Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:53 AM GMT

PDB ID	:	3JQO
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

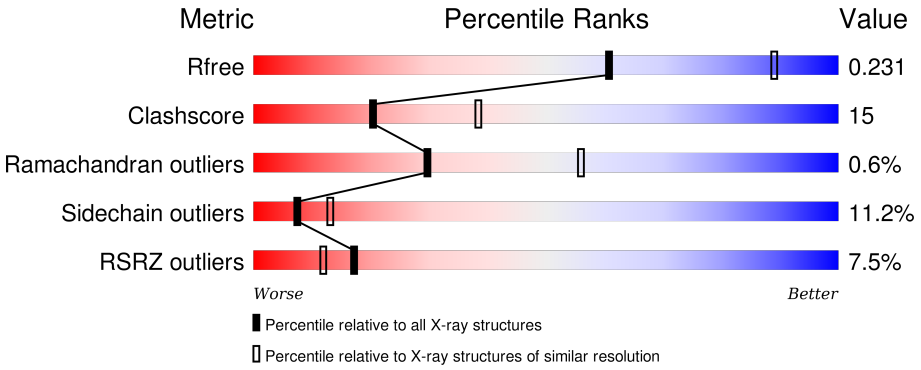
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 61% 20% • • 14%
1	D	227	9% 60% 20% 5% • 14%
1	G	227	8% 61% 19% 5% 15%
1	J	227	11% 59% 22% • 13%
1	M	227	11% 59% 21% 5% • 13%

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Mol	Chain	Length	Quality of chain
1	P	227	11% 61% 20% 6% 13%
1	S	227	10% 64% 16% 5% 13%
1	V	227	10% 62% 20% 14%
1	Y	227	9% 64% 17% 14%
1	b	227	9% 74% 9% 14%
1	e	227	10% 74% 11% 14%
1	h	227	8% 76% 8% 14%
1	k	227	9% 76% 9% 14%
1	n	227	10% 75% 9% 14%
2	B	135	2% 70% 21%
2	E	135	2% 70% 21% 5%
2	H	135	% 64% 27%
2	K	135	2% 71% 18% 7%
2	N	135	2% 68% 23%
2	Q	135	2% 67% 23% 6%
2	T	135	2% 66% 24% 6%
2	W	135	2% 72% 18% 6%
2	Z	135	% 66% 24% 6%
2	c	135	% 84% 10%
2	f	135	% 84% 11%
2	i	135	% 84% 10%
2	l	135	2% 83% 11%
2	o	135	2% 84% 10%
3	C	34	9% 59% 15% 24%
3	F	34	6% 62% 12% 26%

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Mol	Chain	Length	Quality of chain
3	I	34	53% 21% 26%
3	L	34	12% 59% 24% 18%
3	O	34	3% 59% 12% 29%
3	R	34	3% 53% 18% 29%
3	U	34	15% 56% 21% 21%
3	X	34	6% 47% 21% 29%
3	a	34	65% 6% 29%
3	d	34	9% 68% 29%
3	g	34	3% 71% 26%
3	j	34	6% 71% 26%
3	m	34	3% 71% 26%
3	p	34	65% 32%

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
4	MPD	D	1	-	-	X	X
4	MPD	h	2	-	-	-	X
4	MPD	k	3	-	-	-	X
5	LDA	J	1	-	-	X	X

2 Entry composition (i)

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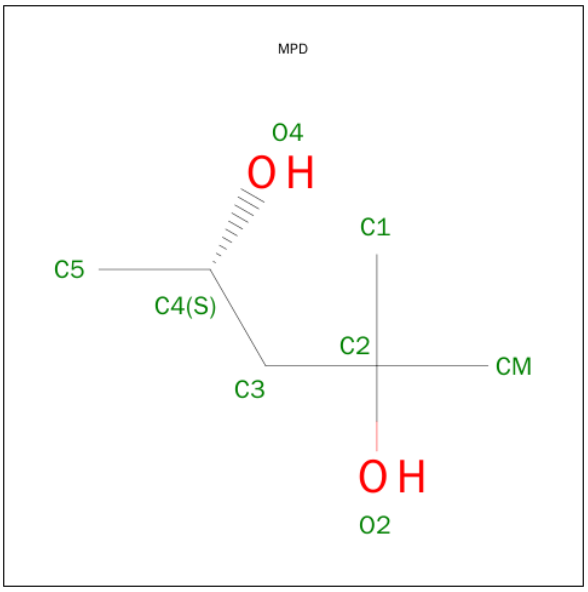
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	o	130	Total	C	N	O	Se	0	0	0
			1032	647	193	189	3			

- Molecule 3 is a protein called TraN protein.

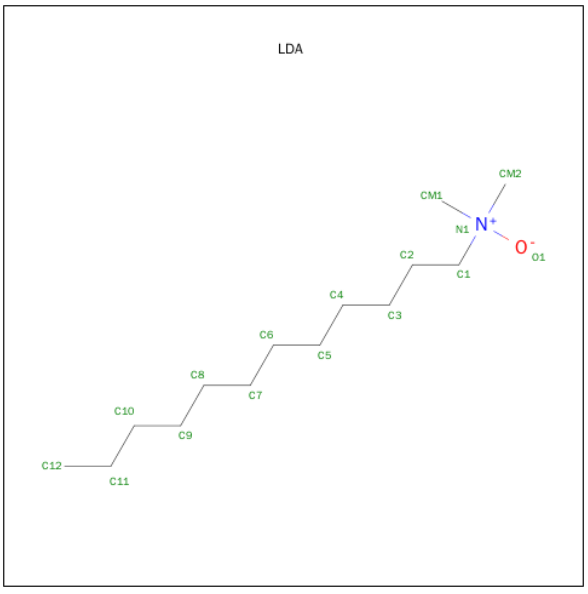
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O		0	0	0
			200	126	34	40				
3	F	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	I	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	L	28	Total	C	N	O	S	0	0	0
			212	132	36	43	1			
3	O	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	R	24	Total	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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: 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	0	0
			65	65		
6	B	31	Total	O	0	0
			31	31		
6	C	7	Total	O	0	0
			7	7		
6	E	28	Total	O	0	0
			28	28		
6	D	65	Total	O	0	0
			65	65		
6	F	9	Total	O	0	0
			9	9		
6	G	50	Total	O	0	0
			50	50		
6	H	22	Total	O	0	0
			22	22		
6	J	49	Total	O	0	0
			49	49		
6	I	9	Total	O	0	0
			9	9		
6	K	30	Total	O	0	0
			30	30		
6	L	12	Total	O	0	0
			12	12		
6	N	35	Total	O	0	0
			35	35		
6	M	48	Total	O	0	0
			48	48		
6	O	11	Total	O	0	0
			11	11		
6	P	58	Total	O	0	0
			58	58		
6	Q	27	Total	O	0	0
			27	27		
6	R	7	Total	O	0	0
			7	7		
6	S	57	Total	O	0	0
			57	57		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	21	Total O 21 21	0	0
6	U	10	Total O 10 10	0	0
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	Z	21	Total O 21 21	0	0
6	Y	57	Total O 57 57	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

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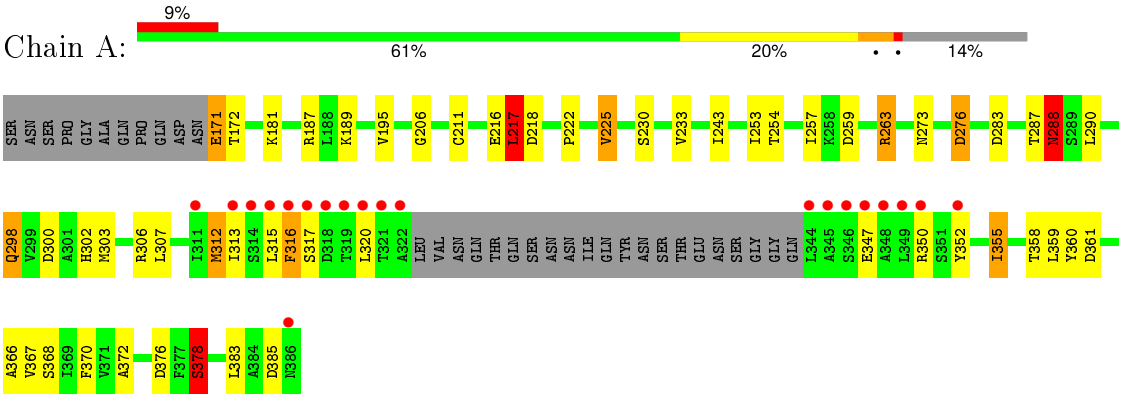
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	o	35	Total O 35 35	0	0
6	p	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

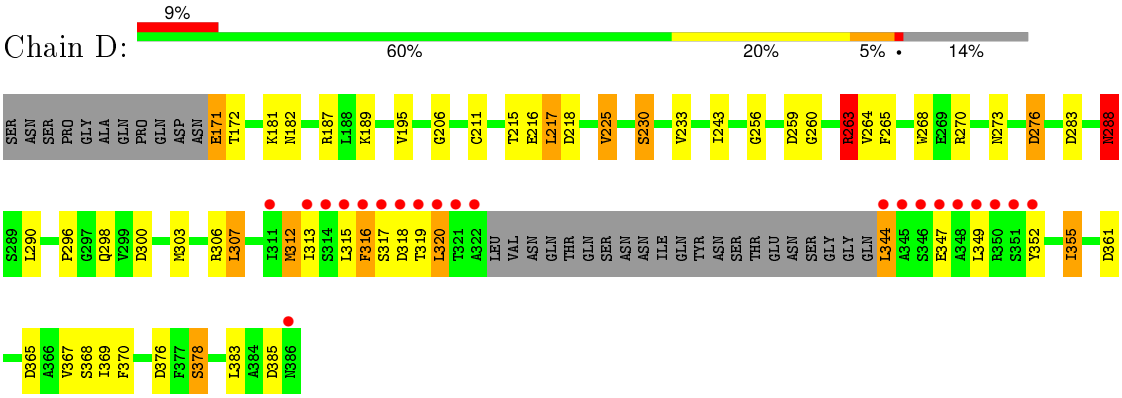
- Molecule 1: TraF protein

Chain A:



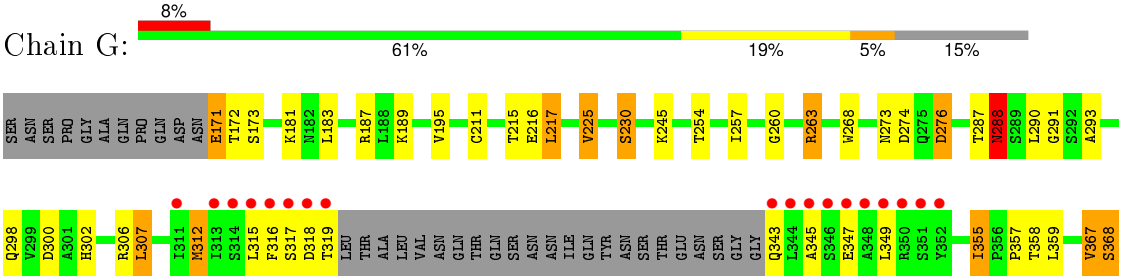
- Molecule 1: TraF protein

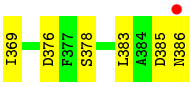
Chain D:



- Molecule 1: TraF protein

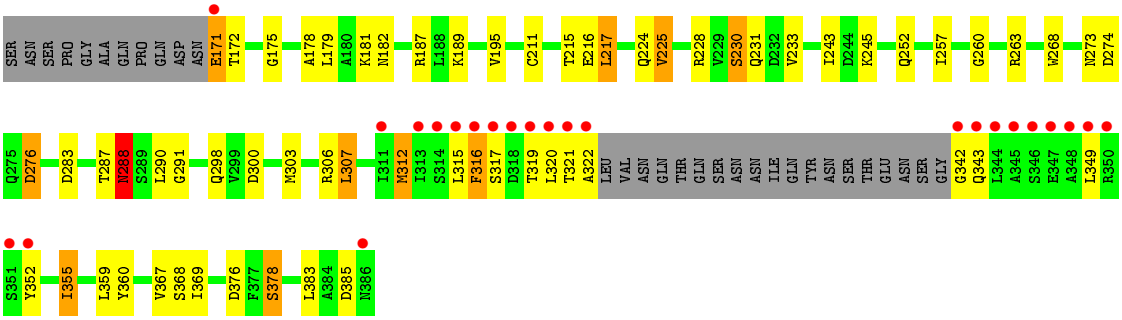
Chain G:





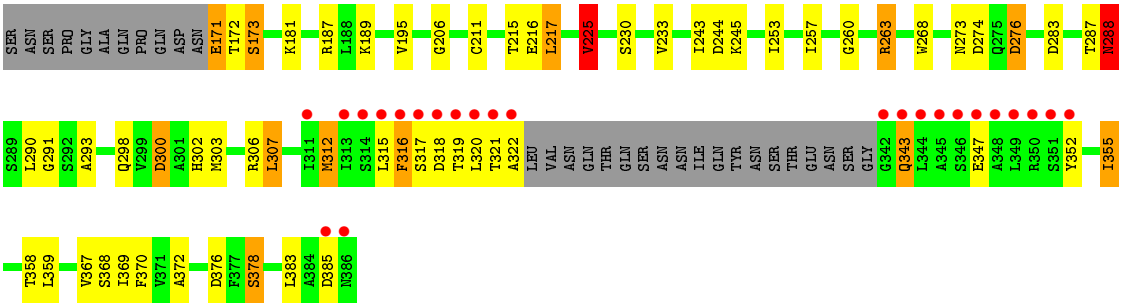
• Molecule 1: TraF protein

Chain J:



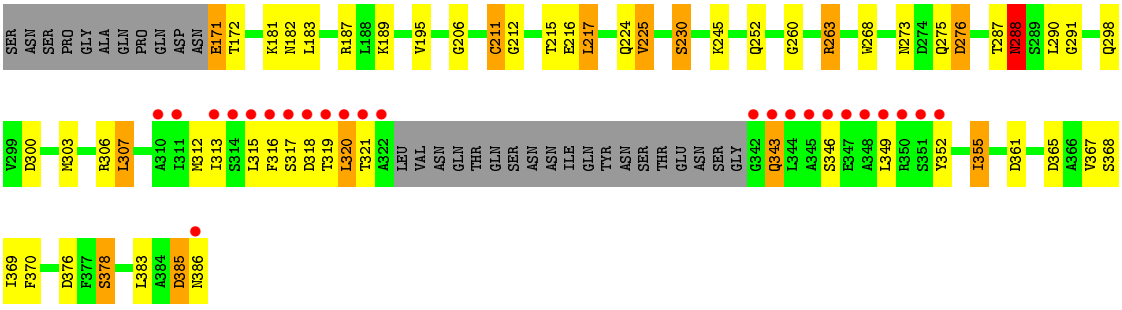
• Molecule 1: TraF protein

Chain M:



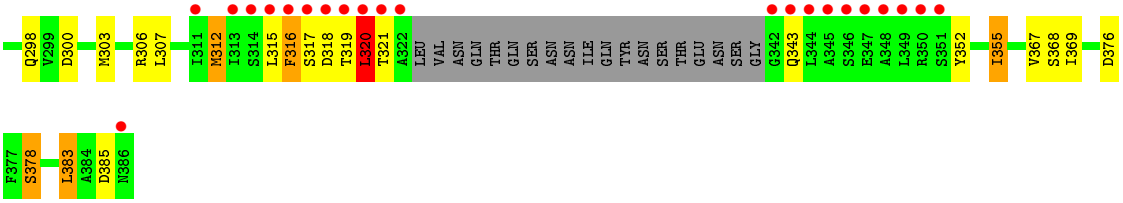
• Molecule 1: TraF protein

Chain P:



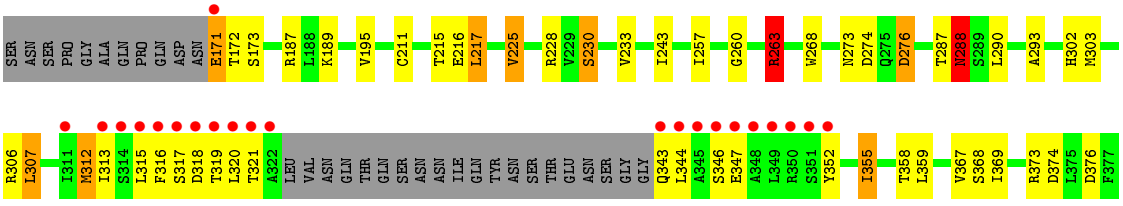
• Molecule 1: TraF protein

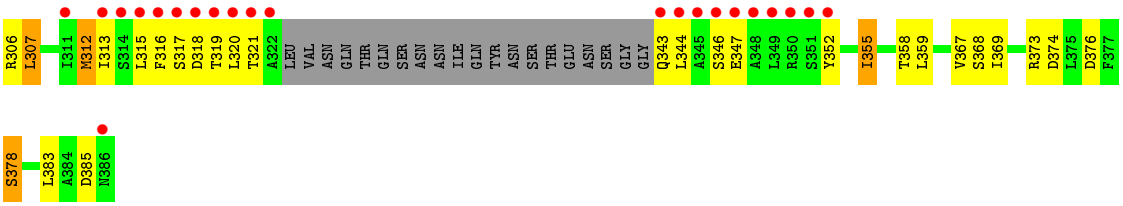
Chain S:



• Molecule 1: TraF protein

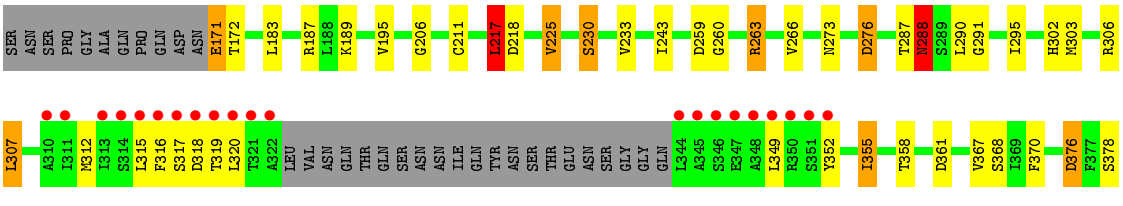
Chain V:

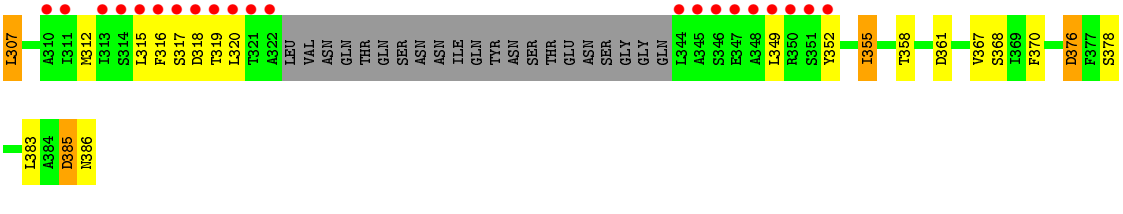




• Molecule 1: TraF protein

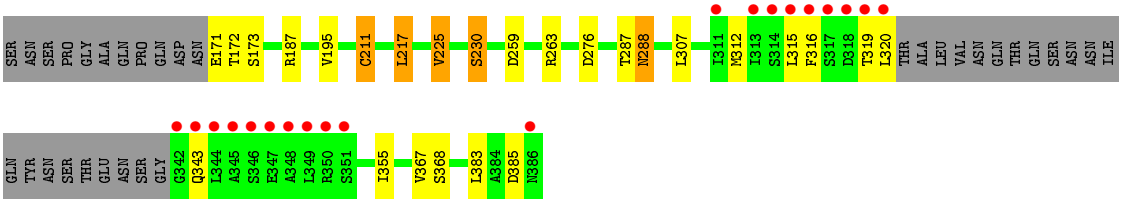
Chain Y:





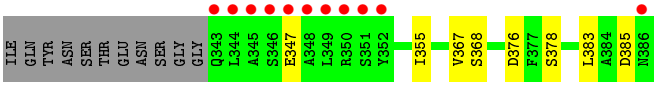
• Molecule 1: TraF protein

Chain b:



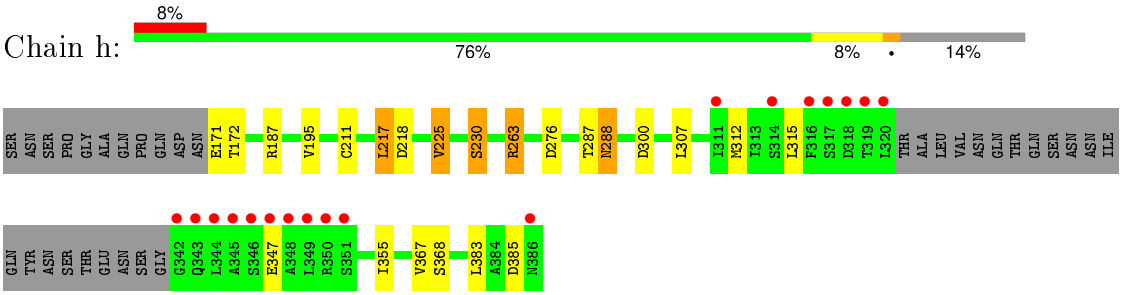
• Molecule 1: TraF protein

Chain e:



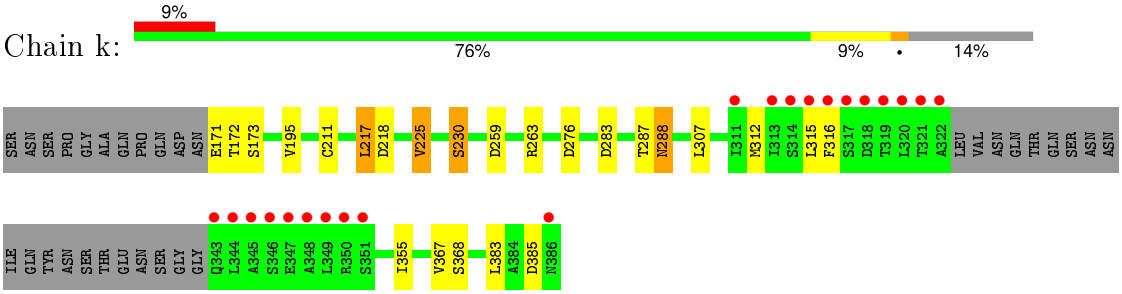
• Molecule 1: TraF protein

Chain h:



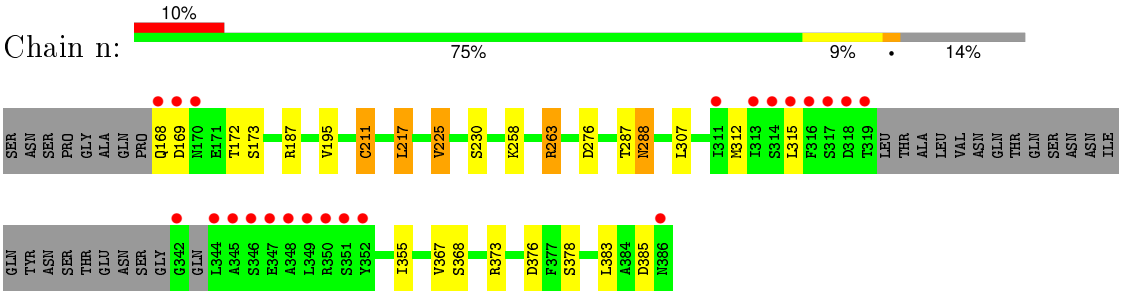
• Molecule 1: TraF protein

Chain k:



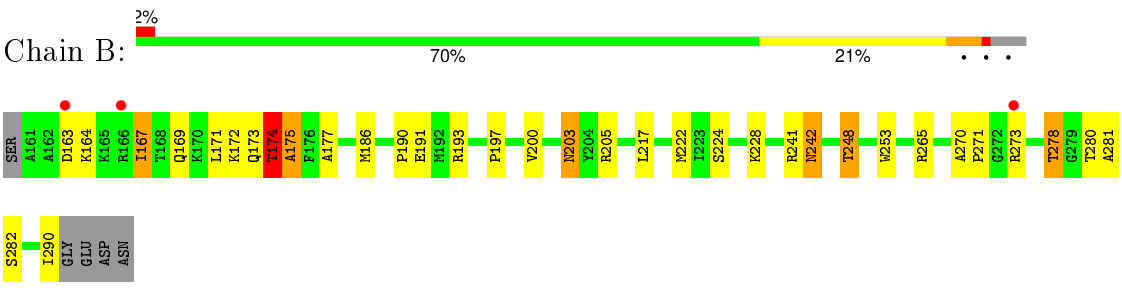
• Molecule 1: TraF protein

Chain n:



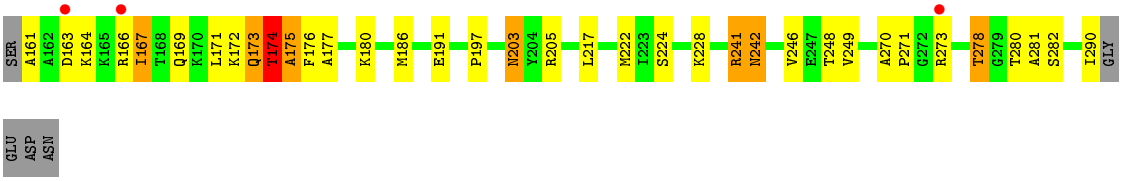
• Molecule 2: TraO protein

Chain B:



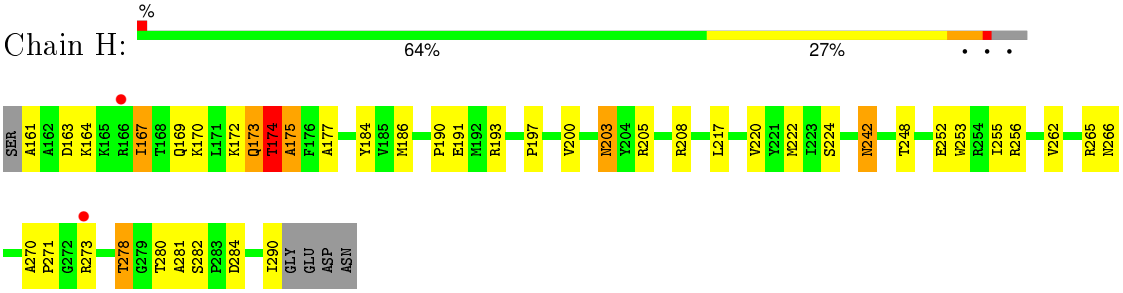
• Molecule 2: TraO protein

Chain E:



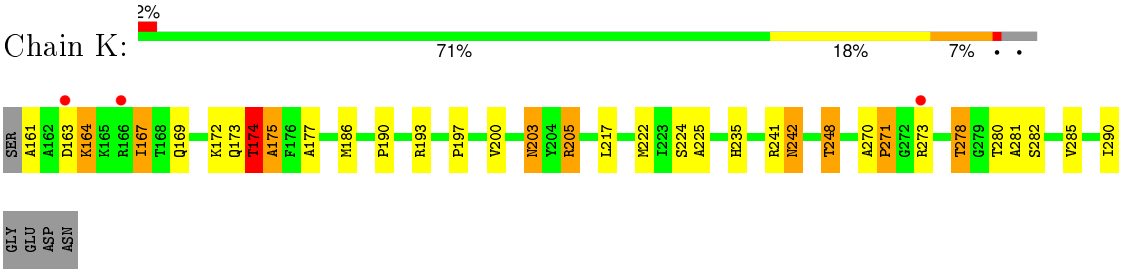
• Molecule 2: TraO protein

Chain H:



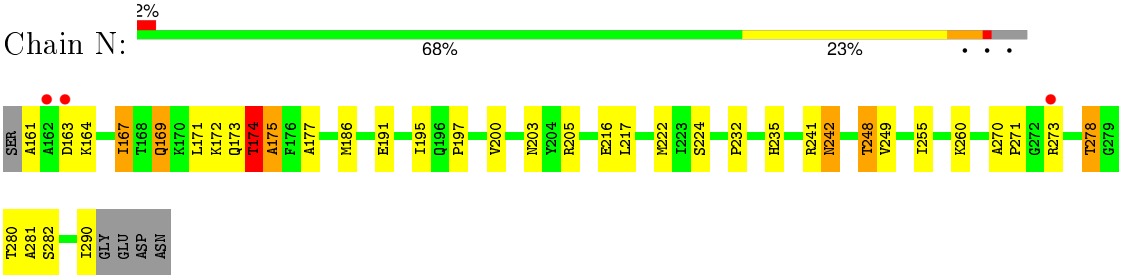
• Molecule 2: TraO protein

Chain K:



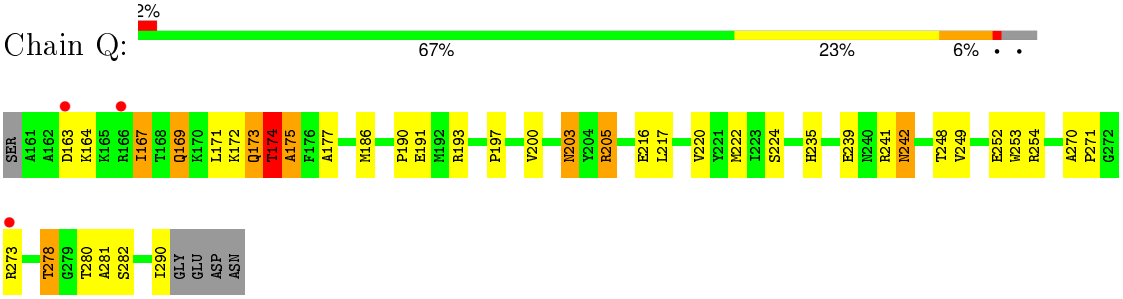
• Molecule 2: TraO protein

Chain N:



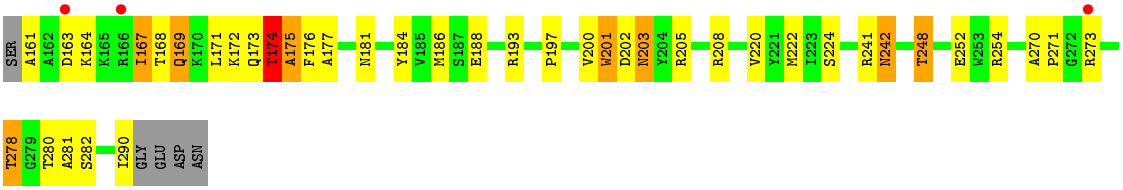
• Molecule 2: TraO protein

Chain Q:



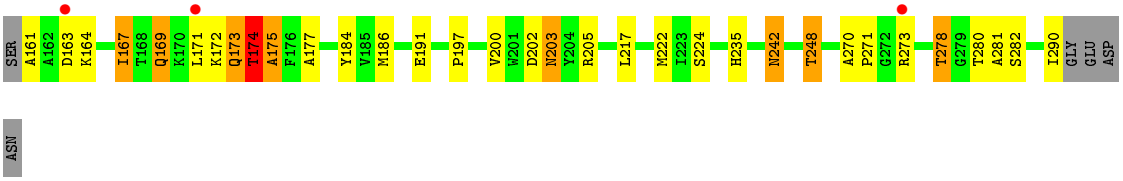
• Molecule 2: TraO protein

Chain T:



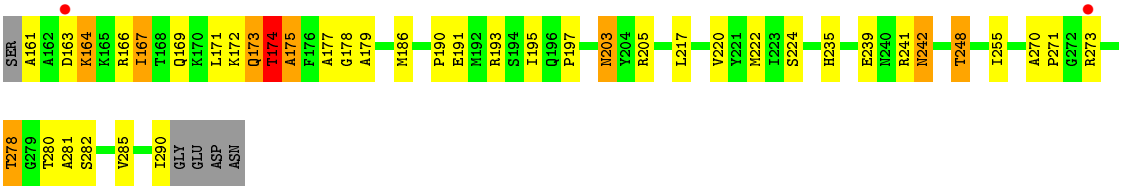
• Molecule 2: TraO protein

Chain W:



• Molecule 2: TraO protein

Chain Z:

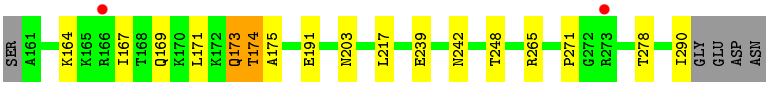


• Molecule 2: TraO protein

Chain c:

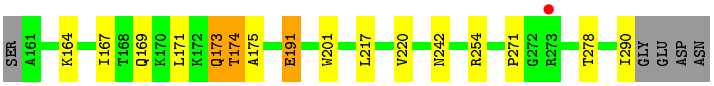
• Molecule 2: TraO protein

Chain f:



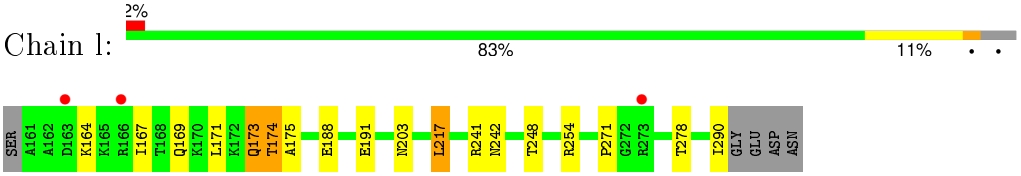
• Molecule 2: TraO protein

Chain i:



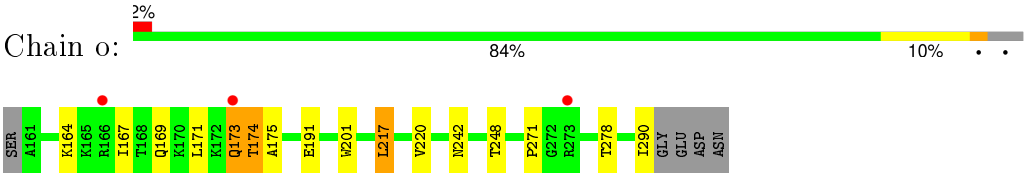
• Molecule 2: TraO protein

Chain l:



• Molecule 2: TraO protein

Chain o:



• Molecule 3: TraN protein

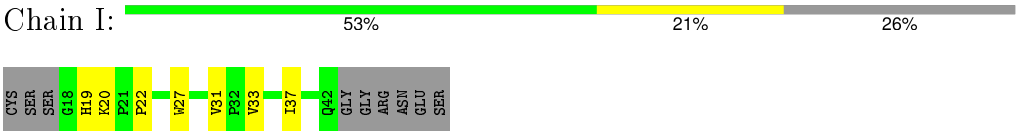
Chain C:

• Molecule 3: TraN protein

Chain F:

• Molecule 3: TraN protein

Chain I:



• Molecule 3: TraN protein

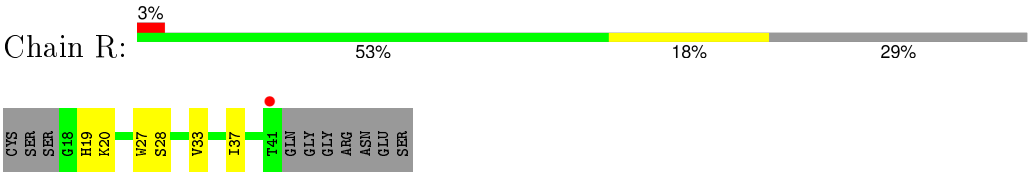
Chain L:

• Molecule 3: TraN protein

Chain O:

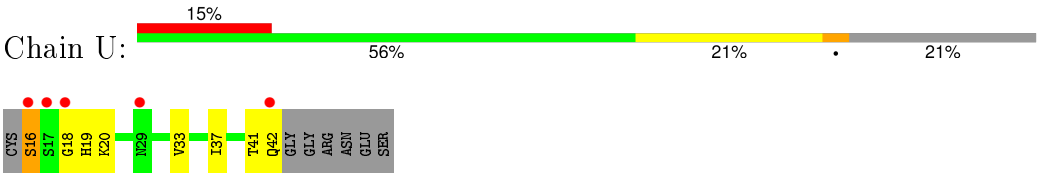
• Molecule 3: TraN protein

Chain R:



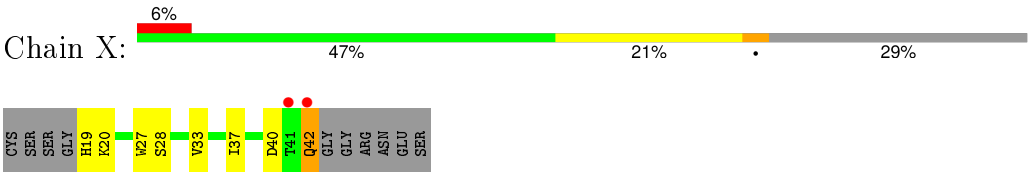
- Molecule 3: TraN protein

Chain U:



- Molecule 3: TraN protein

Chain X:

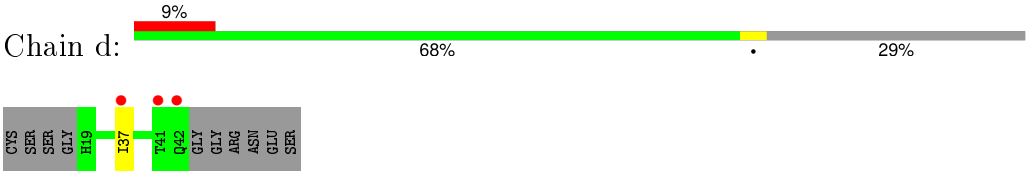


- Molecule 3: TraN protein

Chain a:

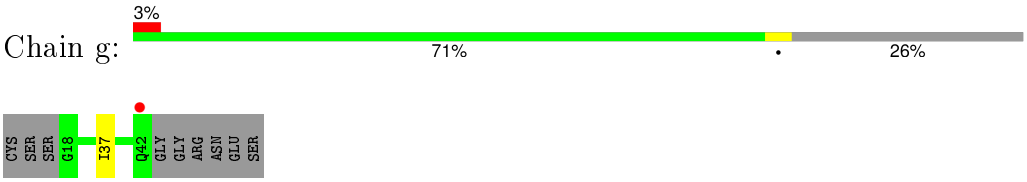
- Molecule 3: TraN protein

Chain d:



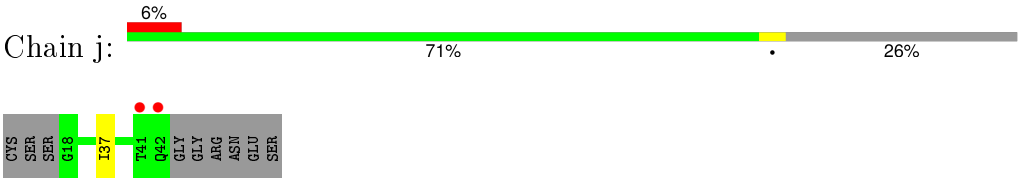
- Molecule 3: TraN protein

Chain g:



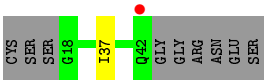
- Molecule 3: TraN protein

Chain j:



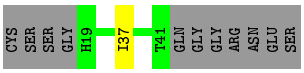
- Molecule 3: TraN protein

Chain m:



- Molecule 3: TraN protein

Chain p:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.26%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.3	EDS
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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	3 of 258767 reflections (0.001%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: LDA, MPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.95	2/1464 (0.1%)	1.04	9/1978 (0.5%)
1	D	0.99	2/1464 (0.1%)	1.11	16/1978 (0.8%)
1	G	0.96	2/1453 (0.1%)	1.01	7/1962 (0.4%)
1	J	0.97	1/1473 (0.1%)	1.03	10/1990 (0.5%)
1	M	0.98	1/1477 (0.1%)	1.05	13/1995 (0.7%)
1	P	0.95	3/1477 (0.2%)	1.03	9/1995 (0.5%)
1	S	0.96	2/1477 (0.1%)	1.04	13/1995 (0.7%)
1	V	0.94	1/1473 (0.1%)	1.03	12/1990 (0.6%)
1	Y	0.97	2/1464 (0.1%)	1.07	13/1978 (0.7%)
1	b	0.95	3/1465 (0.2%)	1.01	10/1978 (0.5%)
1	e	0.99	3/1473 (0.2%)	1.03	10/1990 (0.5%)
1	h	0.99	3/1455 (0.2%)	1.07	13/1966 (0.7%)
1	k	0.96	2/1473 (0.1%)	1.06	12/1990 (0.6%)
1	n	0.98	2/1472 (0.1%)	1.02	11/1986 (0.6%)
2	B	0.96	0/1051	0.97	2/1417 (0.1%)
2	E	0.96	1/1051 (0.1%)	0.97	4/1417 (0.3%)
2	H	1.07	0/1051	0.99	3/1417 (0.2%)
2	K	0.91	0/1051	0.99	3/1417 (0.2%)
2	N	0.88	0/1051	0.95	1/1417 (0.1%)
2	Q	0.93	0/1051	0.97	7/1417 (0.5%)
2	T	0.95	0/1051	0.97	2/1417 (0.1%)
2	W	0.96	0/1051	0.93	2/1417 (0.1%)
2	Z	0.92	0/1051	0.99	4/1417 (0.3%)
2	c	0.93	0/1051	0.98	4/1417 (0.3%)
2	f	0.97	0/1051	0.98	4/1417 (0.3%)
2	i	1.00	1/1051 (0.1%)	0.95	2/1417 (0.1%)
2	l	0.93	0/1051	0.98	6/1417 (0.4%)
2	o	1.01	0/1050	0.94	2/1415 (0.1%)
3	C	0.93	0/208	0.80	0/289
3	F	0.79	0/202	0.75	0/281
3	I	0.86	0/202	0.75	0/281
3	L	0.80	0/220	0.88	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	O	0.68	0/198	0.76	0/276
3	R	0.77	0/193	0.75	0/269
3	U	0.90	0/214	0.93	0/297
3	X	0.71	0/198	0.73	0/276
3	a	0.68	0/198	0.72	0/276
3	d	0.76	0/198	0.77	0/276
3	g	0.86	0/202	0.82	0/281
3	j	0.82	0/202	0.75	0/281
3	m	0.82	0/202	0.75	0/281
3	p	0.78	0/189	0.79	0/264
All	All	0.95	31/38099 (0.1%)	1.00	204/51540 (0.4%)

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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	298	GLN	CD-NE2	-8.19	1.12	1.32
1	e	298	GLN	CD-OE1	-8.10	1.06	1.24
1	A	298	GLN	CD-OE1	-8.09	1.06	1.24
1	n	211	CYS	CB-SG	-7.71	1.69	1.82
1	J	276	ASP	CB-CG	-7.16	1.36	1.51
1	k	276	ASP	CB-CG	-7.06	1.36	1.51
1	M	276	ASP	CB-CG	-6.86	1.37	1.51
1	V	230	SER	CB-OG	-6.80	1.33	1.42
1	h	288	ASN	CB-CG	-6.44	1.36	1.51
1	A	298	GLN	CD-NE2	-6.37	1.17	1.32
2	i	191	GLU	CB-CG	-6.35	1.40	1.52
1	D	276	ASP	CB-CG	-6.32	1.38	1.51
1	P	230	SER	CB-OG	-6.17	1.34	1.42
1	h	276	ASP	CB-CG	-6.16	1.38	1.51
1	S	211	CYS	CB-SG	-6.03	1.72	1.82
1	Y	276	ASP	CB-CG	-5.99	1.39	1.51
1	G	276	ASP	CB-CG	-5.86	1.39	1.51
1	e	276	ASP	CB-CG	-5.84	1.39	1.51
1	P	211	CYS	CB-SG	-5.83	1.72	1.81
1	G	230	SER	CB-OG	-5.80	1.34	1.42
1	b	230	SER	CB-OG	-5.57	1.35	1.42
1	Y	230	SER	CB-OG	-5.50	1.35	1.42
1	n	276	ASP	CB-CG	-5.44	1.40	1.51
1	D	230	SER	CB-OG	-5.43	1.35	1.42
1	b	276	ASP	CB-CG	-5.43	1.40	1.51
1	k	230	SER	CB-OG	-5.38	1.35	1.42
1	P	288	ASN	CB-CG	-5.36	1.38	1.51
1	b	211	CYS	CB-SG	-5.29	1.73	1.81
2	E	246	VAL	CB-CG1	-5.26	1.41	1.52
1	h	230	SER	CB-OG	-5.18	1.35	1.42
1	S	230	SER	CB-OG	-5.03	1.35	1.42

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	217	LEU	CA-CB-CG	10.11	138.54	115.30
1	h	276	ASP	CB-CG-OD1	-9.75	109.53	118.30
1	k	217	LEU	CA-CB-CG	9.54	137.23	115.30
1	S	217	LEU	CA-CB-CG	9.39	136.90	115.30
1	A	217	LEU	CA-CB-CG	9.39	136.89	115.30
1	e	217	LEU	CA-CB-CG	9.37	136.85	115.30
1	M	217	LEU	CA-CB-CG	9.24	136.55	115.30
1	e	276	ASP	CB-CG-OD1	-9.20	110.02	118.30
1	n	217	LEU	CA-CB-CG	9.18	136.42	115.30
1	D	217	LEU	CA-CB-CG	9.13	136.31	115.30
1	e	263	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	M	263	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	D	276	ASP	CB-CG-OD1	-9.00	110.20	118.30
1	J	276	ASP	CB-CG-OD1	-8.84	110.34	118.30
1	J	217	LEU	CA-CB-CG	8.79	135.53	115.30
1	P	217	LEU	CA-CB-CG	8.73	135.37	115.30
1	Y	218	ASP	CB-CG-OD1	8.60	126.04	118.30
1	V	217	LEU	CA-CB-CG	8.60	135.08	115.30
1	h	263	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	b	217	LEU	CA-CB-CG	8.44	134.72	115.30
1	A	276	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	S	263	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	h	217	LEU	CA-CB-CG	8.29	134.37	115.30
1	h	263	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	P	263	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	V	263	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	Y	217	LEU	CA-CB-CG	8.14	134.03	115.30
1	k	263	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	M	263	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	S	288	ASN	CB-CA-C	-7.83	94.74	110.40
1	k	259	ASP	CB-CG-OD1	7.73	125.26	118.30
1	S	259	ASP	CB-CG-OD1	7.65	125.19	118.30
1	J	263	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	Y	276	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	218	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	k	263	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	f	265	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	263	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	218	ASP	CB-CG-OD1	7.20	124.78	118.30
1	G	276	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	S	259	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	M	276	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	n	288	ASN	CB-CA-C	-7.09	96.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	187	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	S	263	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	h	187	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	288	ASN	CB-CA-C	-6.99	96.41	110.40
1	Y	288	ASN	CB-CA-C	-6.92	96.56	110.40
1	e	187	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	288	ASN	CB-CA-C	-6.79	96.82	110.40
1	V	276	ASP	CB-CG-OD1	-6.79	112.19	118.30
2	Z	241	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	Y	259	ASP	CB-CG-OD1	6.78	124.40	118.30
1	k	288	ASN	CB-CA-C	-6.76	96.88	110.40
1	h	288	ASN	CB-CA-C	-6.75	96.89	110.40
2	B	271	PRO	C-N-CA	-6.73	108.16	122.30
1	V	288	ASN	CB-CA-C	-6.73	96.94	110.40
1	J	225	VAL	CB-CA-C	-6.69	98.69	111.40
1	n	263	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	Y	218	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	n	187	ARG	CG-CD-NE	-6.64	97.85	111.80
1	k	218	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	P	263	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	c	254	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	P	276	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	J	288	ASN	CB-CA-C	-6.54	97.32	110.40
1	P	288	ASN	CB-CA-C	-6.49	97.42	110.40
1	G	288	ASN	CB-CA-C	-6.48	97.44	110.40
1	b	276	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	n	263	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	b	288	ASN	CB-CA-C	-6.47	97.46	110.40
1	M	225	VAL	CB-CA-C	-6.47	99.11	111.40
1	D	225	VAL	CB-CA-C	-6.44	99.16	111.40
1	D	187	ARG	CG-CD-NE	-6.41	98.34	111.80
2	K	205	ARG	NE-CZ-NH1	-6.38	117.11	120.30
2	c	271	PRO	C-N-CA	-6.38	108.91	122.30
1	k	276	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	M	288	ASN	CB-CA-C	-6.34	97.73	110.40
1	V	225	VAL	CB-CA-C	-6.33	99.38	111.40
2	N	271	PRO	C-N-CA	-6.31	109.05	122.30
1	D	217	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	Y	376	ASP	CB-CG-OD1	6.24	123.92	118.30
1	D	218	ASP	CB-CG-OD1	6.21	123.89	118.30
2	W	271	PRO	C-N-CA	-6.21	109.26	122.30
1	G	225	VAL	CB-CA-C	-6.17	99.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ASP	CB-CG-OD1	6.17	123.85	118.30
2	K	271	PRO	C-N-CA	-6.17	109.35	122.30
2	Q	271	PRO	C-N-CA	-6.16	109.36	122.30
1	h	218	ASP	CB-CG-OD1	6.15	123.83	118.30
1	V	187	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	b	276	ASP	CB-CA-C	-6.14	98.13	110.40
1	A	187	ARG	CG-CD-NE	-6.13	98.94	111.80
2	E	271	PRO	C-N-CA	-6.11	109.46	122.30
1	M	276	ASP	CB-CA-C	-6.09	98.21	110.40
2	T	203	ASN	N-CA-CB	-6.04	99.73	110.60
1	D	283	ASP	CB-CG-OD1	6.02	123.72	118.30
1	h	225	VAL	CB-CA-C	-6.02	99.97	111.40
2	T	271	PRO	C-N-CA	-6.01	109.68	122.30
1	b	187	ARG	CG-CD-NE	-5.97	99.27	111.80
1	n	225	VAL	CB-CA-C	-5.96	100.07	111.40
1	k	225	VAL	CB-CA-C	-5.95	100.09	111.40
1	e	288	ASN	CB-CA-C	-5.94	98.53	110.40
2	H	203	ASN	CB-CA-C	-5.90	98.59	110.40
2	W	203	ASN	CB-CA-C	-5.89	98.63	110.40
2	H	271	PRO	C-N-CA	-5.88	109.95	122.30
1	S	320	LEU	CA-CB-CG	5.88	128.82	115.30
1	Y	263	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	n	276	ASP	CB-CA-C	-5.86	98.69	110.40
1	n	373	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	Y	225	VAL	CB-CA-C	-5.82	100.34	111.40
2	l	271	PRO	C-N-CA	-5.82	110.09	122.30
1	D	187	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	230	SER	N-CA-CB	-5.77	101.85	110.50
2	E	241	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	G	263	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	b	217	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	P	225	VAL	CB-CA-C	-5.74	100.50	111.40
1	n	217	LEU	CB-CG-CD1	-5.74	101.25	111.00
1	S	276	ASP	CB-CA-C	-5.73	98.93	110.40
1	D	320	LEU	CA-CB-CG	5.73	128.48	115.30
2	i	254	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	k	276	ASP	CB-CA-C	-5.71	98.97	110.40
1	G	263	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	Y	187	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	P	320	LEU	CA-CB-CG	5.66	128.32	115.30
2	Z	203	ASN	CB-CA-C	-5.66	99.08	110.40
1	D	263	ARG	NE-CZ-NH1	5.65	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	187	ARG	CG-CD-NE	-5.65	99.94	111.80
1	J	187	ARG	CG-CD-NE	-5.64	99.94	111.80
1	Y	263	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	J	276	ASP	CB-CA-C	-5.61	99.18	110.40
1	h	276	ASP	N-CA-CB	-5.59	100.54	110.60
1	e	263	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	S	218	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	J	228	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	M	244	ASP	CB-CG-OD1	5.57	123.31	118.30
1	b	263	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	M	217	LEU	CB-CG-CD2	5.55	120.44	111.00
2	c	203	ASN	CB-CA-C	-5.55	99.30	110.40
1	Y	217	LEU	CB-CG-CD1	-5.54	101.58	111.00
2	i	271	PRO	C-N-CA	-5.54	110.67	122.30
1	b	259	ASP	CB-CG-OD1	5.54	123.28	118.30
2	l	203	ASN	CB-CA-C	-5.53	99.33	110.40
2	Z	241	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	M	217	LEU	CB-CG-CD1	-5.53	101.60	111.00
2	l	254	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	l	241	ARG	CG-CD-NE	-5.50	100.24	111.80
1	S	225	VAL	CB-CA-C	-5.50	100.95	111.40
1	S	218	ASP	CB-CG-OD1	5.49	123.24	118.30
2	l	203	ASN	N-CA-CB	-5.49	100.72	110.60
2	E	203	ASN	N-CA-CB	-5.48	100.74	110.60
1	V	228	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	f	271	PRO	C-N-CA	-5.47	110.81	122.30
2	f	203	ASN	CB-CA-C	-5.44	99.52	110.40
1	D	276	ASP	CB-CA-C	-5.44	99.53	110.40
2	B	203	ASN	CB-CA-C	-5.43	99.53	110.40
1	D	259	ASP	CB-CG-OD1	5.43	123.19	118.30
2	E	203	ASN	CB-CA-C	-5.42	99.56	110.40
1	b	225	VAL	CB-CA-C	-5.41	101.12	111.40
1	k	218	ASP	CB-CG-OD1	5.40	123.16	118.30
2	Q	205	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	l	217	LEU	CA-CB-CG	5.37	127.64	115.30
1	P	276	ASP	CB-CA-C	-5.36	99.68	110.40
1	e	225	VAL	CB-CA-C	-5.36	101.22	111.40
1	S	187	ARG	CG-CD-NE	-5.34	100.58	111.80
1	h	217	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	V	276	ASP	CB-CA-C	-5.32	99.77	110.40
1	V	373	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	Q	203	ASN	CB-CA-C	-5.29	99.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	270	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	M	187	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	k	283	ASP	CB-CG-OD1	5.26	123.03	118.30
1	h	300	ASP	CB-CG-OD1	5.26	123.03	118.30
1	V	263	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	V	374	ASP	CB-CG-OD1	5.25	123.03	118.30
1	n	376	ASP	CB-CG-OD1	5.24	123.02	118.30
2	c	203	ASN	N-CA-CB	-5.22	101.20	110.60
2	Z	271	PRO	C-N-CA	-5.22	111.34	122.30
2	K	203	ASN	CB-CA-C	-5.21	99.97	110.40
2	H	208	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	h	218	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	Q	217	LEU	CA-CB-CG	5.18	127.22	115.30
2	o	271	PRO	C-N-CA	-5.15	111.48	122.30
2	Q	205	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	S	187	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	M	187	ARG	CG-CD-NE	-5.13	101.02	111.80
1	D	263	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	V	187	ARG	CG-CD-NE	-5.13	101.03	111.80
1	P	187	ARG	CG-CD-NE	-5.12	101.04	111.80
1	e	218	ASP	CB-CG-OD1	5.12	122.91	118.30
2	o	217	LEU	CA-CB-CG	5.11	127.06	115.30
1	b	230	SER	N-CA-CB	-5.11	102.84	110.50
1	e	376	ASP	CB-CG-OD1	5.09	122.88	118.30
1	J	230	SER	N-CA-CB	-5.09	102.86	110.50
2	Q	254	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	f	239	GLU	CB-CA-C	-5.09	100.22	110.40
1	e	276	ASP	CB-CA-C	-5.09	100.22	110.40
1	G	187	ARG	CG-CD-NE	-5.07	101.14	111.80
1	h	230	SER	N-CA-CB	-5.03	102.96	110.50
1	k	230	SER	N-CA-CB	-5.02	102.97	110.50
1	M	300	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	276	ASP	CB-CA-C	-5.02	100.36	110.40
2	Q	239	GLU	CB-CA-C	-5.01	100.37	110.40
1	n	276	ASP	CB-CG-OD1	-5.00	113.80	118.30

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

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Mol	Chain	Res	Type	Group
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
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	51	0
1	D	1448	0	1434	58	0
1	G	1437	0	1419	51	0
1	J	1457	0	1441	65	0
1	M	1461	0	1445	58	0
1	P	1461	0	1445	57	0
1	S	1461	0	1445	49	0
1	V	1457	0	1442	45	0
1	Y	1448	0	1434	33	0
1	b	1449	0	1433	0	0
1	e	1457	0	1442	0	0
1	h	1439	0	1416	0	0
1	k	1457	0	1442	0	0
1	n	1457	0	1431	0	0
2	B	1033	0	1032	31	0
2	E	1033	0	1032	34	0
2	H	1033	0	1032	38	0
2	K	1033	0	1032	36	0
2	N	1033	0	1032	37	0
2	Q	1033	0	1032	32	0
2	T	1033	0	1032	38	1
2	W	1033	0	1032	36	0
2	Z	1033	0	1032	33	0
2	c	1033	0	1032	0	0
2	f	1033	0	1032	0	0
2	i	1033	0	1032	0	0
2	l	1033	0	1032	0	0
2	o	1032	0	1028	0	0
3	C	200	0	190	8	0
3	F	194	0	185	6	0
3	I	194	0	185	11	1
3	L	212	0	200	11	0
3	O	190	0	182	9	0
3	R	185	0	177	10	0
3	U	206	0	195	14	0
3	X	190	0	182	12	0
3	a	190	0	182	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	d	190	0	182	0	0
3	g	194	0	185	0	0
3	j	194	0	185	0	0
3	m	194	0	185	0	0
3	p	181	0	174	0	0
4	D	8	0	14	6	0
4	h	8	0	14	0	0
4	k	8	0	14	0	0
5	J	16	0	31	33	0
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	0	0
6	c	31	0	0	0	0
6	d	3	0	0	0	0
6	e	52	0	0	0	0
6	f	28	0	0	0	0
6	g	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	h	50	0	0	0	0
6	i	21	0	0	0	0
6	j	11	0	0	0	0
6	k	56	0	0	0	0
6	l	37	0	0	0	0
6	m	8	0	0	0	0
6	n	50	0	0	0	0
6	o	35	0	0	0	0
6	p	12	0	0	0	0
All	All	38842	0	37209	697	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 (697) 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: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:G:298:GLN:HE22	3:L:20:LYS:H	1.09	0.99
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:W:278:THR:HG22	2:W:280:THR:H	1.32	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
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:J:178:ALA:CB	5:J:1:LDA:HM11	1.98	0.90
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:298:GLN:HE22	3:X:20:LYS:H	1.18	0.88
1:A:316:PHE:C	1:A:320:LEU:HG	1.93	0.88
1:P:298:GLN:NE2	3:U:20:LYS:H	1.72	0.86
2:K:278:THR:HG22	2:K:280:THR:H	1.40	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
3:C:17:SER:HB2	6:C:1003:HOH:O	1.76	0.85
1:P:355:ILE:CD1	1:S:260:GLY:HA3	2.06	0.85
1:M:317:SER:HA	1:M:320:LEU:HG	1.56	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
1:A:347:GLU:CG	1:D:349:LEU:HD23	2.04	0.83
2:Z:242:ASN:HD22	2:Z:242:ASN:H	1.25	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: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: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:Q:186:MSE:CE	3:R:33:VAL:HG22	2.10	0.81
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:H:186:MSE:CE	3:I:33:VAL:HG22	2.11	0.80
2:T:205:ARG:NH1	2:T:281:ALA:O	2.15	0.80
1:J:316:PHE:C	1:J:320:LEU:HG	2.03	0.79
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:N:174:THR:O	6:N:1020:HOH:O	1.99	0.78
2:B:242:ASN:HD22	2:B:242:ASN:H	1.28	0.78
1:A:355:ILE:CD1	1:D:260:GLY:HA3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Q:278:THR:HG21	2:Q:282:SER:O	1.85	0.77
2:W:186:MSE:HE3	3:X:33:VAL:HG22	1.66	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
1:M:355:ILE:CD1	1:P:260:GLY:HA3	2.15	0.76
2:H:170:LYS:HD2	6:H:296:HOH:O	1.84	0.76
1:P:288:ASN:HB3	1:P:290:LEU:H	1.50	0.76
2:Z:278:THR:CG2	2:Z:280:THR:H	1.98	0.75
1:V:343:GLN:CG	1:V:344:LEU:H	2.00	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
2:W:186:MSE:CE	3:X:33:VAL:HG22	2.17	0.75
1:V:288:ASN:HB3	1:V:290:LEU:H	1.51	0.75
1:A:254:THR:O	5:J:1:LDA:O1	2.05	0.74
1:M:343:GLN:HG2	1:P:346:SER:OG	1.87	0.74
6:D:398:HOH:O	5:J:1:LDA:H102	1.85	0.74
1:D:288:ASN:HB3	1:D:290:LEU:H	1.51	0.74
2:K:186:MSE:CE	3:L: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:G:288:ASN:HB3	1:G:290:LEU:H	1.52	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:HD22	2:W:242:ASN:H	1.36	0.73
2:W:203:ASN:HB3	2:W:205:ARG:H	1.52	0.72
2:K:270:ALA:HB1	2:K:273:ARG:HG2	1.71	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
6:Y:1308:HOH:O	2:Z:167:ILE:HD13	1.89	0.72
4:D:1:MPD:H52	4:D:1:MPD:O2	1.89	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:317:SER:HA	1:D:320:LEU:HG	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ARG:HG3	1:D:355:ILE:HG12	1.73	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: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:V:317:SER:HA	1:V:320:LEU:HG	1.72	0.70
1:S:288:ASN:HB3	1:S:290:LEU:H	1.56	0.70
2:K:186:MSE:HE3	3:L:33:VAL:HG22	1.73	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: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
1:J:355:ILE:CD1	1:M:260:GLY:HA3	2.23	0.69
2:E:242:ASN:HD22	2:E:242:ASN:H	1.41	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: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
1:S:320:LEU:HD22	1:V:318:ASP:OD2	1.94	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
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:W:278:THR:CG2	2:W:280:THR:H	2.06	0.66
2:K:278:THR:CG2	2:K:280:THR:H	2.08	0.66
2:Z:270:ALA:HB1	2:Z:273:ARG:HG2	1.76	0.66
1:D:182:ASN:ND2	6:D:717:HOH:O	2.27	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
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:M:317:SER:CA	1:M:320:LEU:HG	2.25	0.65
2:H:222:MSE:HE3	2:H:224:SER:HA	1.77	0.65
1:J:179:LEU:HB2	5:J:1:LDA:H11	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:175:GLY:CA	5:J:1:LDA:HM12	2.26	0.65
2:N:172:LYS:NZ	2:N:172:LYS:HB3	2.11	0.65
2:N:203:ASN:HB3	2:N:205:ARG:H	1.62	0.65
1:G:273:ASN:OD1	1:G:276:ASP:HB2	1.97	0.65
2:E:222:MSE:HE3	2:E:224:SER:HA	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
1:G:306:ARG:CG	1:G:355:ILE:HG12	2.26	0.64
2:E:172:LYS:HB3	2:E:172:LYS:NZ	2.12	0.64
2:N:278:THR:CG2	2:N:280:THR:H	2.10	0.64
2:K:203:ASN:HB3	2:K:205:ARG:H	1.62	0.64
2:Q:203:ASN:HB3	2:Q:205:ARG:H	1.63	0.64
2:H:172:LYS:HB3	2:H:172:LYS:NZ	2.13	0.64
2:Q:172:LYS:HB3	2:Q:172:LYS:NZ	2.11	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:M:376:ASP:OD1	1:M:378:SER:HB2	1.99	0.63
1:S:298:GLN:NE2	3:X:20:LYS:H	1.93	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:T:186:MSE:HE3	3:U:33:VAL:CG2	2.26	0.62
2:N:242:ASN:H	2:N:242:ASN:HD22	1.45	0.62
2:E:270:ALA:HB1	2:E:273:ARG:HG2	1.81	0.62
2:E:278:THR:CG2	2:E:280:THR:H	2.11	0.62
2:B:172:LYS:HB3	2:B:172:LYS:NZ	2.13	0.62
2:H:242:ASN:HD22	2:H:242:ASN:H	1.46	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: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
1:S:298:GLN:HE22	3:X:20:LYS:N	1.94	0.61
2:H:186:MSE:HE1	2:H:197:PRO:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:THR:HG22	1:J:291:GLY:HA3	1.81	0.61
1:J:216:GLU:OE2	1:M:288:ASN:ND2	2.34	0.61
1:J:179:LEU:HA	5:J:1:LDA:H32	1.83	0.60
1:J:316:PHE:O	1:J:320:LEU:HG	2.01	0.60
1:J:288:ASN:HB3	1:J:290:LEU:H	1.66	0.60
2:T:172:LYS:C	2:T:174:THR:N	2.54	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:D:320:LEU:HD22	1:G:318:ASP:CG	2.21	0.60
2:B:186:MSE:HE3	3:C:33:VAL:HG13	1.84	0.60
1:Y:306:ARG:CG	1:Y:355:ILE:HG12	2.32	0.59
1:V:306:ARG:CG	1:V:355:ILE:HG12	2.32	0.59
1:J:175:GLY:O	5:J:1:LDA:HM12	1.96	0.59
2:B:278:THR:CG2	2:B:280:THR:H	2.12	0.59
1:S:306:ARG:CG	1:S:355:ILE:HG12	2.32	0.59
2:H:172:LYS:HZ1	2:H:172:LYS:HB3	1.67	0.59
1:A:171:GLU:OE2	1:A:171:GLU:N	2.36	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
2:B:203:ASN:HB3	2:B:205:ARG:H	1.66	0.59
1:A:376:ASP:OD1	1:A:378:SER:HB2	2.02	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:Z:172:LYS:HB3	2:Z:172:LYS:NZ	2.17	0.59
2:T:222:MSE:HE3	2:T:224:SER:HA	1.85	0.59
2:N:186:MSE:HE3	3:O:33:VAL:CG2	2.30	0.58
4:D:1:MPD:HM3	2:E:228:LYS:NZ	2.17	0.58
2:Z:172:LYS:C	2:Z:174:THR:N	2.54	0.58
2:Q:177:ALA:O	2:Q:205:ARG:NH2	2.36	0.58
1:A:288:ASN:HB3	1:A:290:LEU:H	1.68	0.58
1:V:343:GLN:OE1	1:V:344:LEU:HB3	2.04	0.58
2:W:172:LYS:C	2:W:174:THR:N	2.56	0.58
2:Z:203:ASN:HB3	2:Z:205:ARG:H	1.69	0.58
1:G:306:ARG:HG3	1:G:355:ILE:HG12	1.86	0.58
2:H:172:LYS:C	2:H:174:THR:N	2.56	0.58
2:K:172:LYS:NZ	2:K:172:LYS:HB3	2.17	0.58
1:A:298:GLN:HE21	1:A:360:TYR:HD2	1.52	0.58
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
2:K:241:ARG:NH2	6:K:298:HOH:O	2.35	0.57
4:D:1:MPD:CM	2:E:228:LYS:NZ	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:242:ASN:HD22	2:T:242:ASN:H	1.53	0.57
1:M:320:LEU:HA	1:P:318:ASP:OD2	2.05	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:A:181:LYS:HE3	1:D:171:GLU:HA	1.86	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: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:V:317:SER:CA	1:V:320:LEU:HG	2.34	0.56
1:S:376:ASP:OD1	1:S:378:SER:HB2	2.05	0.56
2:K:186:MSE:HE1	2:K:197:PRO:HG2	1.88	0.56
2:W:242:ASN:N	2:W:242:ASN:HD22	2.02	0.56
2:H:278:THR:CG2	2:H:280:THR:H	2.16	0.56
2:B:186:MSE:CE	3:C:33:VAL:HG13	2.34	0.56
1:P:306:ARG:HG2	1:P:355:ILE:HG12	1.88	0.56
1:D:376:ASP:OD1	1:D:378:SER:HB2	2.05	0.56
2:Q:242:ASN:HD22	2:Q:242:ASN:N	2.03	0.56
1:P:171:GLU:HA	6:P:1052:HOH:O	2.06	0.56
2:Q:175:ALA:HB3	2:Q:282:SER:HA	1.88	0.56
2:E:172:LYS:HZ1	2:E:172:LYS:HB3	1.69	0.56
1:M:245:LYS:HE3	2:Q:241:ARG:O	2.06	0.55
2:B:172:LYS:C	2:B:174:THR:N	2.57	0.55
2:B:186:MSE:HE3	3:C:33:VAL:CG2	2.35	0.55
2:E:172:LYS:C	2:E:174:THR:N	2.60	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:H:175:ALA:HB3	2:H:282:SER:HA	1.87	0.55
1:G:376:ASP:OD1	1:G:378:SER:HB2	2.07	0.55
2:K:175:ALA:HB3	2:K:282:SER:HA	1.88	0.55
2:T:174:THR:HG23	3:U:42:GLN:HB2	1.89	0.55
1:P:171:GLU:CA	6:P:1052:HOH:O	2.55	0.55
1:S:273:ASN:OD1	1:S:276:ASP:HB2	2.07	0.55
1:Y:171:GLU:OE2	1:Y:171:GLU:C	2.46	0.55
1:Y:316:PHE:O	1:Y:320:LEU:N	2.35	0.54
2:T:181:ASN:O	2:T:201:TRP:HB2	2.06	0.54
2:B:172:LYS:HB3	2:B:172:LYS:HZ1	1.72	0.54
2:Q:172:LYS:C	2:Q:174:THR:N	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:317:SER:CA	1:S:320:LEU:HG	2.36	0.54
1:S:300:ASP:HB2	3:X:19:HIS:CE1	2.42	0.54
1:D:265:PHE:H	5:J:1:LDA:H101	1.73	0.54
1:D:171:GLU:N	1:D:171:GLU:OE2	2.41	0.54
1:P:245:LYS:HE3	2:T:241:ARG:O	2.07	0.54
1:J:306:ARG:HG3	1:J:355:ILE:HG12	1.89	0.54
1:V:215:THR:HG22	1:Y:291:GLY:HA3	1.90	0.54
2:Z:166:ARG:NH1	6:Z:464:HOH:O	2.41	0.54
2:W:172:LYS:O	2:W:174:THR:N	2.41	0.53
2:W:177:ALA:O	2:W:205:ARG:NH2	2.42	0.53
1:V:343:GLN:HG2	1:V:344:LEU:N	2.22	0.53
4:D:1:MPD:C5	4:D:1:MPD:O2	2.56	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:Q:270:ALA:HB1	2:Q:273:ARG:HG2	1.91	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
2:N:175:ALA:HB3	2:N:282:SER:HA	1.91	0.53
2:E:175:ALA:HB3	2:E: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:T:177:ALA:O	2:T:205:ARG:NH2	2.42	0.53
1:J:320:LEU:CD2	1:M:318:ASP:OD2	2.57	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
1:A:254:THR:HB	5:J:1:LDA:O1	2.09	0.53
2:T:203:ASN:HB3	2:T:205:ARG:H	1.73	0.53
1:G:216:GLU:OE2	1:J:288:ASN:ND2	2.42	0.53
1:V:171:GLU:C	1:V:171:GLU:OE2	2.48	0.52
2:B:242:ASN:N	2:B:242:ASN:HD22	2.03	0.52
2:Z:175:ALA:HB3	2:Z:282:SER:HA	1.90	0.52
2:N:177:ALA:O	2:N:205:ARG:NH2	2.43	0.52
2:K:270:ALA:CB	2:K:273:ARG:HG2	2.38	0.52
1:S:320:LEU:HD22	1:V:318:ASP:CG	2.30	0.52
2:W:186:MSE:HE1	2:W:197:PRO:HD2	1.91	0.52
2:B:222:MSE:HE3	2:B:224:SER:HA	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:J:298:GLN:NE2	3:O:20:LYS:H	1.96	0.52
2:B:175:ALA:HB3	2:B:282:SER:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:171:GLU:N	6:V:396:HOH:O	2.43	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: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:J:320:LEU:HD22	1:M:318:ASP:CG	2.29	0.51
1:P:320:LEU:HD22	1:S:318:ASP:CG	2.31	0.51
2:N:172:LYS:C	2:N:174:THR:N	2.63	0.51
1:A:288:ASN:ND2	2:N:216:GLU:OE2	79.06	0.51
2:T:163:ASP:O	2:T:167:ILE:HG22	2.10	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: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:M:316:PHE:O	1:M:320:LEU:N	2.43	0.51
2:H:172:LYS:O	2:H:174:THR:N	2.43	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
1:Y:171:GLU:OE2	1:Y:171:GLU:CA	2.58	0.51
1:D:344:LEU:HG	1:G:345:ALA:HB1	1.92	0.51
2:Q:172:LYS:HB3	2:Q:172:LYS:HZ1	1.75	0.51
2:Q:190:PRO:O	2:Q:193:ARG:HG3	2.11	0.51
1:Y:273:ASN:OD1	1:Y:276:ASP:HB2	2.10	0.51
1:S:283:ASP:HB3	1:Y:183:LEU:O	2.10	0.51
2:Z:172:LYS:O	2:Z:174:THR:N	2.44	0.50
2:N:222:MSE:SE	2:N:248:THR:HG21	2.60	0.50
1:S:171:GLU:CA	1:S:171:GLU:OE2	2.59	0.50
1:D:273:ASN:OD1	1:D:276:ASP:HB2	2.10	0.50
2:Q:186:MSE:HE2	3:R:33:VAL:HG22	1.91	0.50
1:P:216:GLU:OE2	1:S:288:ASN:ND2	2.45	0.50
2:Q:186:MSE:HE3	3:R:33:VAL:CG2	2.38	0.50
1:M:283:ASP:HB3	1:S:183:LEU:O	2.11	0.50
2:T:222:MSE:SE	2:T:248:THR:HG21	2.62	0.50
1:Y:171:GLU:N	1:Y:171:GLU:OE2	2.45	0.50
1:G:268:TRP:CD1	1:G:369:ILE:HG12	2.46	0.50
1:M:171:GLU:C	1:M:171:GLU:OE2	2.50	0.50
2:Q:186:MSE:HE1	2:Q:197:PRO:HG2	1.94	0.50
2:Z:242:ASN:H	2:Z:242:ASN:ND2	2.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:233:VAL:HB	1:V:243:ILE:HB	1.93	0.50
1:M:298:GLN:HE22	3:R:20:LYS:N	1.94	0.50
1:A:216:GLU:OE2	1:D:288:ASN:ND2	2.45	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
2:T:172:LYS:O	2:T:174:THR:N	2.45	0.50
2:N:222:MSE:HE3	2:N:224:SER:HA	1.93	0.49
1:S:171:GLU:C	1:S:171:GLU:OE2	2.50	0.49
2:N:186:MSE:HE3	3:O:33:VAL:HG13	1.92	0.49
1:S:288:ASN:HB3	1:S:290:LEU:N	2.27	0.49
1:S:171:GLU:N	1:S:171:GLU:OE2	2.45	0.49
1:D:233:VAL:HB	1:D:243:ILE:HB	1.93	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:171:GLU:C	1:P:171:GLU:OE2	2.50	0.49
2:H:163:ASP:O	2:H:167:ILE:HG22	2.11	0.49
1:Y:376:ASP:OD1	1:Y:378:SER:HB2	2.12	0.49
2:Q:242:ASN:ND2	2:Q:242:ASN:H	2.07	0.49
1:J:181:LYS:HE3	1:M:171:GLU:HA	1.94	0.49
1:D:265:PHE:H	5:J:1:LDA:C11	2.25	0.49
1:M:273:ASN:CG	1:M:276:ASP:HB2	2.33	0.49
2:H:186:MSE:HE3	3:I:33:VAL:HG13	1.94	0.49
2:K:186:MSE:HE2	3:L:33:VAL:HG22	1.92	0.49
1:A:233:VAL:HB	1:A:243:ILE:HB	1.95	0.49
1:J:312:MSE:HG2	1:M:307:LEU:CD2	2.43	0.49
2:W:163:ASP:O	2:W:167:ILE:HG22	2.12	0.49
2:Z:172:LYS:HB3	2:Z:172:LYS:HZ1	1.77	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
2:W:222:MSE:SE	2:W:248:THR:HG21	2.63	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:Z:222:MSE:HE3	2:Z:224:SER:HA	1.95	0.48
2:K:172:LYS:C	2:K:174:THR:N	2.64	0.48
1:J:171:GLU:C	1:J:171:GLU:OE2	2.52	0.48
1:J:312:MSE:HG2	1:M:307:LEU:HD21	1.95	0.48
2:Z:239:GLU:HG3	6:Z:297:HOH:O	2.12	0.48
1:M:263:ARG:CD	1:M:293:ALA:O	2.62	0.48
2:Z:163:ASP:O	2:Z:167:ILE:HG22	2.13	0.48
2:K:163:ASP:O	2:K:167:ILE:HG22	2.14	0.48
2:E:186:MSE:CE	3:F:33:VAL:HG13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:186:MSE:CE	2:W:197:PRO:HG2	2.44	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
1:Y:217:LEU:HD13	1:Y:361:ASP:HB3	1.94	0.48
2:Z:186:MSE:HE1	2:Z:197:PRO:HG2	1.94	0.48
1:P:320:LEU:CD2	1:S:318:ASP:OD2	2.61	0.48
1:V:171:GLU:CA	1:V:171:GLU:OE2	2.62	0.48
3:U:16:SER:HA	6:U:891:HOH:O	2.14	0.48
2:H:186:MSE:CE	2:H:197:PRO:HG2	2.43	0.48
1:V:171:GLU:OE2	1:V:171:GLU:N	2.46	0.48
1:J:171:GLU:N	1:J:171:GLU:OE2	2.47	0.48
1:D:265:PHE:H	5:J:1:LDA:C10	2.27	0.48
2:N:161:ALA:HB1	2:N:163:ASP:OD1	2.14	0.48
1:J:257:ILE:HD13	1:J:359:LEU:HB2	1.94	0.48
1:A:317:SER:N	1:A:320:LEU:HG	2.26	0.47
2:T:175:ALA:HB3	2:T:282:SER:HA	1.95	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:N:186:MSE:CE	2:N:197:PRO:HD2	2.44	0.47
2:H:200:VAL:HG23	3:I:33:VAL:HG11	1.96	0.47
1:D:171:GLU:OE2	1:D:171:GLU:C	2.53	0.47
1:P:171:GLU:N	1:P:171:GLU:OE2	2.47	0.47
1:M:171:GLU:N	1:M:171:GLU:OE2	2.47	0.47
2:H:252:GLU:HG3	2:H:265:ARG:HG2	1.96	0.47
2:N:172:LYS:HZ1	2:N:172:LYS:HB3	1.76	0.47
1:V:347:GLU:HG3	1:Y:349:LEU:HD23	1.95	0.47
1:V:268:TRP:CD1	1:V:369:ILE:HG12	2.49	0.47
1:M:171:GLU:CA	1:M:171:GLU:OE2	2.63	0.47
1:M:312:MSE:HG2	1:P:307:LEU:HD21	1.96	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: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:D:171:GLU:OE2	1:D:171:GLU:CA	2.62	0.47
2:Z:177:ALA:O	2:Z:205:ARG:NH2	2.48	0.47
2:W:242:ASN:H	2:W:242:ASN:ND2	2.08	0.47
2:H:222:MSE:HB3	2:H:253:TRP:CZ3	2.49	0.47
1:J:273:ASN:CG	1:J:276:ASP:HB2	2.35	0.47
2:H:161:ALA:HB1	2:H:163:ASP:OD1	2.14	0.47
1:G:343:GLN:OE1	1:J:342:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:HIS:HE1	1:G:358:THR:OG1	1.98	0.47
2:K:242:ASN:N	2:K:242:ASN:HD22	2.10	0.47
1:J:274:ASP:OD1	2:N:235:HIS:HA	2.15	0.47
2:W:175:ALA:HB3	2:W:282:SER:HA	1.96	0.47
1:P:306:ARG:HG3	1:P:355:ILE:HG12	1.97	0.47
2:E:186:MSE:HE1	2:E:197:PRO:HG2	1.96	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:J:231:GLN:HG2	6:K:296:HOH:O	2.14	0.47
2:K:186:MSE:CE	2:K:197:PRO:HG2	2.44	0.46
1:G:189:LYS:HB3	1:G:189:LYS:HE2	1.66	0.46
1:Y:316:PHE:O	1:Y:319:THR:N	2.47	0.46
2:E:166:ARG:NH2	6:E:297:HOH:O	2.48	0.46
2:B:186:MSE:HE1	2:B:197:PRO:HG2	1.98	0.46
1:D:355:ILE:HD12	1:G:260:GLY:HA3	1.97	0.46
1:G:171:GLU:OE2	1:G:171:GLU:C	2.53	0.46
2:T:186:MSE:HE1	2:T:197:PRO:HG2	1.98	0.46
1:J:171:GLU:CA	1:J:171:GLU:OE2	2.63	0.46
1:M:302:HIS:HE1	1:M:358:THR:OG1	1.99	0.46
2:B:242:ASN:ND2	2:B:242:ASN:H	2.05	0.46
2:W:270:ALA:CB	2:W:273:ARG:HG2	2.45	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
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:S:316:PHE:O	1:S:319:THR:N	2.49	0.46
1:S:181:LYS:HE3	1:V:171:GLU:HA	1.98	0.46
1:D:273:ASN:CG	1:D:276:ASP:HB2	2.36	0.46
2:H:190:PRO:O	2:H:193:ARG:HG3	2.16	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: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
2:K:190:PRO:O	2:K:193:ARG:HG3	2.16	0.46
1:S:306:ARG:HG3	1:S:355:ILE:HG12	1.97	0.46
1:M:181:LYS:HE3	1:P:171:GLU:HA	1.97	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
1:M:233:VAL:HB	1:M:243:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:1:MPD:CM	2:E:228:LYS:HZ3	2.29	0.45
1:J:189:LYS:HE2	1:J:189:LYS:HB3	1.73	0.45
1:G:273:ASN:CG	1:G:276:ASP:HB2	2.37	0.45
1:A:300:ASP:HB2	3:F:19:HIS:CE1	2.51	0.45
1:P:189:LYS:HB3	1:P:189:LYS:HE2	1.75	0.45
1:M:189:LYS:HB3	1:M:189:LYS:HE2	1.73	0.45
2:W:186:MSE:HE3	3:X:33:VAL:HG13	1.99	0.45
2:E:172:LYS:O	2:E:174:THR:N	2.49	0.45
1:A:206:GLY:HA2	1:A:370:PHE:CZ	2.51	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
1:D:317:SER:O	1:D:320:LEU:HB2	2.16	0.45
1:P:355:ILE:HG13	1:P:355:ILE:O	2.08	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
2:N:169:GLN:HB3	2:N:169:GLN:HE21	1.52	0.45
1:M:303:MSE:SE	1:M:352:TYR:OH	2.85	0.45
1:A:189:LYS:HB3	1:A:189:LYS:HE2	1.73	0.45
2:W:184:TYR:OH	2:W:202:ASP:OD2	2.29	0.45
1:M:206:GLY:HA2	1:M:370:PHE:CZ	2.52	0.45
1:P:316:PHE:O	1:P:317:SER:C	2.56	0.45
2:E:242:ASN:ND2	2:E:242:ASN:H	2.13	0.45
1:A:303:MSE:SE	1:A:352:TYR:OH	2.85	0.45
2:Q:216:GLU:HG3	6:Q:1323:HOH:O	2.17	0.45
1:P:215:THR:HG22	1:S:291:GLY:HA3	1.99	0.45
1:J:233:VAL:HB	1:J:243:ILE:HB	1.99	0.45
1:D:268:TRP:CD1	1:D:369:ILE:HG12	2.52	0.45
2:W:200:VAL:HG23	3:X:33:VAL:HG11	1.99	0.44
1:S:355:ILE:HD12	1:V:260:GLY:HA3	1.96	0.44
1:G:171:GLU:CA	1:G:171:GLU:OE2	2.65	0.44
1:V:263:ARG:HD2	1:V:293:ALA:O	2.17	0.44
1:M:316:PHE:O	1:M:319:THR:N	2.50	0.44
2:W:161:ALA:HB1	2:W:163:ASP:OD1	2.17	0.44
1:A:273:ASN:CG	1:A:276:ASP:HB2	2.38	0.44
1:V:189:LYS:HB3	1:V:189:LYS:HE2	1.70	0.44
1:D:189:LYS:HB3	1:D:189:LYS:HE2	1.72	0.44
1:V:306:ARG:HG2	1:V:355:ILE:HG12	1.99	0.44
1:A:317:SER:HA	1:A:320:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:274:ASP:OD1	2:Z:235:HIS:HA	2.17	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:D:318:ASP:C	1:D:320:LEU:H	2.20	0.44
2:H:186:MSE:CE	3:I:33:VAL:HG13	2.47	0.44
2:H:184:TYR:CE2	2:H:266:ASN:HB2	2.53	0.44
2:N:186:MSE:CE	3:O:33:VAL:HG13	2.47	0.44
2:T:186:MSE:HE3	3:U:33:VAL:HG13	2.00	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
1:Y:355:ILE:O	1:Y:355:ILE:HG13	2.09	0.44
2:K:222:MSE:SE	2:K:248:THR:HG21	2.68	0.44
2:W:172:LYS:HZ1	2:W:172:LYS:HB3	1.82	0.44
1:G:263:ARG:HD2	1:G:293:ALA:O	2.17	0.44
2:K:186:MSE:HE3	3:L:33:VAL:HG13	1.98	0.44
1:D:355:ILE:HD13	1:G:260:GLY:HA3	2.00	0.44
1:Y:302:HIS:HE1	1:Y:358:THR:OG1	2.01	0.44
2:T:169:GLN:HE21	2:T:169:GLN:HB3	1.49	0.44
1:V:316:PHE:O	1:V:320:LEU:N	2.51	0.44
1:G:316:PHE:O	1:G:319:THR:N	2.51	0.44
1:A:225:VAL:HG22	1:A:253:ILE:HG13	2.00	0.44
1:Y:306:ARG:HG3	1:Y:355:ILE:HG12	1.99	0.43
2:H:242:ASN:HD22	2:H:242:ASN:N	2.13	0.43
1:G:257:ILE:HG13	1:G:357:PRO:HG2	1.99	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
2:Z:161:ALA:HB1	2:Z:163:ASP:OD1	2.17	0.43
1:V:317:SER:HA	1:V:320:LEU:CG	2.45	0.43
1:Y:189:LYS:HB3	1:Y:189:LYS:HE2	1.59	0.43
2:E:270:ALA:CB	2:E:273:ARG:HG2	2.46	0.43
2:T:252:GLU:OE2	2:T:254:ARG:NH1	2.35	0.43
1:A:312:MSE:HG2	1:D:307:LEU:HD21	2.00	0.43
1:S:189:LYS:HE2	1:S:189:LYS:HB3	1.66	0.43
1:M:300:ASP:HB2	3:R:19:HIS:CE1	2.53	0.43
1:J:179:LEU:CB	5:J:1:LDA:H11	2.46	0.43
1:A:316:PHE:HB3	1:A:320:LEU:HD21	2.00	0.43
1:G:316:PHE:O	1:G:317:SER:C	2.56	0.43
1:S:233:VAL:HB	1:S:243:ILE:HB	2.00	0.43
1:G:300:ASP:HB2	3:L:19:HIS:CE1	2.53	0.43
2:T:186:MSE:CE	3:U:33:VAL:HG13	2.49	0.43
1:J:316:PHE:O	1:J:319:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:172:LYS:O	2:Q:174:THR:N	2.51	0.43
2:H:161:ALA:CB	2:H:163:ASP:OD1	2.66	0.43
1:D:265:PHE:CD1	5:J:1:LDA:H51	2.54	0.43
1:J:175:GLY:C	5:J:1:LDA:HM12	2.38	0.43
2:W:186:MSE:CE	2:W:197:PRO:HD2	2.48	0.43
1:M:355:ILE:HD12	1:P:260:GLY:HA3	1.97	0.43
2:B:222:MSE:HB3	2:B:253:TRP:CZ3	2.54	0.43
1:S:268:TRP:CD1	1:S:369:ILE:HG12	2.54	0.43
1:J:224:GLN:HA	1:J:252:GLN:HA	2.00	0.43
2:Z:186:MSE:CE	2:Z:197:PRO:HG2	2.49	0.43
2:K:177:ALA:O	2:K:205:ARG:NH2	2.51	0.43
2:K:172:LYS:HZ1	2:K:172:LYS:HB3	1.82	0.43
2:W:186:MSE:HE3	3:X:33:VAL:CG2	2.43	0.43
2:Q:172:LYS:HE3	2:Q:172:LYS:HB2	1.67	0.43
1:G:312:MSE:HG2	1:J:307:LEU:HD21	2.01	0.43
2:K:186:MSE:CE	3:L:33:VAL:HG13	2.48	0.43
2:H:270:ALA:CB	2:H:273:ARG:HG2	2.48	0.43
1:Y:273:ASN:CG	1:Y:276:ASP:HB2	2.39	0.43
1:D:300:ASP:HB2	3:I:19:HIS:CE1	2.53	0.43
2:K:225:ALA:O	2:N:260:LYS:HD2	2.19	0.43
1:J:355:ILE:HD12	1:M:260:GLY:HA3	1.99	0.43
2:Z:222:MSE:SE	2:Z:248:THR:HG21	2.69	0.43
1:P:316:PHE:C	1:P:320:LEU:HG	2.39	0.43
2:N:161:ALA:CB	2:N:163:ASP:OD1	2.66	0.43
2:T:172:LYS:C	2:T:174:THR:H	2.21	0.43
1:D:181:LYS:HE3	1:G:171:GLU:HA	2.00	0.43
3:X:27:TRP:O	3:X:28:SER:C	2.57	0.43
1:D:182:ASN:HA	1:G:173:SER:HB2	2.01	0.42
1:A:273:ASN:OD1	1:A:276:ASP:HB2	2.19	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:M:320:LEU:C	1:M:322:ALA:H	2.21	0.42
2:B:172:LYS:O	2:B:174:THR:N	2.53	0.42
1:A:171:GLU:OE2	1:A:171:GLU:CA	2.68	0.42
3:R:27:TRP:O	3:R:28:SER:C	2.57	0.42
2:Z:195:ILE:HD12	2:Z:255:ILE:HG22	2.00	0.42
1:S:316:PHE:HA	1:S:319:THR:OG1	2.19	0.42
2:T:242:ASN:HD22	2:T:242:ASN:N	2.18	0.42
1:P:361:ASP:OD2	1:P:365:ASP:OD2	2.37	0.42
1:Y:303:MSE:SE	1:Y:352:TYR:OH	2.87	0.42
1:P:355:ILE:HD13	1:S:260:GLY:HA3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:172:LYS:C	2:Z:174:THR:H	2.22	0.42
1:S:316:PHE:O	1:S:317:SER:C	2.58	0.42
2:W:172:LYS:C	2:W:174:THR:H	2.22	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:W:175:ALA:HB3	2:W:282:SER:HB2	2.02	0.42
1:P:317:SER:O	1:P:321:THR:HG23	2.19	0.42
1:V:306:ARG:HG3	1:V:355:ILE:HG12	1.99	0.42
2:N:195:ILE:HD12	2:N:255:ILE:HG22	2.01	0.42
1:D:206:GLY:HA2	1:D:370:PHE:CZ	2.54	0.42
1:Y:316:PHE:O	1:Y:317:SER:C	2.58	0.42
1:V:302:HIS:HE1	1:V:358:THR:OG1	2.02	0.42
1:D:215:THR:HG22	1:G:291:GLY:HA3	2.02	0.42
1:S:303:MSE:SE	1:S:352:TYR:OH	2.88	0.42
2:Q:169:GLN:HB3	2:Q:169:GLN:HE21	1.52	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
2:E:161:ALA:CB	2:E:163:ASP:OD1	2.67	0.42
2:K:161:ALA:HB1	2:K:163:ASP:OD1	2.19	0.42
1:J:268:TRP:CD1	1:J:369:ILE:HG12	2.55	0.42
2:T:200:VAL:HA	2:T:208:ARG:O	2.20	0.42
1:G:367:VAL:HG13	1:G:368:SER:N	2.35	0.42
2:Z:278:THR:HG23	2:Z:285:VAL:O	2.20	0.42
3:X:42:GLN:NE2	6:X:69:HOH:O	2.52	0.42
2:W:169:GLN:HE21	2:W:169:GLN:HB3	1.54	0.42
2:Q:252:GLU:HG2	2:Q:253:TRP:N	2.35	0.41
2:T:186:MSE:HE3	3:U:33:VAL:CB	2.51	0.41
2:K:161:ALA:HB3	2:K:164:LYS:HB2	2.02	0.41
1:Y:233:VAL:HB	1:Y:243:ILE:HB	2.02	0.41
1:V:313:ILE:HA	1:V:316:PHE:CE2	2.56	0.41
1:V:303:MSE:SE	1:V:352:TYR:OH	2.88	0.41
1:Y:206:GLY:HA2	1:Y:370:PHE:CZ	2.55	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:J:179:LEU:CA	5:J:1:LDA:H11	2.50	0.41
1:A:313:ILE:HA	1:A:316:PHE:CE2	2.55	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:G:312:MSE:HG2	1:J:307:LEU:CD2	2.49	0.41
1:P:268:TRP:CD1	1:P:369:ILE:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ILE:HA	1:D:316:PHE:CE2	2.55	0.41
1:D:316:PHE:O	1:D:317:SER:C	2.59	0.41
1:S:383:LEU:HB3	2:T:168:THR:HG21	2.01	0.41
1:G:386:ASN:HA	2:H:284:ASP:O	2.19	0.41
1:G:347:GLU:HA	1:G:347:GLU:OE2	2.21	0.41
2:W:172:LYS:HE3	2:W:172:LYS:HB2	1.72	0.41
1:G:257:ILE:HD13	1:G:359:LEU:HB2	2.03	0.41
1:D:265:PHE:HB2	5:J:1:LDA:H81	2.02	0.41
2:N:186:MSE:HE1	2:N:197:PRO:CD	2.48	0.41
1:P:317:SER:HA	1:P:320:LEU:CG	2.49	0.41
1:A:306:ARG:HG2	1:A:355:ILE:HG12	2.01	0.41
2:Z:161:ALA:HB3	2:Z:164:LYS:HB2	2.03	0.41
1:V:216:GLU:OE2	1:Y:288:ASN:ND2	2.53	0.41
2:T:172:LYS:HB3	2:T:172:LYS:HZ1	1.84	0.41
2:H:172:LYS:HB2	2:H:172:LYS:HE3	1.70	0.41
2:N:242:ASN:H	2:N:242:ASN:ND2	2.14	0.41
1:A:366:ALA:HB3	2:B:228:LYS:HE2	2.02	0.41
1:P:206:GLY:HA2	1:P:370:PHE:CZ	2.56	0.41
2:T:184:TYR:CE1	2:T:201:TRP:HA	2.56	0.41
1:J:316:PHE:O	1:J:317:SER:C	2.59	0.41
2:E:176:PHE:CE2	2:E:180:LYS:HE3	2.56	0.41
1:D:263:ARG:HB3	1:D:296:PRO:HA	2.03	0.41
1:Y:266:VAL:HG21	1:Y:295:ILE:HG13	2.03	0.41
1:P:316:PHE:HA	1:P:319:THR:OG1	2.20	0.41
1:S:318:ASP:C	1:S:320:LEU:N	2.73	0.41
2:Q:242:ASN:ND2	2:Q:242:ASN:N	2.68	0.41
1:P:224:GLN:HA	1:P:252:GLN:HA	2.01	0.41
1:S:312:MSE:HG2	1:V:307:LEU:HD21	2.03	0.41
1:D:361:ASP:OD2	1:D:365:ASP:OD2	2.38	0.41
1:J:283:ASP:HB3	1:P:183:LEU:O	2.20	0.41
2:K:270:ALA:O	2:K:271:PRO:C	2.60	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
2:B:265:ARG:HD2	2:B:265:ARG:HH11	1.73	0.41
2:B:200:VAL:HG23	3:C:33:VAL:HG11	2.03	0.40
2:K:172:LYS:HE3	2:K:172:LYS:HB2	1.71	0.40
1:A:302:HIS:HE1	1:A:358:THR:OG1	2.04	0.40
1:Y:385:ASP:HA	1:Y:386:ASN:HA	1.95	0.40
2:N:200:VAL:HG23	3:O:33:VAL:HG11	2.02	0.40
2:K:278:THR:HG23	2:K:285:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:MSE:CE	2:E:197:PRO:HG2	2.49	0.40
2:B:222:MSE:SE	2:B:248:THR:HG21	2.71	0.40
1:M:215:THR:HG22	1:P:291:GLY:HA3	2.03	0.40
1:J:182:ASN:HA	1:M:173:SER:HB2	2.02	0.40
4:D:1:MPD:CM	2:E:228:LYS:HZ2	2.34	0.40
2:H:255:ILE:HB	2:H:262:VAL:HB	2.04	0.40
2:Z:190:PRO:O	2:Z:193:ARG:HG3	2.21	0.40
1:M:316:PHE:O	1:M:317:SER:C	2.59	0.40
2:Z:161:ALA:CB	2:Z:163:ASP:OD1	2.69	0.40
1:G:274:ASP:OD1	2:K:235:HIS:HA	2.21	0.40
2:Z:178:GLY:O	2:Z:179:ALA:C	2.60	0.40
1:A:217:LEU:HD13	1:A:361:ASP:HB3	2.03	0.40
1:A:222:PRO:HD2	5:J:1:LDA:H52	2.04	0.40
1:S:273:ASN:CG	1:S:276:ASP:HB2	2.42	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
1:A:283:ASP:HB3	1:G:183:LEU:O	2.22	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/227 (84%)	179 (94%)	10 (5%)	2 (1%)	19	39
1	D	191/227 (84%)	177 (93%)	13 (7%)	1 (0%)	34	60
1	G	189/227 (83%)	176 (93%)	12 (6%)	1 (0%)	34	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	193/227 (85%)	178 (92%)	14 (7%)	1 (0%)	34	60
1	M	193/227 (85%)	178 (92%)	13 (7%)	2 (1%)	19	39
1	P	193/227 (85%)	179 (93%)	13 (7%)	1 (0%)	34	60
1	S	193/227 (85%)	179 (93%)	13 (7%)	1 (0%)	34	60
1	V	192/227 (85%)	179 (93%)	12 (6%)	1 (0%)	34	60
1	Y	191/227 (84%)	179 (94%)	11 (6%)	1 (0%)	34	60
1	b	191/227 (84%)	176 (92%)	13 (7%)	2 (1%)	19	39
1	e	192/227 (85%)	180 (94%)	10 (5%)	2 (1%)	19	39
1	h	191/227 (84%)	179 (94%)	11 (6%)	1 (0%)	34	60
1	k	192/227 (85%)	180 (94%)	11 (6%)	1 (0%)	34	60
1	n	191/227 (84%)	178 (93%)	12 (6%)	1 (0%)	34	60
2	B	128/135 (95%)	118 (92%)	10 (8%)	0	100	100
2	E	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	24	46
2	H	128/135 (95%)	118 (92%)	9 (7%)	1 (1%)	24	46
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%)	24	46
2	T	128/135 (95%)	120 (94%)	8 (6%)	0	100	100
2	W	128/135 (95%)	122 (95%)	5 (4%)	1 (1%)	24	46
2	Z	128/135 (95%)	118 (92%)	9 (7%)	1 (1%)	24	46
2	c	128/135 (95%)	119 (93%)	8 (6%)	1 (1%)	24	46
2	f	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	24	46
2	i	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	24	46
2	l	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	24	46
2	o	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	24	46
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%)	4	5
3	O	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	R	22/34 (65%)	21 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	56

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
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

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Mol	Chain	Res	Type
1	e	319	THR
2	f	173	GLN
2	c	173	GLN

5.3.2 Protein sidechains (i)

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%)	139 (88%)	18 (12%)	7 12
1	D	157/180 (87%)	138 (88%)	19 (12%)	6 11
1	G	156/180 (87%)	141 (90%)	15 (10%)	10 20
1	J	157/180 (87%)	137 (87%)	20 (13%)	5 10
1	M	158/180 (88%)	139 (88%)	19 (12%)	6 11
1	P	158/180 (88%)	140 (89%)	18 (11%)	7 12
1	S	158/180 (88%)	138 (87%)	20 (13%)	5 10
1	V	158/180 (88%)	139 (88%)	19 (12%)	6 11
1	Y	157/180 (87%)	141 (90%)	16 (10%)	9 17
1	b	157/180 (87%)	138 (88%)	19 (12%)	6 11
1	e	158/180 (88%)	138 (87%)	20 (13%)	5 10
1	h	155/180 (86%)	138 (89%)	17 (11%)	8 14
1	k	158/180 (88%)	141 (89%)	17 (11%)	8 15
1	n	158/180 (88%)	138 (87%)	20 (13%)	5 10
2	B	109/110 (99%)	97 (89%)	12 (11%)	8 14
2	E	109/110 (99%)	96 (88%)	13 (12%)	6 11
2	H	109/110 (99%)	97 (89%)	12 (11%)	8 14
2	K	109/110 (99%)	99 (91%)	10 (9%)	11 21
2	N	109/110 (99%)	95 (87%)	14 (13%)	5 10
2	Q	109/110 (99%)	96 (88%)	13 (12%)	6 11
2	T	109/110 (99%)	96 (88%)	13 (12%)	6 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	W	109/110 (99%)	97 (89%)	12 (11%)	8 14
2	Z	109/110 (99%)	96 (88%)	13 (12%)	6 11
2	c	109/110 (99%)	97 (89%)	12 (11%)	8 14
2	f	109/110 (99%)	97 (89%)	12 (11%)	8 14
2	i	109/110 (99%)	96 (88%)	13 (12%)	6 11
2	l	109/110 (99%)	96 (88%)	13 (12%)	6 11
2	o	108/110 (98%)	94 (87%)	14 (13%)	5 9
3	C	25/31 (81%)	22 (88%)	3 (12%)	6 11
3	F	24/31 (77%)	22 (92%)	2 (8%)	14 27
3	I	24/31 (77%)	22 (92%)	2 (8%)	14 27
3	L	27/31 (87%)	25 (93%)	2 (7%)	17 34
3	O	24/31 (77%)	23 (96%)	1 (4%)	36 65
3	R	23/31 (74%)	22 (96%)	1 (4%)	35 64
3	U	26/31 (84%)	24 (92%)	2 (8%)	16 31
3	X	24/31 (77%)	22 (92%)	2 (8%)	14 27
3	a	24/31 (77%)	22 (92%)	2 (8%)	14 27
3	d	24/31 (77%)	23 (96%)	1 (4%)	36 65
3	g	24/31 (77%)	23 (96%)	1 (4%)	36 65
3	j	24/31 (77%)	23 (96%)	1 (4%)	36 65
3	m	24/31 (77%)	23 (96%)	1 (4%)	36 65
3	p	23/31 (74%)	22 (96%)	1 (4%)	35 64
All	All	4067/4494 (90%)	3612 (89%)	455 (11%)	7 13

All (455) 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	263	ARG
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	312	MSE
1	A	315	LEU
1	A	316	PHE
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	191	GLU
2	B	217	LEU
2	B	242	ASN
2	B	248	THR
2	B	278	THR
2	B	290	ILE
3	C	17	SER
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	263	ARG
1	D	307	LEU
1	D	312	MSE
1	D	315	LEU
1	D	316	PHE
1	D	344	LEU
1	D	355	ILE
1	D	367	VAL
1	D	368	SER
1	D	378	SER
1	D	383	LEU

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Mol	Chain	Res	Type
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	242	ASN
2	E	248	THR
2	E	249	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	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
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	278	THR

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Mol	Chain	Res	Type
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	307	LEU
1	J	312	MSE
1	J	315	LEU
1	J	316	PHE
1	J	321	THR
1	J	343	GLN
1	J	355	ILE
1	J	360	TYR
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	173	GLN
2	K	174	THR
2	K	217	LEU
2	K	242	ASN
2	K	248	THR
2	K	278	THR
2	K	290	ILE
3	L	15	CYS
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

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Mol	Chain	Res	Type
1	M	230	SER
1	M	307	LEU
1	M	312	MSE
1	M	315	LEU
1	M	316	PHE
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	232	PRO
2	N	242	ASN
2	N	248	THR
2	N	249	VAL
2	N	278	THR
2	N	290	ILE
3	O	37	ILE
1	P	171	GLU
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	263	ARG
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

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Mol	Chain	Res	Type
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	220	VAL
2	Q	242	ASN
2	Q	248	THR
2	Q	249	VAL
2	Q	278	THR
2	Q	290	ILE
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
1	S	263	ARG
1	S	307	LEU
1	S	312	MSE
1	S	315	LEU
1	S	316	PHE
1	S	320	LEU
1	S	355	ILE
1	S	367	VAL
1	S	368	SER
1	S	378	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

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Mol	Chain	Res	Type
2	T	174	THR
2	T	188	GLU
2	T	201	TRP
2	T	220	VAL
2	T	242	ASN
2	T	248	THR
2	T	278	THR
2	T	290	ILE
3	U	16	SER
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	263	ARG
1	V	307	LEU
1	V	312	MSE
1	V	315	LEU
1	V	321	THR
1	V	355	ILE
1	V	367	VAL
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	242	ASN
2	W	248	THR
2	W	278	THR
2	W	290	ILE
3	X	37	ILE

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Mol	Chain	Res	Type
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	263	ARG
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
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	173	SER
1	b	195	VAL
1	b	211	CYS
1	b	217	LEU
1	b	225	VAL
1	b	230	SER
1	b	307	LEU
1	b	312	MSE

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Mol	Chain	Res	Type
1	b	315	LEU
1	b	316	PHE
1	b	320	LEU
1	b	343	GLN
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	242	ASN
2	c	248	THR
2	c	278	THR
2	c	290	ILE
3	d	37	ILE
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	263	ARG
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

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Mol	Chain	Res	Type
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	242	ASN
2	f	248	THR
2	f	278	THR
2	f	290	ILE
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
1	h	263	ARG
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	201	TRP
2	i	217	LEU
2	i	220	VAL
2	i	242	ASN
2	i	278	THR

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Mol	Chain	Res	Type
2	i	290	ILE
3	j	37	ILE
1	k	171	GLU
1	k	172	THR
1	k	173	SER
1	k	195	VAL
1	k	211	CYS
1	k	217	LEU
1	k	225	VAL
1	k	230	SER
1	k	307	LEU
1	k	312	MSE
1	k	315	LEU
1	k	316	PHE
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
2	l	169	GLN
2	l	171	LEU
2	l	173	GLN
2	l	174	THR
2	l	188	GLU
2	l	191	GLU
2	l	217	LEU
2	l	242	ASN
2	l	248	THR
2	l	278	THR
2	l	290	ILE
3	m	37	ILE
1	n	168	GLN
1	n	169	ASP
1	n	172	THR
1	n	173	SER
1	n	195	VAL
1	n	211	CYS
1	n	217	LEU
1	n	225	VAL
1	n	230	SER

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Mol	Chain	Res	Type
1	n	258	LYS
1	n	263	ARG
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	378	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
2	o	248	THR
2	o	278	THR
2	o	290	ILE
3	p	37	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	302	HIS
2	B	169	GLN
2	B	199	HIS
2	B	242	ASN
2	B	268	ASN
1	D	182	ASN
1	D	298	GLN
1	D	302	HIS
2	E	169	GLN
2	E	219	GLN
2	E	242	ASN

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Mol	Chain	Res	Type
2	E	268	ASN
1	G	182	ASN
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	169	GLN
2	N	219	GLN
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	219	GLN
2	Q	242	ASN
2	Q	268	ASN
3	R	19	HIS
1	S	182	ASN
1	S	298	GLN
1	S	302	HIS
2	T	169	GLN
2	T	199	HIS
2	T	219	GLN
2	T	242	ASN
2	T	268	ASN
3	U	34	ASN
1	V	182	ASN
1	V	298	GLN
1	V	302	HIS

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Mol	Chain	Res	Type
2	W	169	GLN
2	W	219	GLN
2	W	242	ASN
2	W	268	ASN
3	X	19	HIS
3	X	42	GLN
1	Y	182	ASN
1	Y	298	GLN
1	Y	302	HIS
2	Z	169	GLN
2	Z	219	GLN
2	Z	242	ASN
2	Z	268	ASN
3	a	19	HIS
1	b	182	ASN
1	b	298	GLN
1	b	302	HIS
2	c	169	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
1	e	343	GLN
2	f	169	GLN
2	f	199	HIS
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	199	HIS
2	i	219	GLN
2	i	242	ASN
2	i	268	ASN
3	j	34	ASN
1	k	182	ASN
1	k	298	GLN
1	k	302	HIS

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Mol	Chain	Res	Type
1	k	343	GLN
2	l	169	GLN
2	l	219	GLN
2	l	242	ASN
2	l	268	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 carbohydrates 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	$\#\|Z\|>2$
4	MPD	D	1	-	6,7,7	0.24	0	7,10,10	0.41	0
5	LDA	J	1	-	15,15,15	4.57	3 (20%)	16,17,17	2.25	4 (25%)
4	MPD	h	2	-	6,7,7	0.22	0	7,10,10	0.73	0
4	MPD	k	3	-	6,7,7	0.31	0	7,10,10	0.89	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
4	MPD	D	1	-	-	0/5/5/5	0/0/0/0
5	LDA	J	1	-	-	0/13/13/13	0/0/0/0
4	MPD	h	2	-	-	0/5/5/5	0/0/0/0
4	MPD	k	3	-	-	0/5/5/5	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	LDA	O1-N1	-17.04	1.23	1.39
5	J	1	LDA	CM1-N1	-3.65	1.43	1.49
5	J	1	LDA	C1-N1	-2.34	1.47	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	1	LDA	O1-N1-CM1	-7.18	99.45	109.05
5	J	1	LDA	O1-N1-C1	-2.55	107.41	110.27
5	J	1	LDA	CM2-N1-C1	2.21	116.89	109.77
5	J	1	LDA	CM2-N1-CM1	2.82	112.01	108.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	MPD	6	0
5	J	1	LDA	33	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.12	20 (10%)	8	5	19, 27, 76, 95	0
1	D	190/227 (83%)	0.15	21 (11%)	7	4	19, 27, 76, 96	0
1	G	188/227 (82%)	-0.02	19 (10%)	9	5	19, 27, 74, 87	0
1	J	192/227 (84%)	0.14	24 (12%)	5	3	19, 27, 76, 97	0
1	M	192/227 (84%)	0.11	24 (12%)	5	3	19, 27, 77, 93	0
1	P	192/227 (84%)	0.12	24 (12%)	5	3	19, 27, 77, 97	0
1	S	192/227 (84%)	0.08	22 (11%)	6	4	19, 27, 77, 95	0
1	V	191/227 (84%)	0.07	23 (12%)	6	4	19, 27, 77, 95	0
1	Y	190/227 (83%)	0.04	21 (11%)	7	4	19, 27, 76, 95	0
1	b	190/227 (83%)	0.06	20 (10%)	8	5	19, 27, 76, 90	0
1	e	191/227 (84%)	0.18	22 (11%)	6	4	19, 27, 76, 97	0
1	h	190/227 (83%)	0.16	18 (9%)	10	6	19, 27, 76, 89	0
1	k	191/227 (84%)	0.17	21 (10%)	7	4	19, 27, 77, 98	0
1	n	191/227 (84%)	0.13	22 (11%)	6	4	19, 27, 75, 126	0
2	B	127/135 (94%)	-0.26	3 (2%)	62	56	24, 33, 68, 93	0
2	E	127/135 (94%)	-0.30	3 (2%)	62	56	24, 33, 68, 93	0
2	H	127/135 (94%)	-0.31	2 (1%)	74	69	24, 33, 68, 93	0
2	K	127/135 (94%)	-0.27	3 (2%)	62	56	24, 33, 68, 93	0
2	N	127/135 (94%)	-0.35	3 (2%)	62	56	25, 33, 68, 93	0
2	Q	127/135 (94%)	-0.38	3 (2%)	62	56	25, 33, 68, 93	0
2	T	127/135 (94%)	-0.26	3 (2%)	62	56	24, 33, 68, 93	0
2	W	127/135 (94%)	-0.35	3 (2%)	62	56	24, 33, 68, 93	0
2	Z	127/135 (94%)	-0.40	2 (1%)	74	69	24, 33, 68, 93	0
2	c	127/135 (94%)	-0.39	2 (1%)	74	69	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%)	-0.17	2 (1%) 74 69	24, 33, 68, 93	0
2	i	127/135 (94%)	-0.35	1 (0%) 87 85	24, 33, 68, 93	0
2	l	127/135 (94%)	-0.40	3 (2%) 62 56	25, 33, 68, 93	0
2	o	127/135 (94%)	-0.24	3 (2%) 62 56	24, 33, 68, 93	0
3	C	26/34 (76%)	0.26	3 (11%) 6 4	30, 40, 76, 83	0
3	F	25/34 (73%)	0.14	2 (8%) 15 10	31, 37, 76, 84	0
3	I	25/34 (73%)	-0.07	0 100 100	30, 37, 76, 82	0
3	L	28/34 (82%)	0.16	4 (14%) 4 2	30, 41, 79, 82	0
3	O	24/34 (70%)	-0.09	1 (4%) 40 32	30, 37, 76, 85	0
3	R	24/34 (70%)	-0.35	1 (4%) 40 32	30, 37, 69, 81	0
3	U	27/34 (79%)	0.57	5 (18%) 2 1	30, 40, 76, 84	0
3	X	24/34 (70%)	-0.13	2 (8%) 14 9	30, 37, 76, 84	0
3	a	24/34 (70%)	-0.23	0 100 100	31, 37, 76, 83	0
3	d	24/34 (70%)	0.20	3 (12%) 5 3	30, 37, 76, 85	0
3	g	25/34 (73%)	-0.13	1 (4%) 42 34	30, 37, 76, 86	0
3	j	25/34 (73%)	0.01	2 (8%) 15 10	30, 37, 76, 84	0
3	m	25/34 (73%)	-0.14	1 (4%) 42 34	30, 37, 76, 84	0
3	p	23/34 (67%)	-0.32	0 100 100	30, 37, 69, 81	0
All	All	4797/5544 (86%)	-0.06	362 (7%) 17 12	19, 31, 77, 126	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	342	GLY	12.5
1	n	345	ALA	9.3
1	h	349	LEU	9.3
1	G	349	LEU	9.2
1	A	345	ALA	8.9
1	b	343	GLN	8.6
1	D	345	ALA	8.5
1	k	345	ALA	8.4
1	b	342	GLY	8.4
1	J	343	GLN	8.4
1	b	316	PHE	8.4
1	e	317	SER	8.3
1	V	316	PHE	8.3

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Mol	Chain	Res	Type	RSRZ
1	b	317	SER	8.3
1	e	316	PHE	8.2
1	h	342	GLY	8.2
1	h	318	ASP	8.2
1	e	344	LEU	8.2
1	e	343	GLN	8.2
1	M	316	PHE	8.2
1	P	316	PHE	8.2
1	D	344	LEU	8.0
1	h	344	LEU	8.0
1	k	349	LEU	8.0
1	Y	318	ASP	7.9
1	P	349	LEU	7.9
1	D	321	THR	7.8
1	M	320	LEU	7.8
1	J	349	LEU	7.8
1	M	343	GLN	7.7
1	A	316	PHE	7.6
1	b	345	ALA	7.6
1	k	318	ASP	7.6
1	S	345	ALA	7.5
1	e	318	ASP	7.5
1	n	316	PHE	7.4
1	k	321	THR	7.4
1	n	319	THR	7.3
1	h	316	PHE	7.3
1	D	316	PHE	7.3
1	Y	316	PHE	7.3
1	h	345	ALA	7.2
1	P	313	ILE	7.2
1	k	320	LEU	7.1
1	S	316	PHE	7.1
1	k	316	PHE	7.1
1	G	344	LEU	7.1
1	P	342	GLY	7.0
1	A	318	ASP	7.0
1	G	317	SER	7.0
1	M	344	LEU	7.0
1	P	345	ALA	6.9
1	b	320	LEU	6.9
1	M	318	ASP	6.9
1	b	318	ASP	6.9

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Mol	Chain	Res	Type	RSRZ
1	e	346	SER	6.9
1	J	321	THR	6.8
1	n	168	GLN	6.7
1	P	348	ALA	6.7
1	J	318	ASP	6.7
1	A	320	LEU	6.6
1	Y	321	THR	6.6
1	V	318	ASP	6.5
1	V	317	SER	6.5
1	D	320	LEU	6.5
1	k	344	LEU	6.5
1	h	317	SER	6.4
1	V	349	LEU	6.4
1	n	169	ASP	6.4
1	D	348	ALA	6.4
1	h	343	GLN	6.3
1	P	318	ASP	6.3
1	Y	320	LEU	6.2
1	k	348	ALA	6.2
1	M	342	GLY	6.2
1	S	321	THR	6.2
1	e	347	GLU	6.1
1	J	344	LEU	6.1
1	e	349	LEU	6.1
1	k	346	SER	6.1
1	P	320	LEU	6.0
1	k	315	LEU	6.0
1	Y	317	SER	6.0
1	S	348	ALA	6.0
1	e	348	ALA	5.9
1	G	318	ASP	5.9
1	P	314	SER	5.9
1	Y	344	LEU	5.9
1	G	316	PHE	5.9
1	V	319	THR	5.8
1	P	321	THR	5.8
1	S	344	LEU	5.8
1	S	342	GLY	5.8
1	M	321	THR	5.8
1	h	346	SER	5.8
1	J	345	ALA	5.8
1	S	314	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	P	344	LEU	5.7
1	b	319	THR	5.7
1	h	320	LEU	5.7
1	D	317	SER	5.7
1	n	349	LEU	5.7
1	M	349	LEU	5.6
1	V	320	LEU	5.6
1	V	344	LEU	5.6
1	h	319	THR	5.6
1	G	345	ALA	5.6
1	e	321	THR	5.6
1	V	321	THR	5.6
1	J	316	PHE	5.5
1	S	349	LEU	5.5
1	M	317	SER	5.4
1	S	318	ASP	5.4
1	n	314	SER	5.4
1	D	349	LEU	5.4
1	J	346	SER	5.4
1	k	317	SER	5.4
1	b	349	LEU	5.3
1	M	319	THR	5.3
1	Y	345	ALA	5.3
1	V	347	GLU	5.3
1	S	317	SER	5.3
1	V	345	ALA	5.2
1	G	346	SER	5.2
1	n	318	ASP	5.2
1	M	315	LEU	5.2
1	J	320	LEU	5.1
1	b	344	LEU	5.1
3	U	16	SER	5.1
1	V	348	ALA	5.1
1	G	314	SER	5.0
1	A	344	LEU	5.0
1	D	315	LEU	5.0
1	S	320	LEU	5.0
1	S	343	GLN	5.0
1	M	348	ALA	5.0
1	P	343	GLN	5.0
1	e	322	ALA	4.9
1	e	345	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	317	SER	4.9
1	e	320	LEU	4.9
1	G	343	GLN	4.9
1	n	170	ASN	4.9
1	P	315	LEU	4.9
2	W	163	ASP	4.8
1	D	347	GLU	4.8
1	M	346	SER	4.8
1	n	348	ALA	4.8
1	Y	315	LEU	4.8
1	V	315	LEU	4.8
1	G	319	THR	4.8
1	h	348	ALA	4.7
1	D	318	ASP	4.7
1	Y	350	ARG	4.7
1	Y	349	LEU	4.7
1	Y	319	THR	4.7
2	o	273	ARG	4.7
1	A	317	SER	4.6
1	P	322	ALA	4.6
1	P	317	SER	4.6
1	J	348	ALA	4.5
1	M	313	ILE	4.5
1	Y	313	ILE	4.5
1	A	348	ALA	4.5
1	h	347	GLU	4.4
1	k	347	GLU	4.4
1	b	348	ALA	4.4
1	n	317	SER	4.4
1	n	344	LEU	4.4
1	A	314	SER	4.4
1	A	346	SER	4.4
1	D	351	SER	4.4
1	S	351	SER	4.4
1	P	351	SER	4.3
1	b	346	SER	4.3
2	f	273	ARG	4.3
1	D	322	ALA	4.3
1	J	314	SER	4.2
1	n	351	SER	4.2
1	P	347	GLU	4.2
1	J	350	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	Z	273	ARG	4.2
1	V	313	ILE	4.2
1	k	343	GLN	4.1
1	k	314	SER	4.1
1	k	322	ALA	4.1
1	G	313	ILE	4.1
1	G	348	ALA	4.1
1	A	349	LEU	4.1
3	C	17	SER	4.1
1	S	315	LEU	4.0
1	b	311	ILE	4.0
1	D	319	THR	4.0
1	S	347	GLU	4.0
1	Y	314	SER	4.0
1	G	347	GLU	4.0
1	k	351	SER	4.0
1	A	319	THR	4.0
1	P	319	THR	4.0
1	G	315	LEU	4.0
1	e	319	THR	4.0
1	S	311	ILE	3.9
1	S	350	ARG	3.9
1	S	322	ALA	3.9
1	J	351	SER	3.9
1	M	314	SER	3.9
1	J	319	THR	3.9
2	i	273	ARG	3.9
1	D	311	ILE	3.8
2	N	273	ARG	3.8
2	T	273	ARG	3.8
1	G	386	ASN	3.8
1	M	345	ALA	3.8
1	J	315	LEU	3.8
1	M	311	ILE	3.8
3	U	18	GLY	3.7
1	S	319	THR	3.7
3	U	17	SER	3.7
2	Q	273	ARG	3.7
1	G	350	ARG	3.7
1	b	350	ARG	3.7
1	A	347	GLU	3.6
1	e	313	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	P	346	SER	3.6
1	Y	347	GLU	3.6
3	L	17	SER	3.6
1	n	347	GLU	3.6
1	b	347	GLU	3.6
3	d	42	GLN	3.6
1	V	311	ILE	3.5
1	P	352	TYR	3.5
3	O	41	THR	3.5
1	e	315	LEU	3.5
2	N	163	ASP	3.5
1	M	351	SER	3.5
1	J	313	ILE	3.4
3	X	42	GLN	3.4
1	M	347	GLU	3.4
2	l	166	ARG	3.4
2	H	166	ARG	3.4
1	b	314	SER	3.4
1	e	386	ASN	3.3
1	n	346	SER	3.3
2	W	273	ARG	3.3
1	S	346	SER	3.3
1	J	347	GLU	3.3
1	h	351	SER	3.3
1	k	319	THR	3.3
1	D	313	ILE	3.3
2	H	273	ARG	3.3
1	Y	346	SER	3.2
3	d	41	THR	3.2
1	Y	348	ALA	3.2
3	L	15	CYS	3.2
3	g	42	GLN	3.2
2	K	273	ARG	3.2
1	Y	351	SER	3.2
1	A	311	ILE	3.2
1	e	314	SER	3.2
1	A	321	THR	3.2
3	F	41	THR	3.1
1	b	313	ILE	3.1
1	D	386	ASN	3.1
1	D	346	SER	3.1
2	c	273	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	322	ALA	3.1
1	k	350	ARG	3.1
1	J	322	ALA	3.0
2	f	166	ARG	3.0
3	U	42	GLN	3.0
3	j	42	GLN	3.0
1	k	313	ILE	3.0
3	X	41	THR	3.0
2	B	273	ARG	3.0
1	Y	352	TYR	3.0
3	L	41	THR	3.0
2	E	273	ARG	2.9
1	G	351	SER	2.9
2	c	163	ASP	2.9
2	l	273	ARG	2.9
1	M	350	ARG	2.9
3	d	37	ILE	2.9
1	e	351	SER	2.9
1	S	386	ASN	2.9
1	D	350	ARG	2.8
1	h	314	SER	2.8
2	K	163	ASP	2.8
1	J	352	TYR	2.8
1	Y	311	ILE	2.8
1	b	315	LEU	2.8
1	k	311	ILE	2.8
1	h	386	ASN	2.8
1	V	352	TYR	2.8
1	M	322	ALA	2.8
1	J	311	ILE	2.8
1	M	386	ASN	2.8
1	V	322	ALA	2.8
1	b	386	ASN	2.8
1	n	386	ASN	2.7
1	V	350	ARG	2.7
1	G	352	TYR	2.7
1	G	311	ILE	2.7
1	A	315	LEU	2.7
1	n	313	ILE	2.7
3	R	41	THR	2.7
1	P	386	ASN	2.6
2	Z	163	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	Q	163	ASP	2.6
1	V	346	SER	2.6
1	A	313	ILE	2.6
1	V	314	SER	2.6
1	n	315	LEU	2.5
2	T	163	ASP	2.5
1	h	350	ARG	2.5
2	B	163	ASP	2.5
1	Y	322	ALA	2.5
1	e	311	ILE	2.5
1	n	350	ARG	2.5
2	B	166	ARG	2.5
2	Q	166	ARG	2.5
3	F	18	GLY	2.5
1	k	386	ASN	2.5
3	m	42	GLN	2.4
1	b	351	SER	2.4
1	V	171	GLU	2.4
1	V	343	GLN	2.4
2	T	166	ARG	2.4
1	M	352	TYR	2.4
1	P	311	ILE	2.4
2	W	171	LEU	2.3
3	L	16	SER	2.3
2	o	166	ARG	2.3
1	n	342	GLY	2.3
3	C	39	VAL	2.3
1	J	386	ASN	2.3
1	P	350	ARG	2.3
2	l	163	ASP	2.3
1	J	171	GLU	2.3
1	n	311	ILE	2.3
1	A	350	ARG	2.2
1	e	352	TYR	2.2
1	e	350	ARG	2.2
1	S	313	ILE	2.2
2	E	166	ARG	2.1
1	n	352	TYR	2.1
1	V	386	ASN	2.1
1	A	386	ASN	2.1
3	U	29	ASN	2.1
1	A	352	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	352	TYR	2.1
1	P	310	ALA	2.1
2	E	163	ASP	2.1
2	o	173	GLN	2.1
1	M	385	ASP	2.1
1	D	314	SER	2.1
1	V	351	SER	2.0
1	Y	310	ALA	2.0
2	N	162	ALA	2.0
2	K	166	ARG	2.0
3	j	41	THR	2.0
1	h	311	ILE	2.0
3	C	18	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	LDA	J	1	16/16	0.75	0.50	11.03	11,42,48,52	0
4	MPD	D	1	8/8	0.91	0.25	5.07	62,63,64,67	0
4	MPD	h	2	8/8	0.91	0.19	3.44	50,52,56,59	0
4	MPD	k	3	8/8	0.94	0.20	2.27	44,45,48,53	0

6.5 Other polymers (i)

There are no such residues in this entry.