SER	3.0
1	e	386	ASN	3.0
2	Q	169	GLN	3.0
2	o	163	ASP	3.0
1	M	347	GLU	2.9
1	n	347	GLU	2.9
3	F	41	THR	2.9
3	I	41	THR	2.9
3	U	41	THR	2.9
3	I	29	ASN	2.9
1	b	348	ALA	2.9
2	o	162	ALA	2.9
1	M	315	LEU	2.9
1	h	315	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	311	ILE	2.9
3	F	39	VAL	2.9
2	Q	170	LYS	2.9
2	W	164	LYS	2.9
2	W	171	LEU	2.9
1	P	350	ARG	2.9
3	m	18	GLY	2.9
2	E	164	LYS	2.9
2	K	171	LEU	2.9
2	Q	165	LYS	2.9
1	G	347	GLU	2.8
1	b	347	GLU	2.8
1	G	343	GLN	2.8
1	b	311	ILE	2.8
1	n	311	ILE	2.8
2	K	290	ILE	2.8
3	U	39	VAL	2.8
2	c	169	GLN	2.8
2	H	290	ILE	2.8
1	G	315	LEU	2.8
1	G	310	ALA	2.8
2	K	273	ARG	2.8
2	f	166	ARG	2.8
2	E	173	GLN	2.8
2	f	173	GLN	2.8
2	Z	167	ILE	2.8
1	Y	346	SER	2.8
2	i	174	THR	2.8
3	C	41	THR	2.8
1	D	350	ARG	2.8
2	H	166	ARG	2.8
2	f	169	GLN	2.8
2	B	167	ILE	2.8
1	M	348	ALA	2.8
2	c	174	THR	2.8
2	i	175	ALA	2.8
2	l	174	THR	2.8
1	n	350	ARG	2.8
2	H	165	LYS	2.7
2	T	165	LYS	2.7
2	o	174	THR	2.7
3	j	40	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	172	LYS	2.7
2	i	165	LYS	2.7
2	l	290	ILE	2.7
2	T	174	THR	2.7
2	i	166	ARG	2.7
3	m	40	ASP	2.7
2	B	174	THR	2.7
3	O	39	VAL	2.7
3	d	39	VAL	2.7
3	m	41	THR	2.7
1	n	315	LEU	2.7
2	B	272	GLY	2.7
1	Y	310	ALA	2.7
3	I	39	VAL	2.7
2	N	173	GLN	2.6
2	l	173	GLN	2.6
2	f	165	LYS	2.6
1	A	310	ALA	2.6
1	M	351	SER	2.6
3	C	39	VAL	2.6
3	p	40	ASP	2.6
2	f	162	ALA	2.6
1	D	314	SER	2.6
2	H	173	GLN	2.6
3	X	42	GLN	2.6
1	M	311	ILE	2.6
1	Y	311	ILE	2.6
2	o	251	LYS	2.6
2	T	175	ALA	2.6
2	l	203	ASN	2.6
1	S	346	SER	2.5
2	l	165	LYS	2.5
2	l	170	LYS	2.5
1	e	352	TYR	2.5
1	S	310	ALA	2.5
1	Y	384	ALA	2.5
1	n	310	ALA	2.5
2	o	175	ALA	2.5
3	L	16	SER	2.5
3	L	17	SER	2.5
1	e	313	ILE	2.5
2	K	166	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	165	LYS	2.5
2	f	265	ARG	2.5
1	D	352	TYR	2.5
2	N	272	GLY	2.5
2	c	162	ALA	2.5
1	D	386	ASN	2.5
2	H	174	THR	2.5
3	X	41	THR	2.5
1	b	351	SER	2.5
3	R	40	ASP	2.5
1	n	352	TYR	2.5
3	j	39	VAL	2.5
1	S	311	ILE	2.5
1	n	346	SER	2.5
2	N	174	THR	2.4
1	Y	386	ASN	2.4
1	h	311	ILE	2.4
1	h	351	SER	2.4
1	J	385	ASP	2.4
3	R	18	GLY	2.4
2	B	265	ARG	2.4
2	Q	166	ARG	2.4
2	N	290	ILE	2.4
3	d	19	HIS	2.4
1	V	309	GLY	2.4
2	B	172	LYS	2.4
2	K	172	LYS	2.4
1	A	384	ALA	2.4
1	G	385	ASP	2.4
2	H	175	ALA	2.4
2	K	174	THR	2.4
1	n	386	ASN	2.4
2	B	165	LYS	2.4
2	c	172	LYS	2.4
2	i	169	GLN	2.4
2	Z	175	ALA	2.4
2	T	171	LEU	2.3
1	P	355	ILE	2.3
2	H	167	ILE	2.3
2	W	170	LYS	2.3
2	i	163	ASP	2.3
2	l	172	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	o	170	LYS	2.3
3	L	39	VAL	2.3
1	b	310	ALA	2.3
2	K	175	ALA	2.3
3	a	41	THR	2.3
2	K	165	LYS	2.3
1	J	310	ALA	2.3
2	K	162	ALA	2.3
1	A	352	TYR	2.3
2	B	164	LYS	2.3
2	W	173	GLN	2.3
3	g	18	GLY	2.3
3	X	39	VAL	2.3
2	H	172	LYS	2.3
1	h	310	ALA	2.2
2	c	165	LYS	2.2
1	h	386	ASN	2.2
1	Y	351	SER	2.2
1	n	354	SER	2.2
2	W	174	THR	2.2
1	P	386	ASN	2.2
2	f	172	LYS	2.2
1	A	313	ILE	2.2
2	W	175	ALA	2.2
2	c	173	GLN	2.2
1	M	385	ASP	2.2
1	Y	385	ASP	2.2
2	Z	174	THR	2.2
2	T	170	LYS	2.2
3	X	35	LYS	2.2
1	e	355	ILE	2.2
1	V	386	ASN	2.1
2	i	170	LYS	2.1
2	Q	272	GLY	2.1
1	k	311	ILE	2.1
2	W	290	ILE	2.1
1	n	171	GLU	2.1
1	V	352	TYR	2.1
2	T	162	ALA	2.1
1	e	171	GLU	2.1
1	M	386	ASN	2.1
3	d	29	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	272	GLY	2.1
1	J	311	ILE	2.1
3	g	39	VAL	2.1
1	S	351	SER	2.1
1	J	352	TYR	2.1
1	V	355	ILE	2.1
1	n	355	ILE	2.1
2	B	290	ILE	2.1
2	f	170	LYS	2.0
2	f	171	LEU	2.0
2	Z	166	ARG	2.0
3	U	19	HIS	2.0
2	T	290	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($\text{\AA}^2$)	Q<0.9
5	LDA	J	1	16/16	0.73	0.23	11,42,48,52	0
4	MPD	D	1	8/8	0.88	0.23	62,63,64,67	0
4	MPD	k	3	8/8	0.89	0.17	44,45,48,53	0
4	MPD	h	2	8/8	0.91	0.17	50,52,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.