



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:23 AM UTC

PDB ID : 2BR2 / pdb_00002br2
Title : RNase PH core of the archaeal exosome
Authors : lorentzen, E.; Fribourg, S.; Conti, E.
Deposited on : 2005-04-30
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

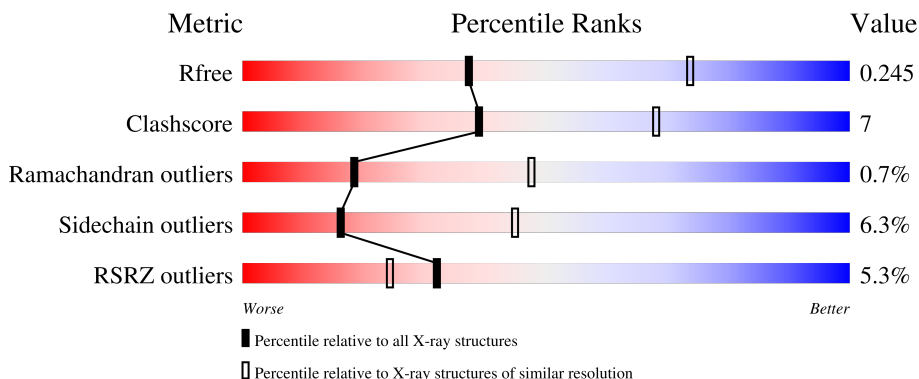
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	 8% 82% 11% • 5%
1	C	275	 6% 78% 15% • 5%
1	E	275	 5% 81% 12% • 5%
1	G	275	 7% 83% 11% • 5%
1	I	275	 6% 81% 12% • 5%

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Mol	Chain	Length	Quality of chain
1	K	275	
1	M	275	
1	O	275	
1	Q	275	
1	S	275	
1	U	275	
1	W	275	
2	B	248	
2	D	248	
2	F	248	
2	H	248	
2	J	248	
2	L	248	
2	N	248	
2	P	248	
2	R	248	
2	T	248	
2	V	248	
2	X	248	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46287 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 EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	Total 1960	C 1248	N 323	O 384	S 5	0	0	0
1	C	260	Total 1972	C 1255	N 325	O 387	S 5	0	0	0
1	E	260	Total 1968	C 1253	N 324	O 386	S 5	0	0	0
1	G	260	Total 1964	C 1251	N 324	O 384	S 5	0	0	0
1	I	260	Total 1961	C 1250	N 323	O 383	S 5	0	0	0
1	K	260	Total 1964	C 1251	N 324	O 384	S 5	0	0	0
1	M	260	Total 1972	C 1255	N 325	O 387	S 5	0	0	0
1	O	260	Total 1968	C 1253	N 325	O 385	S 5	0	0	0
1	Q	260	Total 1968	C 1253	N 325	O 385	S 5	0	0	0
1	S	260	Total 1967	C 1253	N 324	O 385	S 5	0	0	0
1	U	260	Total 1968	C 1253	N 325	O 385	S 5	0	0	0
1	W	260	Total 1968	C 1253	N 324	O 386	S 5	0	0	0

- Molecule 2 is a protein called EXOSOME COMPLEX EXONUCLEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	241	Total 1863	C 1175	N 322	O 356	S 10	0	0	0
2	D	247	Total 1905	C 1202	N 329	O 363	S 11	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	H	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	J	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	L	247	Total	C	N	O	S	0	0	0
			1909	1204	329	365	11			
2	N	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			
2	P	248	Total	C	N	O	S	0	0	0
			1907	1204	327	364	12			
2	R	245	Total	C	N	O	S	0	0	0
			1889	1192	327	359	11			
2	T	247	Total	C	N	O	S	0	0	0
			1905	1202	329	363	11			
2	V	244	Total	C	N	O	S	0	0	0
			1883	1189	325	359	10			
2	X	241	Total	C	N	O	S	0	0	0
			1863	1175	322	356	10			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	L	1	Total	Cl	0	0
			1	1		
3	M	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		
3	P	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total Cl 1 1	0	0
3	T	1	Total Cl 1 1	0	0
3	V	1	Total Cl 1 1	0	0
3	X	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	5	Total O 5 5	0	0
4	C	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0
4	E	6	Total O 6 6	0	0
4	F	4	Total O 4 4	0	0
4	G	2	Total O 2 2	0	0
4	H	3	Total O 3 3	0	0
4	I	1	Total O 1 1	0	0
4	J	5	Total O 5 5	0	0
4	K	3	Total O 3 3	0	0
4	L	3	Total O 3 3	0	0
4	M	8	Total O 8 8	0	0
4	N	4	Total O 4 4	0	0
4	O	9	Total O 9 9	0	0

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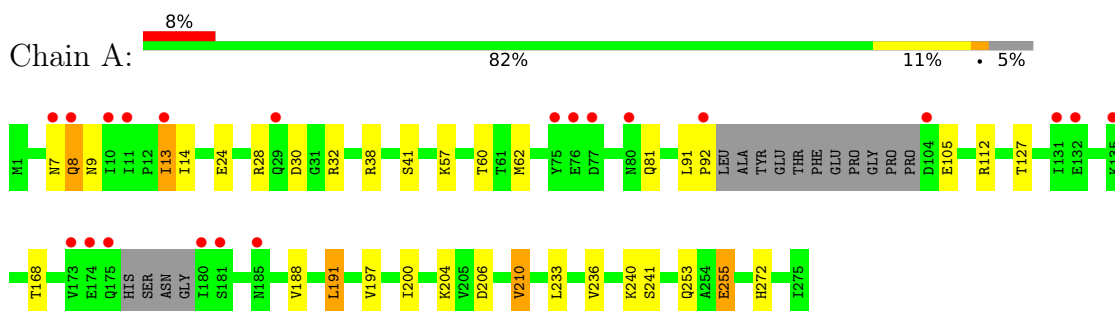
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	6	Total O 6 6	0	0
4	Q	4	Total O 4 4	0	0
4	R	5	Total O 5 5	0	0
4	S	6	Total O 6 6	0	0
4	T	4	Total O 4 4	0	0
4	U	3	Total O 3 3	0	0
4	V	3	Total O 3 3	0	0
4	W	2	Total O 2 2	0	0
4	X	1	Total O 1 1	0	0

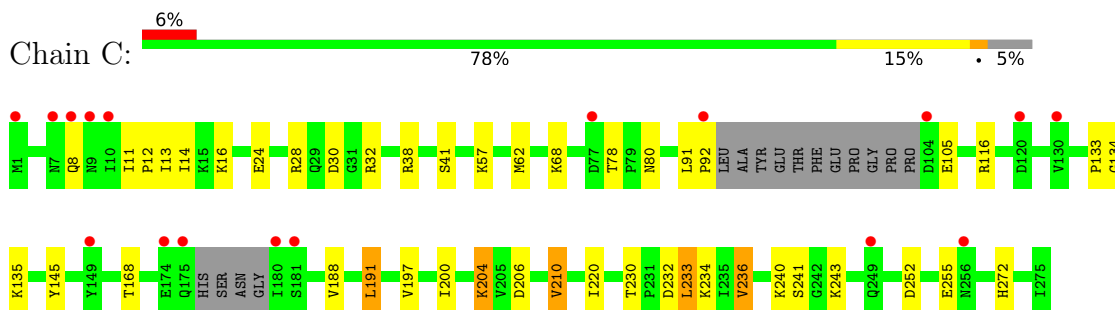
3 Residue-property plots [i](#)

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

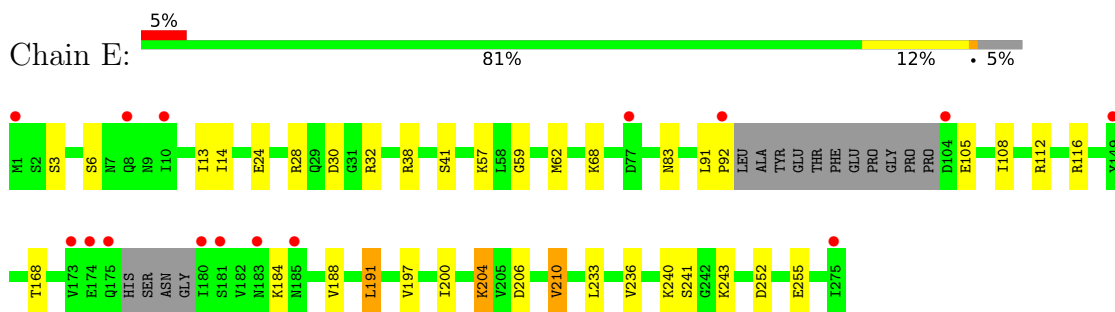
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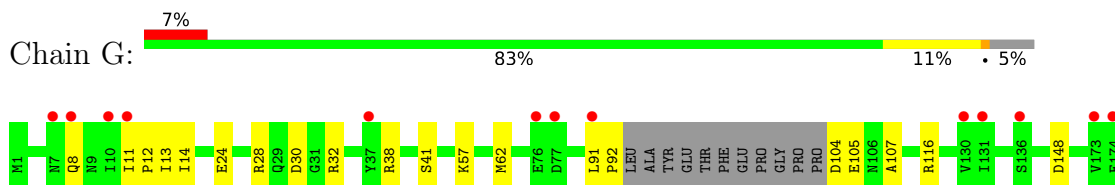
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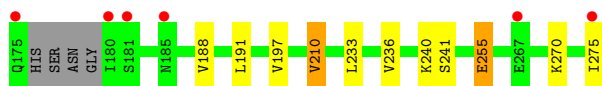


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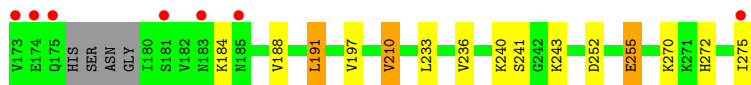
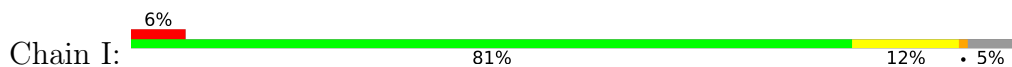


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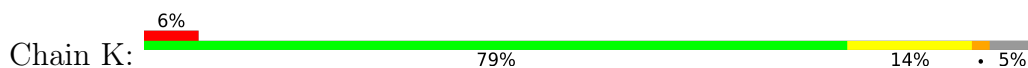




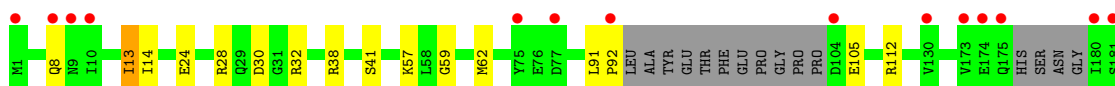
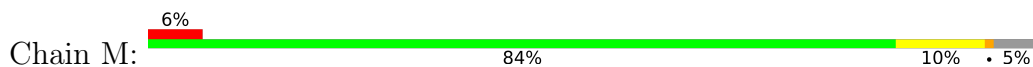
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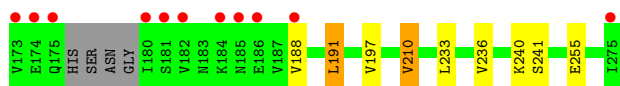
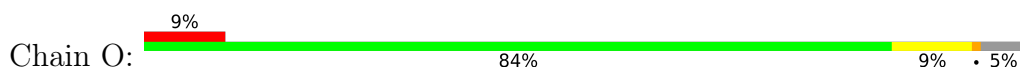
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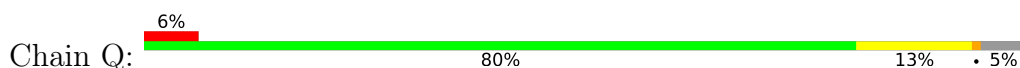
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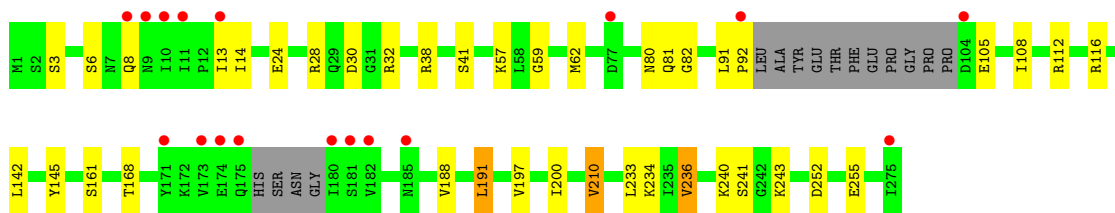


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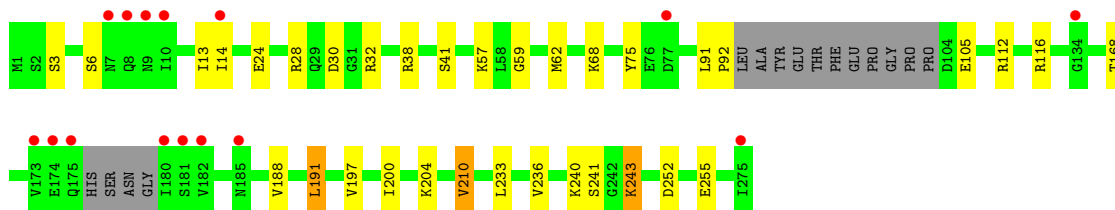
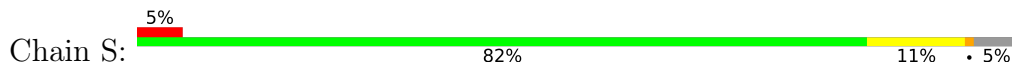


- Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

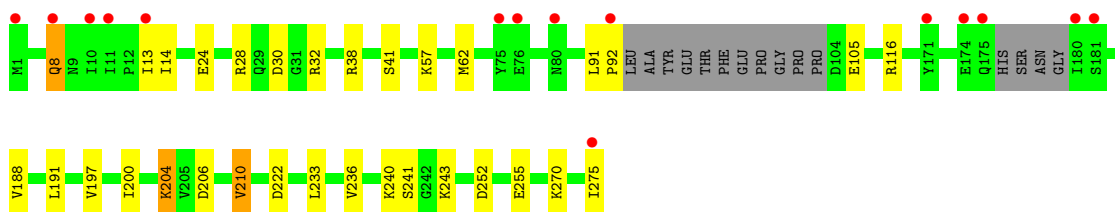
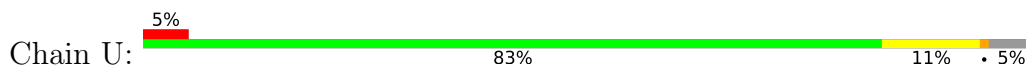




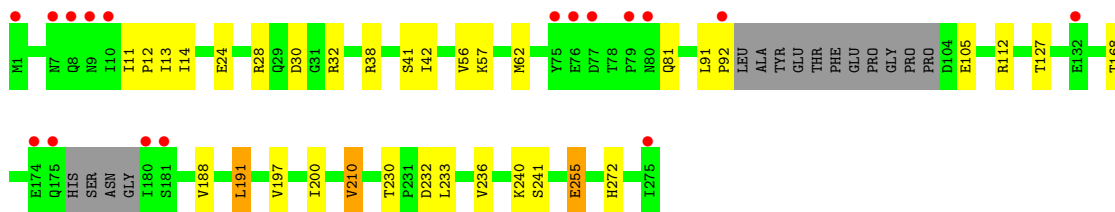
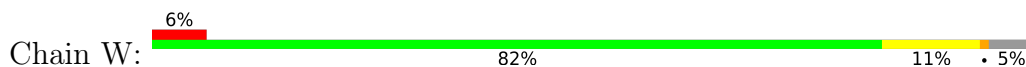
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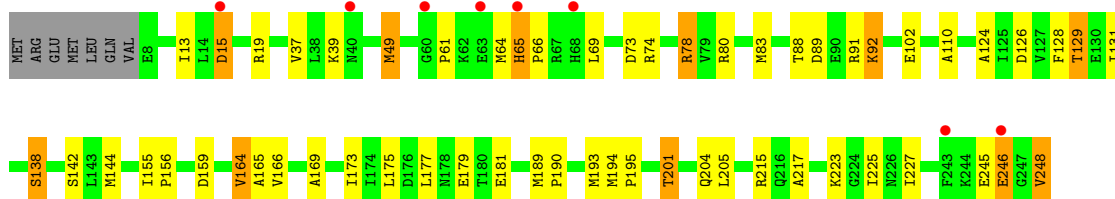
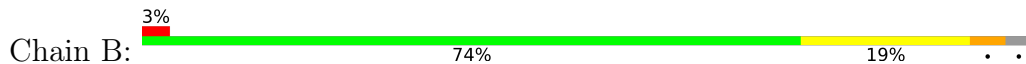
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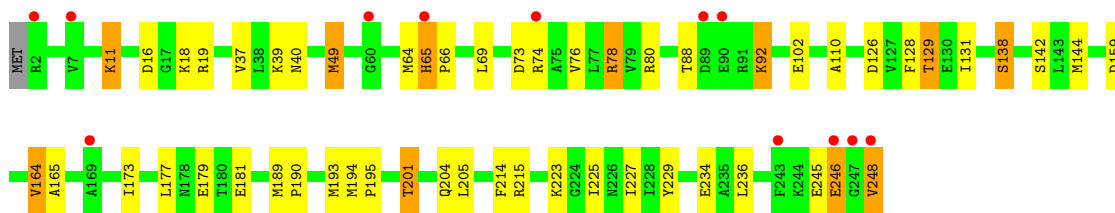


• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

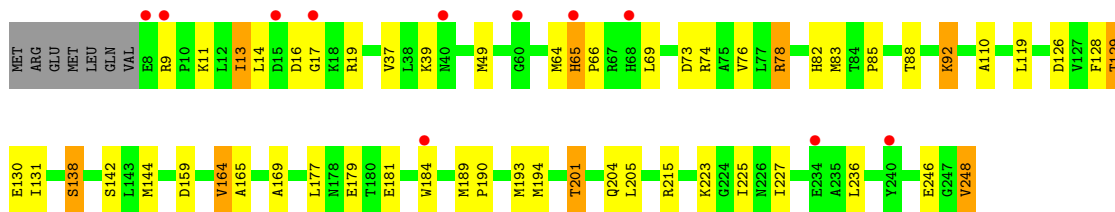


• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

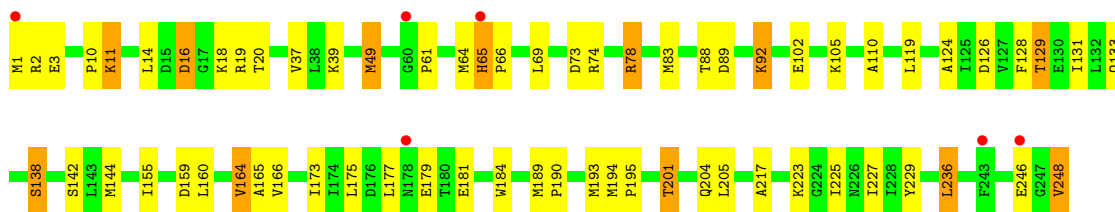




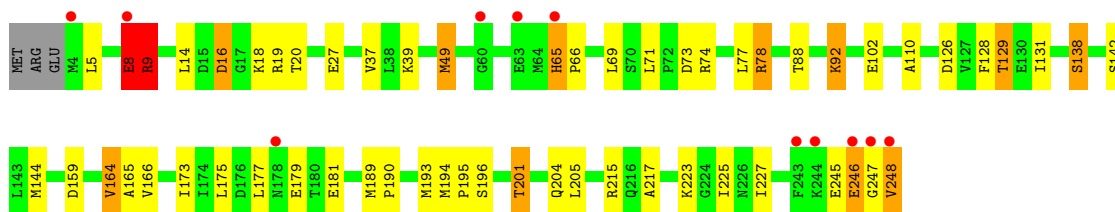
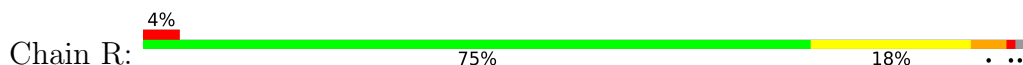
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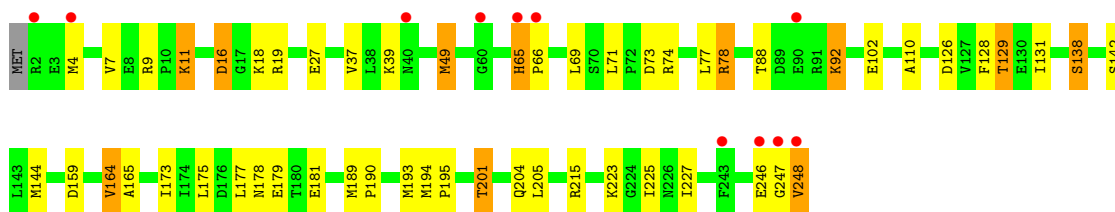
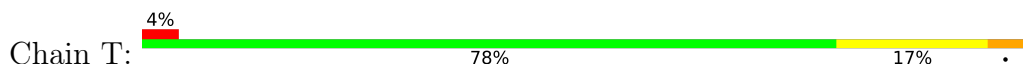
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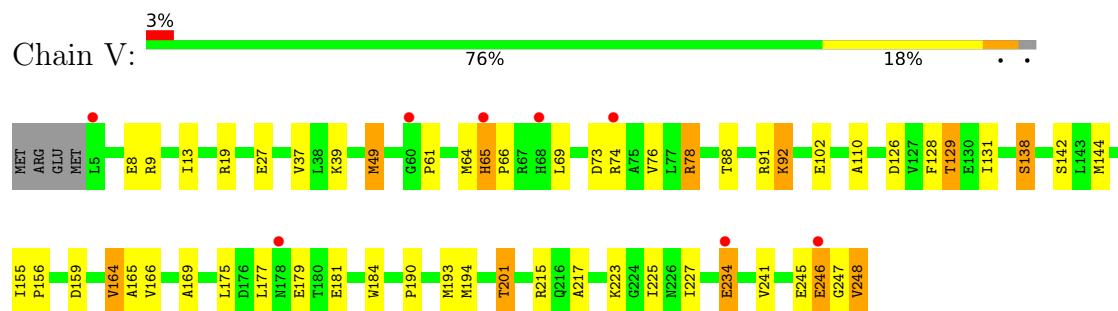
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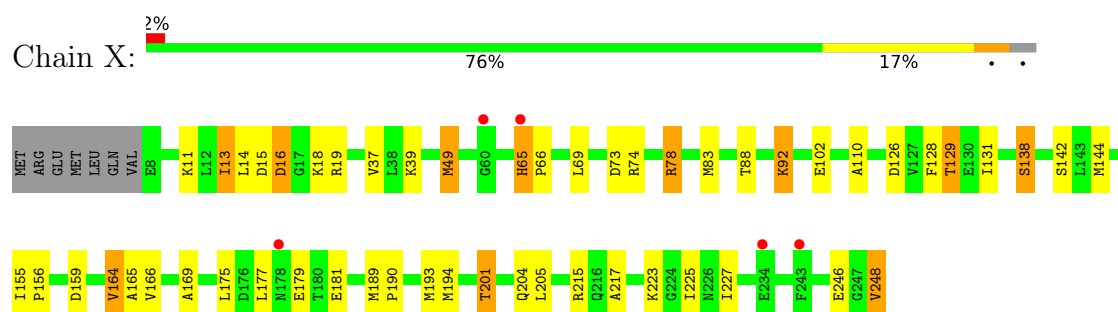
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



- Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



- Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	206.88Å 212.72Å 434.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	218.22 – 2.80 217.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (218.22-2.80) 99.8 (217.03-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.82Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.237 0.227 , 0.245	Depositor DCC
R_{free} test set	7031 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.033 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	46287	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.56	0/1985	0.80	0/2697
1	C	0.62	1/1997 (0.1%)	0.83	3/2711 (0.1%)
1	E	0.57	0/1993	0.80	0/2706
1	G	0.58	0/1989	0.79	0/2701
1	I	0.57	0/1986	0.81	0/2697
1	K	0.63	1/1989 (0.1%)	0.82	3/2701 (0.1%)
1	M	0.57	0/1997	0.80	0/2711
1	O	0.65	2/1993 (0.1%)	0.83	0/2706
1	Q	0.61	1/1993 (0.1%)	0.82	1/2706 (0.0%)
1	S	0.60	0/1992	0.82	0/2706
1	U	0.58	0/1993	0.80	0/2706
1	W	0.57	0/1993	0.78	0/2706
2	B	0.57	0/1891	0.86	3/2553 (0.1%)
2	D	0.58	0/1933	0.88	4/2610 (0.2%)
2	F	0.58	0/1891	0.86	3/2553 (0.1%)
2	H	0.55	0/1891	0.85	1/2553 (0.0%)
2	J	0.57	0/1891	0.85	3/2553 (0.1%)
2	L	0.59	0/1937	0.88	4/2615 (0.2%)
2	N	0.56	0/1891	0.86	2/2553 (0.1%)
2	P	0.61	0/1935	0.87	3/2613 (0.1%)
2	R	0.61	0/1917	0.90	6/2588 (0.2%)
2	T	0.58	0/1933	0.88	1/2610 (0.0%)
2	V	0.58	0/1911	0.85	1/2581 (0.0%)
2	X	0.56	0/1891	0.85	1/2553 (0.0%)
All	All	0.59	5/46812 (0.0%)	0.84	39/63389 (0.1%)

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	O	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	25	LYS	C-N	6.69	1.42	1.33
1	C	234	LYS	C-N	5.82	1.41	1.33
1	K	234	LYS	C-N	5.65	1.41	1.33
1	Q	234	LYS	C-N	5.64	1.41	1.33
1	O	24	GLU	C-N	5.39	1.40	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	8	GLU	CA-C-N	7.44	135.09	121.70
2	R	8	GLU	C-N-CA	7.44	135.09	121.70
1	C	236	VAL	CB-CA-C	6.66	117.30	110.70
2	L	18	LYS	N-CA-C	6.52	120.17	110.52
1	Q	236	VAL	CB-CA-C	6.12	116.76	110.70
2	R	9	ARG	N-CA-CB	5.84	120.44	110.50
2	D	246	GLU	N-CA-C	5.80	117.35	108.42
2	R	246	GLU	CA-C-N	5.76	125.45	119.92
2	R	246	GLU	C-N-CA	5.76	125.45	119.92
2	F	246	GLU	N-CA-C	5.73	117.25	108.42
2	P	246	GLU	N-CA-C	5.71	116.82	108.14
2	T	246	GLU	N-CA-C	5.71	117.22	108.42
2	H	246	GLU	N-CA-C	5.71	116.81	108.14
1	K	236	VAL	CB-CA-C	5.67	116.31	110.70
2	N	246	GLU	N-CA-C	5.66	117.14	108.42
1	C	78	THR	CA-C-N	5.63	125.48	119.28
1	C	78	THR	C-N-CA	5.63	125.48	119.28
2	D	18	LYS	N-CA-C	5.61	118.82	110.52
2	B	246	GLU	N-CA-C	5.60	117.04	108.42
2	L	246	GLU	CA-C-N	5.59	125.28	119.92
2	L	246	GLU	C-N-CA	5.59	125.28	119.92
2	X	246	GLU	N-CA-C	5.57	116.61	108.14
2	J	246	GLU	N-CA-C	5.56	116.98	108.42
2	V	246	GLU	N-CA-C	5.48	116.86	108.42
2	J	246	GLU	CA-C-N	5.47	125.17	119.92
2	J	246	GLU	C-N-CA	5.47	125.17	119.92
1	K	78	THR	CA-C-N	5.40	125.07	119.56
1	K	78	THR	C-N-CA	5.40	125.07	119.56
2	D	246	GLU	CA-C-N	5.39	125.10	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	246	GLU	C-N-CA	5.39	125.10	119.92
2	R	246	GLU	N-CA-C	5.38	116.71	108.42
2	N	17	GLY	N-CA-C	-5.30	107.79	115.27
2	F	246	GLU	CA-C-N	5.28	124.99	119.92
2	F	246	GLU	C-N-CA	5.28	124.99	119.92
2	B	246	GLU	CA-C-N	5.21	124.92	119.92
2	B	246	GLU	C-N-CA	5.21	124.92	119.92
2	L	246	GLU	N-CA-C	5.17	116.38	108.42
2	P	246	GLU	CA-C-N	5.14	124.85	119.92
2	P	246	GLU	C-N-CA	5.14	124.85	119.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	24	GLU	Mainchain

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	1960	0	1996	20	0
1	C	1972	0	2017	23	0
1	E	1968	0	2011	22	0
1	G	1964	0	2007	15	0
1	I	1961	0	2003	26	0
1	K	1964	0	2007	30	0
1	M	1972	0	2017	16	0
1	O	1968	0	2013	17	0
1	Q	1968	0	2013	26	0
1	S	1967	0	2011	22	0
1	U	1968	0	2013	16	0
1	W	1968	0	2011	16	0
2	B	1863	0	1895	38	0
2	D	1905	0	1936	34	0
2	F	1863	0	1895	38	0
2	H	1863	0	1895	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1863	0	1895	50	0
2	L	1909	0	1940	37	0
2	N	1863	0	1895	36	0
2	P	1907	0	1937	44	0
2	R	1889	0	1921	43	0
2	T	1905	0	1936	40	0
2	V	1883	0	1917	37	0
2	X	1863	0	1895	31	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
4	A	6	0	0	2	0
4	B	5	0	0	2	0
4	C	4	0	0	1	0
4	D	1	0	0	0	0
4	E	6	0	0	1	0
4	F	4	0	0	0	0
4	G	2	0	0	0	0
4	H	3	0	0	0	0
4	I	1	0	0	1	0
4	J	5	0	0	0	0
4	K	3	0	0	1	0
4	L	3	0	0	2	0
4	M	8	0	0	2	0
4	N	4	0	0	0	0
4	O	9	0	0	1	0
4	P	6	0	0	0	0
4	Q	4	0	0	1	0
4	R	5	0	0	0	0
4	S	6	0	0	0	0
4	T	4	0	0	0	0
4	U	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	3	0	0	0	0
4	W	2	0	0	1	0
4	X	1	0	0	0	0
All	All	46287	0	47076	638	0

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

All (638) 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:O:62:MET:HE3	4:O:2003:HOH:O	1.59	1.02
2:P:110:ALA:HB1	2:P:201:THR:HG23	1.45	0.99
1:A:272:HIS:HD2	4:A:2001:HOH:O	1.49	0.94
2:T:110:ALA:HB1	2:T:201:THR:HG23	1.50	0.91
2:N:110:ALA:HB1	2:N:201:THR:HG23	1.50	0.91
2:L:110:ALA:HB1	2:L:201:THR:HG23	1.54	0.90
2:D:110:ALA:HB1	2:D:201:THR:HG23	1.53	0.89
2:B:110:ALA:HB1	2:B:201:THR:HG23	1.56	0.87
2:J:110:ALA:HB1	2:J:201:THR:HG23	1.55	0.86
2:X:110:ALA:HB1	2:X:201:THR:HG23	1.56	0.86
2:V:110:ALA:HB1	2:V:201:THR:HG23	1.56	0.86
2:H:110:ALA:HB1	2:H:201:THR:HG23	1.60	0.84
2:R:110:ALA:HB1	2:R:201:THR:HG23	1.60	0.83
2:N:9:ARG:NH2	2:N:184:TRP:O	2.13	0.82
2:F:110:ALA:HB1	2:F:201:THR:HG23	1.61	0.80
1:I:272:HIS:HD2	4:I:2001:HOH:O	1.63	0.80
2:T:19:ARG:HD2	2:T:181:GLU:OE2	1.87	0.74
1:A:253:GLN:HG2	4:A:2006:HOH:O	1.87	0.73
2:X:19:ARG:HD2	2:X:181:GLU:OE2	1.89	0.73
2:L:19:ARG:HD2	2:L:181:GLU:OE2	1.89	0.73
2:P:19:ARG:HD2	2:P:181:GLU:OE2	1.88	0.73
2:D:19:ARG:HD2	2:D:181:GLU:OE2	1.89	0.72
2:N:9:ARG:HG3	2:N:184:TRP:CE3	2.24	0.72
2:P:1:MET:HE3	2:P:2:ARG:H	1.54	0.72
2:P:1:MET:HG3	2:P:3:GLU:H	1.54	0.72
2:P:110:ALA:HB1	2:P:201:THR:CG2	2.18	0.71
2:R:19:ARG:HD2	2:R:181:GLU:OE2	1.91	0.71
1:W:272:HIS:HD2	4:W:2001:HOH:O	1.74	0.70
2:B:19:ARG:HD2	2:B:181:GLU:OE2	1.92	0.70
2:V:19:ARG:HD2	2:V:181:GLU:OE2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:ARG:HD2	2:H:181:GLU:OE2	1.92	0.70
1:K:272:HIS:HD2	4:K:2002:HOH:O	1.76	0.69
2:T:65:HIS:CB	2:T:66:PRO:HD3	2.23	0.68
2:N:19:ARG:HD2	2:N:181:GLU:OE2	1.92	0.68
2:R:65:HIS:CB	2:R:66:PRO:HD3	2.23	0.68
1:O:57:LYS:HG2	1:O:62:MET:HG2	1.74	0.68
2:X:110:ALA:HB1	2:X:201:THR:CG2	2.24	0.68
1:C:243:LYS:HD3	2:D:74:ARG:HH12	1.58	0.68
1:M:112:ARG:NH2	3:M:1276:CL:CL	2.62	0.68
2:T:110:ALA:HB1	2:T:201:THR:CG2	2.23	0.67
2:F:65:HIS:CB	2:F:66:PRO:HD3	2.24	0.67
4:M:2002:HOH:O	2:P:133:GLN:HG2	1.93	0.67
2:F:19:ARG:HD2	2:F:181:GLU:OE2	1.94	0.67
1:S:57:LYS:HG2	1:S:62:MET:HG2	1.76	0.67
2:H:65:HIS:CB	2:H:66:PRO:HD3	2.24	0.67
2:P:65:HIS:CB	2:P:66:PRO:HD3	2.24	0.67
2:J:65:HIS:CB	2:J:66:PRO:HD3	2.25	0.67
2:N:65:HIS:CB	2:N:66:PRO:HD3	2.25	0.67
1:I:243:LYS:HD3	2:J:74:ARG:HH12	1.60	0.66
2:J:110:ALA:HB1	2:J:201:THR:CG2	2.26	0.66
2:B:110:ALA:HB1	2:B:201:THR:CG2	2.24	0.66
2:L:65:HIS:CB	2:L:66:PRO:HD3	2.25	0.66
2:P:110:ALA:CB	2:P:201:THR:HG23	2.22	0.66
2:L:110:ALA:HB1	2:L:201:THR:CG2	2.25	0.65
2:X:65:HIS:CB	2:X:66:PRO:HD3	2.25	0.65
2:D:65:HIS:CB	2:D:66:PRO:HD3	2.26	0.65
2:L:223:LYS:HB3	2:L:248:VAL:HG13	1.78	0.65
2:J:19:ARG:HD2	2:J:181:GLU:OE2	1.96	0.65
2:L:66:PRO:HG2	2:L:69:LEU:HD12	1.78	0.65
1:C:57:LYS:HG2	1:C:62:MET:HG2	1.77	0.65
2:V:65:HIS:CB	2:V:66:PRO:HD3	2.25	0.65
2:B:65:HIS:CB	2:B:66:PRO:HD3	2.26	0.65
1:G:57:LYS:HG2	1:G:62:MET:HG2	1.79	0.65
2:R:8:GLU:CB	2:R:9:ARG:HB2	2.27	0.65
2:T:110:ALA:CB	2:T:201:THR:HG23	2.26	0.65
2:L:110:ALA:CB	2:L:201:THR:HG23	2.27	0.65
2:T:66:PRO:HG2	2:T:69:LEU:HD12	1.78	0.64
1:W:57:LYS:HG2	1:W:62:MET:HG2	1.79	0.64
1:I:57:LYS:HG2	1:I:62:MET:HG2	1.78	0.64
2:B:80:ARG:HD3	4:B:2003:HOH:O	1.97	0.64
1:E:57:LYS:HG2	1:E:62:MET:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:223:LYS:HB3	2:T:248:VAL:HG13	1.80	0.64
2:B:66:PRO:HG2	2:B:69:LEU:HD12	1.80	0.63
2:D:110:ALA:HB1	2:D:201:THR:CG2	2.27	0.63
2:D:223:LYS:HB3	2:D:248:VAL:HG13	1.79	0.63
1:M:57:LYS:HG2	1:M:62:MET:HG2	1.79	0.63
2:F:193:MET:HG3	2:F:225:ILE:HD13	1.81	0.63
2:J:223:LYS:HB3	2:J:248:VAL:HG13	1.80	0.63
2:R:223:LYS:HB3	2:R:248:VAL:HG13	1.80	0.63
2:X:66:PRO:HG2	2:X:69:LEU:HD12	1.81	0.63
2:V:13:ILE:HD11	2:V:169:ALA:HB3	1.79	0.63
2:V:223:LYS:HB3	2:V:248:VAL:HG13	1.81	0.63
2:T:131:ILE:HG12	2:T:138:SER:HB3	1.81	0.62
2:V:66:PRO:HG2	2:V:69:LEU:HD12	1.81	0.62
1:K:57:LYS:HG2	1:K:62:MET:HG2	1.81	0.62
1:Q:57:LYS:HG2	1:Q:62:MET:HG2	1.81	0.62
2:L:131:ILE:HG12	2:L:138:SER:HB3	1.81	0.62
2:H:8:GLU:OE2	2:H:8:GLU:HA	1.99	0.62
2:H:71:LEU:HD13	2:H:74:ARG:HD2	1.81	0.62
2:H:227:ILE:HD12	2:H:248:VAL:HG22	1.82	0.62
2:R:110:ALA:HB1	2:R:201:THR:CG2	2.28	0.62
2:J:66:PRO:HG2	2:J:69:LEU:HD12	1.79	0.62
2:N:78:ARG:HD3	2:N:126:ASP:OD1	1.99	0.62
1:A:81:GLN:HG2	1:A:127:THR:HG22	1.82	0.62
1:U:57:LYS:HG2	1:U:62:MET:HG2	1.81	0.62
2:P:223:LYS:HB3	2:P:248:VAL:HG13	1.81	0.62
2:X:110:ALA:CB	2:X:201:THR:HG23	2.30	0.62
2:D:110:ALA:CB	2:D:201:THR:HG23	2.28	0.62
2:P:73:ASP:OD2	2:P:74:ARG:HG3	2.00	0.62
2:H:66:PRO:HG2	2:H:69:LEU:HD12	1.82	0.61
2:N:66:PRO:HG2	2:N:69:LEU:HD12	1.81	0.61
2:N:110:ALA:HB1	2:N:201:THR:CG2	2.26	0.61
2:V:110:ALA:HB1	2:V:201:THR:CG2	2.28	0.61
2:V:110:ALA:CB	2:V:201:THR:HG23	2.30	0.61
2:B:131:ILE:HG12	2:B:138:SER:HB3	1.82	0.61
2:D:129:THR:HG21	2:D:142:SER:OG	2.00	0.61
2:J:110:ALA:CB	2:J:201:THR:HG23	2.28	0.61
2:N:110:ALA:CB	2:N:201:THR:HG23	2.27	0.61
2:D:78:ARG:HD3	2:D:126:ASP:OD1	2.01	0.61
2:H:91:ARG:HB2	1:I:68:LYS:HG2	1.81	0.61
2:P:193:MET:HG3	2:P:225:ILE:HD13	1.83	0.61
2:R:66:PRO:HG2	2:R:69:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:110:ALA:CB	2:R:201:THR:HG23	2.31	0.61
2:D:66:PRO:HG2	2:D:69:LEU:HD12	1.81	0.61
2:N:73:ASP:OD2	2:N:74:ARG:HG3	2.01	0.61
2:B:227:ILE:HD12	2:B:248:VAL:HG22	1.83	0.61
2:F:223:LYS:HB3	2:F:248:VAL:HG13	1.82	0.61
2:P:66:PRO:HG2	2:P:69:LEU:HD12	1.82	0.60
2:V:129:THR:HG21	2:V:142:SER:OG	2.01	0.60
2:X:223:LYS:HB3	2:X:248:VAL:HG13	1.82	0.60
2:F:78:ARG:HD3	2:F:126:ASP:OD1	2.02	0.60
2:F:131:ILE:HG12	2:F:138:SER:HB3	1.83	0.60
2:B:78:ARG:HD3	2:B:126:ASP:OD1	2.02	0.60
2:N:129:THR:HG21	2:N:142:SER:OG	2.01	0.60
2:B:110:ALA:CB	2:B:201:THR:HG23	2.28	0.60
2:H:223:LYS:HB3	2:H:248:VAL:HG13	1.82	0.60
2:L:73:ASP:OD2	2:L:74:ARG:HG3	2.02	0.60
2:B:223:LYS:HB3	2:B:248:VAL:HG13	1.84	0.60
2:D:227:ILE:HD12	2:D:248:VAL:HG22	1.84	0.60
2:T:78:ARG:HD3	2:T:126:ASP:OD1	2.02	0.60
2:V:164:VAL:HG22	2:V:225:ILE:HG13	1.84	0.60
2:H:89:ASP:O	1:I:184:LYS:NZ	2.34	0.59
2:R:78:ARG:HD3	2:R:126:ASP:OD1	2.01	0.59
2:T:164:VAL:HG22	2:T:225:ILE:HG13	1.83	0.59
2:D:193:MET:HG3	2:D:225:ILE:HD13	1.85	0.59
2:N:131:ILE:HG12	2:N:138:SER:HB3	1.82	0.59
2:X:73:ASP:OD2	2:X:74:ARG:HG3	2.03	0.59
2:V:73:ASP:OD2	2:V:74:ARG:HG3	2.02	0.59
2:L:129:THR:HG21	2:L:142:SER:OG	2.02	0.59
1:A:57:LYS:HG2	1:A:62:MET:HG2	1.84	0.59
2:R:164:VAL:HG22	2:R:225:ILE:HG13	1.85	0.59
2:B:89:ASP:O	1:E:184:LYS:NZ	2.35	0.59
2:F:66:PRO:HG2	2:F:69:LEU:HD12	1.83	0.59
2:V:131:ILE:HG12	2:V:138:SER:HB3	1.85	0.59
2:B:73:ASP:OD2	2:B:74:ARG:HG3	2.02	0.58
2:B:129:THR:HG21	2:B:142:SER:OG	2.03	0.58
2:L:78:ARG:HD3	2:L:126:ASP:OD1	2.03	0.58
2:P:78:ARG:HD3	2:P:126:ASP:OD1	2.03	0.58
2:J:131:ILE:HG12	2:J:138:SER:HB3	1.83	0.58
2:J:193:MET:HG3	2:J:225:ILE:HD13	1.85	0.58
2:V:78:ARG:HD3	2:V:126:ASP:OD1	2.03	0.58
2:L:227:ILE:HD12	2:L:248:VAL:HG22	1.86	0.58
2:F:227:ILE:HD12	2:F:248:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:227:ILE:HD12	2:T:248:VAL:HG22	1.86	0.58
2:X:78:ARG:HD3	2:X:126:ASP:OD1	2.03	0.58
2:D:73:ASP:OD2	2:D:74:ARG:HG3	2.04	0.58
2:V:227:ILE:HD12	2:V:248:VAL:HG22	1.86	0.58
2:F:73:ASP:OD2	2:F:74:ARG:HG3	2.04	0.58
2:R:131:ILE:HG12	2:R:138:SER:HB3	1.86	0.58
2:H:78:ARG:HD3	2:H:126:ASP:OD1	2.04	0.57
2:T:129:THR:HG21	2:T:142:SER:OG	2.04	0.57
2:P:131:ILE:HG12	2:P:138:SER:HB3	1.85	0.57
2:B:193:MET:HG3	2:B:225:ILE:HD13	1.86	0.57
2:J:78:ARG:HD3	2:J:126:ASP:OD1	2.03	0.57
2:P:227:ILE:HD12	2:P:248:VAL:HG22	1.87	0.57
2:J:9:ARG:NH2	2:J:184:TRP:O	2.38	0.57
2:N:223:LYS:HB3	2:N:248:VAL:HG13	1.85	0.57
2:T:193:MET:HG3	2:T:225:ILE:HD13	1.87	0.57
2:B:164:VAL:HG22	2:B:225:ILE:HG13	1.86	0.57
2:F:129:THR:HG21	2:F:142:SER:OG	2.05	0.57
2:H:131:ILE:HG12	2:H:138:SER:HB3	1.86	0.57
1:I:252:ASP:OD1	2:J:215:ARG:NH1	2.36	0.57
2:L:193:MET:HG3	2:L:225:ILE:HD13	1.87	0.57
2:R:73:ASP:OD2	2:R:74:ARG:HG3	2.04	0.57
2:N:193:MET:HG3	2:N:225:ILE:HD13	1.86	0.57
2:R:227:ILE:HD12	2:R:248:VAL:HG22	1.86	0.57
1:C:272:HIS:HD2	4:C:2001:HOH:O	1.88	0.57
2:F:164:VAL:HG22	2:F:225:ILE:HG13	1.86	0.57
2:N:164:VAL:HG22	2:N:225:ILE:HG13	1.87	0.57
1:C:252:ASP:OD1	2:D:215:ARG:NH1	2.37	0.56
2:X:131:ILE:HG12	2:X:138:SER:HB3	1.87	0.56
2:J:73:ASP:OD2	2:J:74:ARG:HG3	2.05	0.56
2:D:131:ILE:HG12	2:D:138:SER:HB3	1.87	0.56
2:H:110:ALA:CB	2:H:201:THR:HG23	2.35	0.56
2:T:73:ASP:OD2	2:T:74:ARG:HG3	2.05	0.56
1:Q:6:SER:HA	2:R:71:LEU:HD21	1.86	0.56
2:X:129:THR:HG21	2:X:142:SER:OG	2.05	0.56
2:H:110:ALA:HB1	2:H:201:THR:CG2	2.32	0.56
2:H:193:MET:HG3	2:H:225:ILE:HD13	1.87	0.56
1:W:230:THR:OG1	1:W:232:ASP:OD1	2.16	0.56
2:X:164:VAL:HG22	2:X:225:ILE:HG13	1.89	0.56
2:L:164:VAL:HG22	2:L:225:ILE:HG13	1.87	0.55
2:J:164:VAL:HG22	2:J:225:ILE:HG13	1.89	0.55
2:N:227:ILE:HD12	2:N:248:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ILE:HD11	2:B:169:ALA:HB3	1.87	0.55
1:E:116:ARG:NH2	2:F:102:GLU:OE1	2.39	0.55
2:X:193:MET:HG3	2:X:225:ILE:HD13	1.88	0.55
2:F:110:ALA:HB1	2:F:201:THR:CG2	2.35	0.55
1:U:204:LYS:HG2	1:U:222:ASP:HB2	1.88	0.55
2:P:164:VAL:HG22	2:P:225:ILE:HG13	1.88	0.55
2:H:164:VAL:HG22	2:H:225:ILE:HG13	1.88	0.54
1:K:116:ARG:NH2	2:L:102:GLU:OE1	2.40	0.54
2:L:80:ARG:HD3	4:L:2003:HOH:O	2.06	0.54
2:P:14:LEU:HD11	2:P:20:THR:HG22	1.89	0.54
2:R:193:MET:HG3	2:R:225:ILE:HD13	1.90	0.54
2:B:91:ARG:HB2	1:E:68:LYS:HG2	1.88	0.54
2:J:129:THR:HG21	2:J:142:SER:OG	2.08	0.54
1:K:28:ARG:NH1	1:K:210:VAL:HG13	2.23	0.54
2:X:227:ILE:HD12	2:X:248:VAL:HG22	1.90	0.54
2:J:15:ASP:OD1	2:J:15:ASP:N	2.35	0.54
2:D:223:LYS:HB3	2:D:248:VAL:CG1	2.38	0.54
2:J:227:ILE:HD12	2:J:248:VAL:HG22	1.89	0.53
1:M:41:SER:HB2	1:M:57:LYS:HB2	1.91	0.53
1:O:28:ARG:NH1	1:O:210:VAL:HG13	2.23	0.53
2:P:129:THR:HG21	2:P:142:SER:OG	2.08	0.53
1:A:7:ASN:O	1:A:8:GLN:C	2.50	0.53
1:S:116:ARG:NH2	2:T:102:GLU:OE1	2.41	0.53
2:D:234:GLU:HG3	2:D:241:VAL:CG2	2.38	0.53
1:G:28:ARG:NH1	1:G:210:VAL:HG13	2.24	0.53
2:N:85:PRO:HD3	1:Q:145:TYR:OH	2.08	0.53
1:W:30:ASP:OD1	1:W:32:ARG:HG2	2.09	0.53
1:S:3:SER:HB3	2:T:78:ARG:HG3	1.91	0.52
2:H:129:THR:HG21	2:H:142:SER:OG	2.10	0.52
2:L:223:LYS:HB3	2:L:248:VAL:CG1	2.39	0.52
1:S:6:SER:HA	2:T:71:LEU:HD21	1.91	0.52
2:D:159:ASP:HB3	2:D:194:MET:HB3	1.92	0.52
1:G:41:SER:HB2	1:G:57:LYS:HB2	1.92	0.52
1:Q:28:ARG:NH1	1:Q:210:VAL:HG13	2.25	0.52
2:N:88:THR:HG21	2:N:92:LYS:HE3	1.92	0.52
2:N:13:ILE:HD11	2:N:169:ALA:HB3	1.92	0.52
2:J:9:ARG:HG2	2:J:184:TRP:CE3	2.45	0.52
2:N:11:LYS:HE3	2:N:14:LEU:HA	1.92	0.52
1:C:116:ARG:NH2	2:D:102:GLU:OE1	2.42	0.51
2:L:159:ASP:HB3	2:L:194:MET:HB3	1.92	0.51
1:G:14:ILE:HD12	1:G:14:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:ARG:NH2	2:J:102:GLU:OE1	2.44	0.51
2:J:166:VAL:HG13	2:J:217:ALA:HB1	1.92	0.51
2:V:49:MET:HE2	2:V:144:MET:HE1	1.93	0.51
1:G:148:ASP:OD1	2:L:40:ASN:HB2	2.10	0.51
1:O:30:ASP:OD1	1:O:32:ARG:HG2	2.11	0.51
1:E:28:ARG:NH1	1:E:210:VAL:HG13	2.25	0.51
2:J:89:ASP:O	1:K:184:LYS:NZ	2.43	0.51
2:V:223:LYS:HB3	2:V:248:VAL:CG1	2.40	0.51
2:D:88:THR:HG21	2:D:92:LYS:HE3	1.93	0.51
1:S:28:ARG:NH1	1:S:210:VAL:HG13	2.25	0.51
1:U:41:SER:HB2	1:U:57:LYS:HB2	1.91	0.51
2:D:189:MET:HE3	2:D:205:LEU:HD13	1.93	0.51
2:R:129:THR:HG21	2:R:142:SER:OG	2.09	0.51
1:E:240:LYS:HG2	1:E:241:SER:N	2.25	0.51
1:K:252:ASP:OD1	2:L:215:ARG:NH1	2.41	0.51
1:C:28:ARG:NH1	1:C:210:VAL:HG13	2.26	0.51
1:S:3:SER:HA	2:T:77:LEU:O	2.11	0.51
1:U:28:ARG:NH1	1:U:210:VAL:HG13	2.26	0.51
2:D:164:VAL:HG22	2:D:225:ILE:HG13	1.93	0.51
2:P:1:MET:HE3	2:P:2:ARG:N	2.24	0.51
1:Q:3:SER:HA	2:R:77:LEU:O	2.11	0.51
2:H:126:ASP:HB3	2:H:128:PHE:CE1	2.46	0.50
2:H:106:VAL:HG12	2:H:202:LEU:HD22	1.93	0.50
2:P:16:ASP:C	2:P:18:LYS:H	2.19	0.50
1:U:30:ASP:OD1	1:U:32:ARG:HG2	2.11	0.50
2:R:223:LYS:HB3	2:R:248:VAL:CG1	2.41	0.50
2:J:133:GLN:NE2	1:K:48:LYS:HB2	2.27	0.50
1:M:14:ILE:H	1:M:14:ILE:HD12	1.77	0.50
1:M:30:ASP:OD1	1:M:32:ARG:HG2	2.12	0.50
1:Q:240:LYS:HG2	1:Q:241:SER:N	2.26	0.50
2:J:223:LYS:HB3	2:J:248:VAL:CG1	2.42	0.50
2:N:9:ARG:HG2	2:N:9:ARG:HH11	1.77	0.50
2:X:16:ASP:OD2	2:X:18:LYS:HB2	2.11	0.50
1:A:28:ARG:NH1	1:A:210:VAL:HG13	2.27	0.50
2:V:88:THR:HG21	2:V:92:LYS:HE3	1.93	0.50
1:E:14:ILE:HD12	1:E:14:ILE:H	1.76	0.50
2:V:193:MET:HG3	2:V:225:ILE:HD13	1.93	0.50
1:O:112:ARG:HD3	2:P:102:GLU:OE1	2.12	0.49
2:H:9:ARG:NH2	2:H:184:TRP:O	2.44	0.49
1:S:68:LYS:HG2	2:V:91:ARG:HB2	1.94	0.49
1:A:7:ASN:O	1:A:8:GLN:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:ALA:CB	2:F:201:THR:HG23	2.37	0.49
2:J:196:SER:HB3	1:O:27:ILE:HG21	1.95	0.49
2:D:126:ASP:HB3	2:D:128:PHE:CE1	2.48	0.49
2:P:73:ASP:CG	2:P:74:ARG:HG3	2.38	0.49
1:W:81:GLN:HG2	1:W:127:THR:HG22	1.95	0.49
1:I:28:ARG:NH1	1:I:210:VAL:HG13	2.27	0.49
2:J:13:ILE:HD11	2:J:169:ALA:HB3	1.94	0.49
2:P:190:PRO:HG2	2:P:204:GLN:HB2	1.95	0.49
2:T:189:MET:HE3	2:T:205:LEU:HD13	1.95	0.49
1:U:14:ILE:HD12	1:U:14:ILE:H	1.77	0.49
1:C:204:LYS:HE2	1:C:206:ASP:O	2.13	0.48
2:F:106:VAL:HG12	2:F:202:LEU:HD22	1.95	0.48
2:H:88:THR:HG21	2:H:92:LYS:HE3	1.95	0.48
1:I:30:ASP:OD1	1:I:32:ARG:HG2	2.13	0.48
2:T:4:MET:O	2:T:4:MET:HG3	2.13	0.48
2:V:126:ASP:HB3	2:V:128:PHE:CE1	2.48	0.48
2:J:88:THR:HG21	2:J:92:LYS:HE3	1.94	0.48
1:K:116:ARG:HH22	2:L:102:GLU:CD	2.21	0.48
1:Q:14:ILE:HD12	1:Q:14:ILE:H	1.77	0.48
2:R:126:ASP:HB3	2:R:128:PHE:CE1	2.49	0.48
1:Q:252:ASP:OD1	2:R:215:ARG:NH1	2.46	0.48
1:A:112:ARG:HD3	2:B:102:GLU:OE1	2.14	0.48
2:T:223:LYS:HB3	2:T:248:VAL:CG1	2.42	0.48
2:B:159:ASP:HB3	2:B:194:MET:HB3	1.94	0.48
2:B:88:THR:HG21	2:B:92:LYS:HE3	1.95	0.48
1:I:14:ILE:HD12	1:I:14:ILE:H	1.79	0.48
2:X:49:MET:HE2	2:X:144:MET:HE1	1.95	0.48
2:F:15:ASP:OD1	2:F:15:ASP:N	2.47	0.48
1:K:240:LYS:HG2	1:K:241:SER:N	2.28	0.48
2:L:190:PRO:HG2	2:L:204:GLN:HB2	1.95	0.48
1:U:116:ARG:NH2	2:V:102:GLU:OE1	2.47	0.48
2:J:159:ASP:HB3	2:J:194:MET:HB3	1.95	0.48
1:Q:116:ARG:NH2	2:R:102:GLU:OE1	2.46	0.48
1:W:14:ILE:HD12	1:W:14:ILE:H	1.79	0.48
2:X:88:THR:HG21	2:X:92:LYS:HE3	1.94	0.48
2:X:126:ASP:HB3	2:X:128:PHE:CE1	2.49	0.48
1:I:240:LYS:HG2	1:I:241:SER:N	2.28	0.48
2:P:49:MET:HE2	2:P:144:MET:HE1	1.95	0.48
2:H:82:HIS:HE1	1:I:145:TYR:OH	1.97	0.47
2:L:49:MET:HE2	2:L:144:MET:HE1	1.96	0.47
1:O:41:SER:HB2	1:O:57:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:49:MET:HE2	2:R:144:MET:HE1	1.96	0.47
1:S:240:LYS:HG2	1:S:241:SER:N	2.29	0.47
1:A:14:ILE:HD12	1:A:14:ILE:H	1.79	0.47
2:B:126:ASP:HB3	2:B:128:PHE:CE1	2.48	0.47
2:F:223:LYS:HB3	2:F:248:VAL:CG1	2.44	0.47
2:H:223:LYS:HB3	2:H:248:VAL:CG1	2.44	0.47
2:L:11:LYS:HD2	2:L:11:LYS:HA	1.68	0.47
1:S:3:SER:HB3	2:T:78:ARG:CG	2.45	0.47
1:E:252:ASP:OD1	2:F:215:ARG:NH1	2.45	0.47
2:H:159:ASP:HB3	2:H:194:MET:HB3	1.96	0.47
2:J:82:HIS:HE1	1:K:145:TYR:OH	1.98	0.47
2:V:13:ILE:CD1	2:V:169:ALA:HB3	2.44	0.47
2:X:223:LYS:HB3	2:X:248:VAL:CG1	2.44	0.47
1:O:28:ARG:CZ	1:O:210:VAL:HG13	2.45	0.47
1:U:243:LYS:HD3	2:V:74:ARG:HH12	1.80	0.47
1:C:14:ILE:H	1:C:14:ILE:HD12	1.80	0.47
2:N:13:ILE:CD1	2:N:169:ALA:HB3	2.45	0.47
2:N:126:ASP:HB3	2:N:128:PHE:CE1	2.50	0.47
2:T:88:THR:HG21	2:T:92:LYS:HE3	1.97	0.47
2:P:159:ASP:HB3	2:P:194:MET:HB3	1.97	0.47
1:K:230:THR:OG1	1:K:232:ASP:OD1	2.29	0.46
1:O:240:LYS:HG2	1:O:241:SER:N	2.29	0.46
1:U:240:LYS:HG2	1:U:241:SER:N	2.29	0.46
2:V:9:ARG:NH2	2:V:184:TRP:O	2.48	0.46
2:V:19:ARG:NH2	2:V:175:LEU:O	2.41	0.46
1:G:28:ARG:CZ	1:G:210:VAL:HG13	2.45	0.46
1:I:3:SER:HB3	2:J:78:ARG:CG	2.45	0.46
1:K:28:ARG:CZ	1:K:210:VAL:HG13	2.45	0.46
1:M:240:LYS:HG2	1:M:241:SER:N	2.30	0.46
1:S:30:ASP:OD1	1:S:32:ARG:HG2	2.16	0.46
1:S:112:ARG:HD3	2:T:102:GLU:OE1	2.15	0.46
2:F:126:ASP:HB3	2:F:128:PHE:CE1	2.51	0.46
2:P:19:ARG:NH2	2:P:175:LEU:O	2.41	0.46
2:P:223:LYS:HB3	2:P:248:VAL:CG1	2.43	0.46
1:Q:3:SER:HB3	2:R:78:ARG:HG3	1.97	0.46
1:K:243:LYS:HD3	2:L:74:ARG:HH12	1.80	0.46
1:Q:41:SER:HB2	1:Q:57:LYS:HB2	1.96	0.46
1:W:28:ARG:NH1	1:W:210:VAL:HG13	2.30	0.46
1:G:30:ASP:OD1	1:G:32:ARG:HG2	2.15	0.46
1:G:240:LYS:HG2	1:G:241:SER:N	2.31	0.46
1:K:14:ILE:HD12	1:K:14:ILE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:LEU:N	1:O:92:PRO:CD	2.79	0.46
2:P:126:ASP:HB3	2:P:128:PHE:CE1	2.50	0.46
1:Q:91:LEU:N	1:Q:92:PRO:CD	2.79	0.46
1:S:14:ILE:HD12	1:S:14:ILE:H	1.79	0.46
1:S:116:ARG:HH22	2:T:102:GLU:CD	2.23	0.46
1:K:30:ASP:OD1	1:K:32:ARG:HG2	2.15	0.46
2:L:73:ASP:CG	2:L:74:ARG:HG3	2.41	0.46
2:L:126:ASP:HB3	2:L:128:PHE:CE1	2.50	0.46
1:Q:28:ARG:CZ	1:Q:210:VAL:HG13	2.45	0.46
2:R:19:ARG:NH2	2:R:175:LEU:O	2.42	0.46
2:R:165:ALA:HA	2:R:190:PRO:HA	1.98	0.46
1:W:112:ARG:HD3	2:X:102:GLU:OE1	2.15	0.46
1:W:240:LYS:HG2	1:W:241:SER:N	2.29	0.46
2:N:189:MET:HE3	2:N:205:LEU:HD13	1.97	0.46
2:T:126:ASP:HB3	2:T:128:PHE:CE1	2.51	0.46
1:C:116:ARG:HH22	2:D:102:GLU:CD	2.24	0.46
2:D:49:MET:HE2	2:D:144:MET:HE1	1.98	0.46
2:R:159:ASP:HB3	2:R:194:MET:HB3	1.98	0.46
2:F:190:PRO:HG2	2:F:204:GLN:HB2	1.98	0.46
1:I:13:ILE:H	1:I:13:ILE:HG13	1.58	0.46
1:W:42:ILE:HG12	1:W:56:VAL:HG22	1.98	0.46
2:F:19:ARG:NH2	2:F:175:LEU:O	2.41	0.45
2:F:49:MET:HE2	2:F:144:MET:HE1	1.97	0.45
1:K:91:LEU:N	1:K:92:PRO:CD	2.78	0.45
1:A:240:LYS:HG2	1:A:241:SER:N	2.31	0.45
2:B:138:SER:OG	4:B:2005:HOH:O	2.21	0.45
2:D:11:LYS:HD2	2:D:11:LYS:HA	1.71	0.45
1:E:32:ARG:CZ	1:E:38:ARG:HG3	2.46	0.45
2:H:64:MET:HE2	2:H:124:ALA:HB2	1.98	0.45
1:K:41:SER:HB2	1:K:57:LYS:HB2	1.96	0.45
2:T:159:ASP:HB3	2:T:194:MET:HB3	1.97	0.45
2:X:165:ALA:HA	2:X:190:PRO:HA	1.97	0.45
1:A:91:LEU:N	1:A:92:PRO:CD	2.80	0.45
2:H:15:ASP:OD1	2:H:15:ASP:N	2.45	0.45
2:H:165:ALA:HA	2:H:190:PRO:HA	1.98	0.45
2:R:88:THR:HG21	2:R:92:LYS:HE3	1.97	0.45
2:X:11:LYS:HE3	2:X:14:LEU:HA	1.99	0.45
1:C:91:LEU:N	1:C:92:PRO:CD	2.80	0.45
2:D:165:ALA:HA	2:D:190:PRO:HA	1.99	0.45
2:F:165:ALA:HA	2:F:190:PRO:HA	1.99	0.45
1:I:270:LYS:HB3	1:I:275:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:189:MET:HE3	2:P:205:LEU:HD13	1.98	0.45
2:F:73:ASP:CG	2:F:74:ARG:HG3	2.42	0.45
1:S:91:LEU:N	1:S:92:PRO:CD	2.80	0.45
2:T:193:MET:O	2:T:195:PRO:HD3	2.17	0.45
1:W:91:LEU:N	1:W:92:PRO:CD	2.79	0.45
1:G:91:LEU:N	1:G:92:PRO:CD	2.79	0.45
2:J:49:MET:HE2	2:J:144:MET:HE1	1.99	0.45
2:N:130:GLU:HG3	1:Q:91:LEU:HD13	1.99	0.45
2:R:14:LEU:HD11	2:R:20:THR:HA	1.99	0.45
2:F:88:THR:HG21	2:F:92:LYS:HE3	1.99	0.45
1:Q:30:ASP:OD1	1:Q:32:ARG:HG2	2.17	0.45
2:V:73:ASP:CG	2:V:74:ARG:HG3	2.41	0.45
1:C:145:TYR:OH	2:F:85:PRO:HD3	2.16	0.45
2:D:73:ASP:CG	2:D:74:ARG:HG3	2.42	0.45
1:I:3:SER:HB3	2:J:78:ARG:HG3	1.99	0.45
1:O:14:ILE:H	1:O:14:ILE:HD12	1.82	0.45
2:H:190:PRO:HG2	2:H:204:GLN:HB2	1.99	0.45
1:I:116:ARG:HH22	2:J:102:GLU:CD	2.25	0.45
2:N:49:MET:HE2	2:N:144:MET:HE1	1.99	0.45
1:U:91:LEU:N	1:U:92:PRO:CD	2.80	0.45
1:E:116:ARG:HH22	2:F:102:GLU:CD	2.25	0.45
2:F:159:ASP:HB3	2:F:194:MET:HB3	1.99	0.45
2:H:64:MET:HE1	2:H:76:VAL:HB	1.99	0.45
2:J:126:ASP:HB3	2:J:128:PHE:CE1	2.52	0.45
1:O:168:THR:HB	1:O:191:LEU:HD22	1.99	0.45
1:Q:240:LYS:NZ	4:Q:2004:HOH:O	2.48	0.45
2:B:189:MET:HE3	2:B:205:LEU:HD13	1.98	0.44
2:B:223:LYS:HB3	2:B:248:VAL:CG1	2.45	0.44
1:E:204:LYS:HE3	1:E:206:ASP:O	2.17	0.44
1:K:168:THR:HB	1:K:191:LEU:HD22	1.99	0.44
1:S:75:TYR:N	1:S:75:TYR:CD1	2.85	0.44
2:V:159:ASP:HB3	2:V:194:MET:HB3	1.99	0.44
2:V:165:ALA:HA	2:V:190:PRO:HA	1.99	0.44
2:H:86:PHE:HB2	1:I:50:ALA:HB2	2.00	0.44
1:K:133:PRO:C	1:K:135:LYS:H	2.25	0.44
1:M:28:ARG:NH1	1:M:210:VAL:HG13	2.32	0.44
1:Q:168:THR:HB	1:Q:191:LEU:HD22	2.00	0.44
2:T:65:HIS:CB	2:T:66:PRO:CD	2.95	0.44
2:T:73:ASP:CG	2:T:74:ARG:HG3	2.42	0.44
1:I:41:SER:HB2	1:I:57:LYS:HB2	1.98	0.44
2:N:159:ASP:HB3	2:N:194:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:168:THR:HB	1:S:191:LEU:HD22	1.99	0.44
1:A:255:GLU:OE2	2:B:215:ARG:NH2	2.50	0.44
2:B:190:PRO:HG2	2:B:204:GLN:HB2	1.99	0.44
2:R:189:MET:HE3	2:R:205:LEU:HD13	1.99	0.44
2:X:73:ASP:CG	2:X:74:ARG:HG3	2.42	0.44
1:A:28:ARG:CZ	1:A:210:VAL:HG13	2.48	0.44
1:C:168:THR:HB	1:C:191:LEU:HD22	1.99	0.44
1:E:3:SER:HB3	2:F:78:ARG:CG	2.47	0.44
1:E:91:LEU:N	1:E:92:PRO:CD	2.80	0.44
2:B:15:ASP:OD1	2:B:15:ASP:N	2.50	0.44
1:E:243:LYS:HD3	2:F:74:ARG:HH12	1.82	0.44
1:M:91:LEU:N	1:M:92:PRO:CD	2.80	0.44
1:M:184:LYS:NZ	2:P:89:ASP:O	2.51	0.44
2:P:88:THR:HG21	2:P:92:LYS:HE3	1.99	0.44
1:A:41:SER:HB2	1:A:57:LYS:HB2	1.98	0.44
2:J:155:ILE:HA	2:J:156:PRO:HD3	1.86	0.44
2:N:223:LYS:HB3	2:N:248:VAL:CG1	2.48	0.44
2:R:73:ASP:CG	2:R:74:ARG:HG3	2.42	0.44
2:L:88:THR:HG21	2:L:92:LYS:HE3	1.98	0.44
1:O:3:SER:HB3	2:P:78:ARG:CG	2.48	0.44
1:S:252:ASP:OD1	2:T:215:ARG:NH1	2.51	0.44
2:T:190:PRO:HG2	2:T:204:GLN:HB2	2.00	0.44
2:B:73:ASP:CG	2:B:74:ARG:HG3	2.42	0.44
1:C:28:ARG:CZ	1:C:210:VAL:HG13	2.48	0.44
2:X:13:ILE:CD1	2:X:169:ALA:HB3	2.48	0.44
2:B:166:VAL:HG13	2:B:217:ALA:HB1	2.00	0.43
1:G:11:ILE:HA	1:G:12:PRO:HD3	1.94	0.43
1:I:91:LEU:N	1:I:92:PRO:CD	2.81	0.43
1:Q:3:SER:HB3	2:R:78:ARG:CG	2.48	0.43
2:T:165:ALA:HA	2:T:190:PRO:HA	2.00	0.43
2:B:61:PRO:HD3	2:B:155:ILE:HD11	2.00	0.43
1:C:32:ARG:CZ	1:C:38:ARG:HG3	2.48	0.43
2:H:65:HIS:CB	2:H:66:PRO:CD	2.96	0.43
2:J:91:ARG:HB2	1:K:68:LYS:HG2	1.99	0.43
1:K:255:GLU:HG2	2:L:214:PHE:CE2	2.53	0.43
2:L:165:ALA:HA	2:L:190:PRO:HA	2.00	0.43
2:P:65:HIS:CB	2:P:66:PRO:CD	2.96	0.43
2:X:190:PRO:HG2	2:X:204:GLN:HB2	1.99	0.43
1:K:27:ILE:HG21	2:R:196:SER:HB3	2.00	0.43
2:P:165:ALA:HA	2:P:190:PRO:HA	1.99	0.43
1:C:41:SER:HB2	1:C:57:LYS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:HG2	1:C:241:SER:N	2.33	0.43
2:H:49:MET:HE2	2:H:144:MET:HE1	1.99	0.43
2:J:165:ALA:HA	2:J:190:PRO:HA	2.00	0.43
1:M:243:LYS:HD3	2:N:74:ARG:HH12	1.83	0.43
2:T:11:LYS:HD2	2:T:11:LYS:HA	1.59	0.43
2:B:49:MET:HE2	2:B:144:MET:HE1	2.00	0.43
2:N:73:ASP:CG	2:N:74:ARG:HG3	2.43	0.43
2:T:49:MET:HE2	2:T:144:MET:HE1	1.99	0.43
1:E:41:SER:HB2	1:E:57:LYS:HB2	2.01	0.43
1:M:252:ASP:OD1	2:N:215:ARG:NH1	2.51	0.43
1:S:38:ARG:HD2	1:S:59:GLY:HA3	2.01	0.43
1:W:255:GLU:OE2	2:X:215:ARG:NH2	2.51	0.43
1:E:38:ARG:HD2	1:E:59:GLY:HA3	2.01	0.43
1:O:106:ASN:OD1	2:P:105:LYS:HE3	2.18	0.43
2:J:9:ARG:HB3	2:J:9:ARG:NH1	2.33	0.43
1:K:42:ILE:HG12	1:K:56:VAL:HG22	2.01	0.43
2:P:166:VAL:HG13	2:P:217:ALA:HB1	2.00	0.43
2:J:85:PRO:HD3	1:K:145:TYR:OH	2.18	0.43
2:X:159:ASP:HB3	2:X:194:MET:HB3	2.00	0.43
2:J:86:PHE:HB2	1:K:50:ALA:HB2	2.01	0.43
2:J:190:PRO:HG2	2:J:204:GLN:HB2	2.00	0.43
2:N:64:MET:HE1	2:N:76:VAL:HB	2.01	0.43
2:P:14:LEU:HD12	2:P:20:THR:HA	2.01	0.43
1:C:68:LYS:HG2	2:F:91:ARG:HB2	2.01	0.42
1:E:108:ILE:O	1:E:112:ARG:HG3	2.19	0.42
1:G:116:ARG:NH2	2:H:102:GLU:OE1	2.52	0.42
1:K:32:ARG:CZ	1:K:38:ARG:HG3	2.50	0.42
2:D:155:ILE:HA	2:D:156:PRO:HD3	1.87	0.42
2:L:195:PRO:HG2	2:L:229:TYR:CD1	2.54	0.42
1:A:204:LYS:HE3	1:A:206:ASP:O	2.19	0.42
1:I:168:THR:HB	1:I:191:LEU:HD22	2.02	0.42
1:K:13:ILE:H	1:K:13:ILE:HG13	1.59	0.42
2:R:190:PRO:HG2	2:R:204:GLN:HB2	2.00	0.42
1:U:32:ARG:CZ	1:U:38:ARG:HG3	2.49	0.42
1:C:11:ILE:HA	1:C:12:PRO:HD3	1.94	0.42
1:E:168:THR:HB	1:E:191:LEU:HD22	2.01	0.42
2:F:65:HIS:CB	2:F:66:PRO:CD	2.96	0.42
2:J:189:MET:HE3	2:J:205:LEU:HD13	2.02	0.42
1:U:204:LYS:HE2	1:U:206:ASP:O	2.18	0.42
1:W:11:ILE:HA	1:W:12:PRO:HD3	1.93	0.42
2:X:166:VAL:HG13	2:X:217:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:VAL:HG13	2:H:217:ALA:HB1	2.02	0.42
1:Q:38:ARG:HD2	1:Q:59:GLY:HA3	2.00	0.42
1:S:28:ARG:CZ	1:S:210:VAL:HG13	2.50	0.42
2:V:61:PRO:HD3	2:V:155:ILE:HD11	2.01	0.42
2:H:189:MET:HE3	2:H:205:LEU:HD13	2.01	0.42
2:J:193:MET:O	2:J:195:PRO:HD3	2.20	0.42
1:Q:112:ARG:HD3	2:R:102:GLU:OE1	2.19	0.42
2:B:165:ALA:HA	2:B:190:PRO:HA	2.02	0.42
1:E:28:ARG:CZ	1:E:210:VAL:HG13	2.49	0.42
2:L:189:MET:HE3	2:L:205:LEU:HD13	2.01	0.42
1:M:13:ILE:H	1:M:13:ILE:HG13	1.60	0.42
2:N:65:HIS:CB	2:N:66:PRO:CD	2.97	0.42
1:Q:116:ARG:HH22	2:R:102:GLU:CD	2.28	0.42
2:R:193:MET:O	2:R:195:PRO:HD3	2.19	0.42
2:V:155:ILE:HA	2:V:156:PRO:HD3	1.87	0.42
2:B:155:ILE:HA	2:B:156:PRO:HD3	1.84	0.42
1:I:28:ARG:CZ	1:I:210:VAL:HG13	2.49	0.42
2:R:14:LEU:CD1	2:R:20:THR:HA	2.50	0.42
2:B:193:MET:O	2:B:195:PRO:HD3	2.20	0.42
1:M:272:HIS:HD2	4:M:2001:HOH:O	2.01	0.42
1:S:41:SER:HB2	1:S:57:LYS:HB2	2.02	0.42
2:V:245:GLU:O	2:V:246:GLU:HB3	2.19	0.42
1:C:133:PRO:C	1:C:135:LYS:H	2.28	0.42
2:P:160:LEU:HD11	2:P:236:LEU:HD22	2.02	0.42
1:U:28:ARG:CZ	1:U:210:VAL:HG13	2.50	0.42
2:V:27:GLU:HG2	2:V:247:GLY:HA2	2.02	0.42
1:C:16:LYS:HG3	1:C:220:ILE:HB	2.02	0.41
1:I:32:ARG:CZ	1:I:38:ARG:HG3	2.50	0.41
2:J:13:ILE:CD1	2:J:169:ALA:HB3	2.50	0.41
2:N:190:PRO:HG2	2:N:204:GLN:HB2	2.02	0.41
1:O:32:ARG:CZ	1:O:38:ARG:HG3	2.50	0.41
2:R:65:HIS:CB	2:R:66:PRO:CD	2.95	0.41
2:V:64:MET:HE1	2:V:76:VAL:HB	2.01	0.41
1:C:232:ASP:O	1:C:233:LEU:HB2	2.20	0.41
2:F:61:PRO:HD3	2:F:155:ILE:HD11	2.01	0.41
1:G:32:ARG:CZ	1:G:38:ARG:HG3	2.50	0.41
2:H:126:ASP:HB3	2:H:128:PHE:HE1	1.84	0.41
1:I:255:GLU:HG2	2:J:214:PHE:CE2	2.55	0.41
2:J:64:MET:HE1	2:J:76:VAL:HB	2.02	0.41
2:L:65:HIS:CB	2:L:66:PRO:CD	2.97	0.41
2:P:64:MET:HE2	2:P:124:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ASP:OD1	1:E:32:ARG:HG2	2.20	0.41
1:M:28:ARG:CZ	1:M:210:VAL:HG13	2.50	0.41
1:M:38:ARG:HD2	1:M:59:GLY:HA3	2.02	0.41
2:P:195:PRO:HG2	2:P:229:TYR:CD1	2.55	0.41
2:T:19:ARG:NH2	2:T:175:LEU:O	2.44	0.41
2:X:155:ILE:HA	2:X:156:PRO:HD3	1.86	0.41
2:H:195:PRO:HG2	2:H:229:TYR:CD1	2.55	0.41
2:J:73:ASP:CG	2:J:74:ARG:HG3	2.45	0.41
1:M:32:ARG:CZ	1:M:38:ARG:HG3	2.50	0.41
1:Q:91:LEU:H	1:Q:92:PRO:HD3	1.86	0.41
2:R:16:ASP:C	2:R:18:LYS:H	2.29	0.41
1:A:30:ASP:OD1	1:A:32:ARG:HG2	2.21	0.41
2:B:64:MET:HE2	2:B:124:ALA:HB2	2.03	0.41
2:F:64:MET:HE1	2:F:76:VAL:HB	2.02	0.41
2:J:65:HIS:CB	2:J:66:PRO:CD	2.97	0.41
2:N:165:ALA:HA	2:N:190:PRO:HA	2.02	0.41
1:S:243:LYS:HE2	2:T:74:ARG:HH12	1.85	0.41
1:U:270:LYS:HB3	1:U:275:ILE:HG12	2.03	0.41
1:G:255:GLU:OE2	2:H:215:ARG:NH2	2.52	0.41
2:P:16:ASP:O	2:P:18:LYS:N	2.54	0.41
1:K:3:SER:HB3	2:L:78:ARG:HG3	2.01	0.41
2:P:11:LYS:HD2	2:P:11:LYS:HA	1.60	0.41
2:V:166:VAL:HG13	2:V:217:ALA:HB1	2.03	0.41
1:A:13:ILE:H	1:A:13:ILE:HG13	1.62	0.41
1:A:168:THR:HB	1:A:191:LEU:HD22	2.02	0.41
2:F:189:MET:HE3	2:F:205:LEU:HD13	2.01	0.41
1:I:38:ARG:HD2	1:I:59:GLY:HA3	2.02	0.41
2:J:166:VAL:CG1	2:J:217:ALA:HB1	2.51	0.41
1:Q:142:LEU:HD21	1:Q:161:SER:HB3	2.02	0.41
2:D:65:HIS:CB	2:D:66:PRO:CD	2.98	0.41
2:F:166:VAL:HG13	2:F:217:ALA:HB1	2.02	0.41
2:L:245:GLU:O	2:L:246:GLU:HB3	2.20	0.41
1:Q:81:GLN:HG2	1:Q:82:GLY:O	2.21	0.41
2:T:178:ASN:HB2	2:T:181:GLU:H	1.86	0.41
1:U:252:ASP:OD1	2:V:215:ARG:NH1	2.52	0.41
1:W:168:THR:HB	1:W:191:LEU:HD22	2.03	0.41
2:X:189:MET:HE3	2:X:205:LEU:HD13	2.02	0.41
1:A:60:THR:HG22	2:D:39:LYS:HG2	2.03	0.41
2:B:19:ARG:NH2	2:B:175:LEU:O	2.45	0.41
2:D:190:PRO:HG2	2:D:204:GLN:HB2	2.02	0.41
2:H:160:LEU:HD11	2:H:236:LEU:HD22	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:82:HIS:HE1	1:Q:145:TYR:OH	2.04	0.41
2:P:61:PRO:HD3	2:P:155:ILE:HD11	2.03	0.41
2:H:245:GLU:O	2:H:246:GLU:HB3	2.20	0.40
2:L:65:HIS:HA	4:L:2001:HOH:O	2.20	0.40
1:O:91:LEU:HD12	1:O:147:LEU:HD23	2.03	0.40
2:P:10:PRO:HD2	2:P:184:TRP:CD2	2.56	0.40
2:R:8:GLU:CB	2:R:9:ARG:CB	2.97	0.40
1:A:32:ARG:CZ	1:A:38:ARG:HG3	2.52	0.40
1:C:230:THR:OG1	1:C:232:ASP:OD1	2.36	0.40
2:J:88:THR:O	1:K:68:LYS:CE	2.69	0.40
2:R:27:GLU:HG2	2:R:247:GLY:HA2	2.02	0.40
2:R:166:VAL:HG13	2:R:217:ALA:HB1	2.03	0.40
2:T:16:ASP:C	2:T:18:LYS:H	2.30	0.40
1:W:41:SER:HB2	1:W:57:LYS:HB2	2.03	0.40
2:X:19:ARG:NH2	2:X:175:LEU:O	2.45	0.40
1:G:104:ASP:HB3	1:G:107:ALA:HB3	2.02	0.40
1:I:11:ILE:HA	1:I:12:PRO:HD3	1.92	0.40
1:O:91:LEU:H	1:O:92:PRO:HD3	1.86	0.40
2:B:245:GLU:O	2:B:246:GLU:HB3	2.21	0.40
2:D:166:VAL:HG13	2:D:217:ALA:HB1	2.03	0.40
2:D:234:GLU:HG3	2:D:241:VAL:HG21	2.03	0.40
1:E:6:SER:HA	2:F:71:LEU:HD21	2.04	0.40
1:E:83:ASN:HA	4:E:2003:HOH:O	2.20	0.40
1:G:270:LYS:HB3	1:G:275:ILE:HG12	2.02	0.40
2:L:64:MET:HE1	2:L:76:VAL:HB	2.03	0.40
1:Q:108:ILE:O	1:Q:112:ARG:HG3	2.21	0.40
2:T:27:GLU:HG2	2:T:247:GLY:HA2	2.03	0.40
1:U:116:ARG:HH22	2:V:102:GLU:CD	2.29	0.40
2:V:234:GLU:HB3	2:V:241:VAL:HG21	2.03	0.40
1:W:32:ARG:CZ	1:W:38:ARG:HG3	2.51	0.40
1:C:30:ASP:OD1	1:C:32:ARG:HG2	2.20	0.40
1:K:91:LEU:H	1:K:92:PRO:HD3	1.87	0.40
2:R:245:GLU:O	2:R:246:GLU:HB3	2.21	0.40
1:S:75:TYR:N	1:S:75:TYR:HD1	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	16	44
1	C	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	16	44
1	E	254/275 (92%)	247 (97%)	6 (2%)	1 (0%)	30	60
1	G	254/275 (92%)	247 (97%)	5 (2%)	2 (1%)	16	44
1	I	254/275 (92%)	243 (96%)	9 (4%)	2 (1%)	16	44
1	K	254/275 (92%)	245 (96%)	8 (3%)	1 (0%)	30	60
1	M	254/275 (92%)	244 (96%)	9 (4%)	1 (0%)	30	60
1	O	254/275 (92%)	245 (96%)	8 (3%)	1 (0%)	30	60
1	Q	254/275 (92%)	243 (96%)	9 (4%)	2 (1%)	16	44
1	S	254/275 (92%)	248 (98%)	5 (2%)	1 (0%)	30	60
1	U	254/275 (92%)	244 (96%)	8 (3%)	2 (1%)	16	44
1	W	254/275 (92%)	247 (97%)	6 (2%)	1 (0%)	30	60
2	B	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	30	60
2	D	245/248 (99%)	231 (94%)	12 (5%)	2 (1%)	16	44
2	F	239/248 (96%)	228 (95%)	9 (4%)	2 (1%)	16	44
2	H	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	30	60
2	J	239/248 (96%)	228 (95%)	10 (4%)	1 (0%)	30	60
2	L	245/248 (99%)	230 (94%)	13 (5%)	2 (1%)	16	44
2	N	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	30	60
2	P	246/248 (99%)	232 (94%)	12 (5%)	2 (1%)	16	44
2	R	243/248 (98%)	226 (93%)	13 (5%)	4 (2%)	7	27
2	T	245/248 (99%)	229 (94%)	14 (6%)	2 (1%)	16	44
2	V	242/248 (98%)	229 (95%)	11 (4%)	2 (1%)	16	44
2	X	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	30	60
All	All	5948/6276 (95%)	5684 (96%)	225 (4%)	39 (1%)	18	47

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
1	C	105	GLU
1	E	105	GLU
1	G	105	GLU
1	I	105	GLU
1	K	105	GLU
1	M	105	GLU
1	O	105	GLU
1	Q	105	GLU
2	R	9	ARG
1	S	105	GLU
1	U	105	GLU
1	W	105	GLU
1	A	8	GLN
1	G	8	GLN
1	I	8	GLN
2	P	16	ASP
1	Q	8	GLN
2	R	8	GLU
2	R	16	ASP
2	T	16	ASP
2	V	8	GLU
2	D	16	ASP
2	L	16	ASP
2	T	65	HIS
1	U	8	GLN
2	B	65	HIS
2	D	65	HIS
2	F	65	HIS
2	F	136	ALA
2	J	65	HIS
2	L	65	HIS
2	N	65	HIS
2	P	65	HIS
2	R	65	HIS
2	V	65	HIS
2	X	65	HIS
2	H	65	HIS
1	C	134	GLY

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	216/242 (89%)	205 (95%)	11 (5%)	21	54
1	C	219/242 (90%)	206 (94%)	13 (6%)	18	48
1	E	218/242 (90%)	207 (95%)	11 (5%)	22	54
1	G	217/242 (90%)	208 (96%)	9 (4%)	27	62
1	I	216/242 (89%)	207 (96%)	9 (4%)	26	61
1	K	217/242 (90%)	206 (95%)	11 (5%)	21	54
1	M	219/242 (90%)	208 (95%)	11 (5%)	22	54
1	O	218/242 (90%)	209 (96%)	9 (4%)	27	62
1	Q	218/242 (90%)	206 (94%)	12 (6%)	19	51
1	S	218/242 (90%)	206 (94%)	12 (6%)	19	51
1	U	218/242 (90%)	206 (94%)	12 (6%)	19	51
1	W	218/242 (90%)	208 (95%)	10 (5%)	24	58
2	B	199/208 (96%)	184 (92%)	15 (8%)	12	37
2	D	203/208 (98%)	187 (92%)	16 (8%)	11	35
2	F	199/208 (96%)	183 (92%)	16 (8%)	11	34
2	H	199/208 (96%)	181 (91%)	18 (9%)	9	28
2	J	199/208 (96%)	185 (93%)	14 (7%)	14	40
2	L	204/208 (98%)	188 (92%)	16 (8%)	11	35
2	N	199/208 (96%)	183 (92%)	16 (8%)	11	34
2	P	203/208 (98%)	186 (92%)	17 (8%)	10	32
2	R	201/208 (97%)	187 (93%)	14 (7%)	14	40
2	T	203/208 (98%)	187 (92%)	16 (8%)	11	35
2	V	201/208 (97%)	188 (94%)	13 (6%)	15	43
2	X	199/208 (96%)	183 (92%)	16 (8%)	11	34
All	All	5021/5400 (93%)	4704 (94%)	317 (6%)	16	45

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	ILE
1	A	24	GLU
1	A	188	VAL
1	A	191	LEU
1	A	197	VAL
1	A	200	ILE
1	A	210	VAL
1	A	233	LEU
1	A	236	VAL
1	A	255	GLU
2	B	15	ASP
2	B	37	VAL
2	B	39	LYS
2	B	49	MET
2	B	78	ARG
2	B	83	MET
2	B	92	LYS
2	B	129	THR
2	B	138	SER
2	B	164	VAL
2	B	173	ILE
2	B	177	LEU
2	B	179	GLU
2	B	201	THR
2	B	248	VAL
1	C	8	GLN
1	C	13	ILE
1	C	24	GLU
1	C	80	ASN
1	C	188	VAL
1	C	191	LEU
1	C	197	VAL
1	C	200	ILE
1	C	204	LYS
1	C	210	VAL
1	C	233	LEU
1	C	236	VAL
1	C	255	GLU
2	D	5	LEU
2	D	7	VAL
2	D	11	LYS
2	D	37	VAL

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Mol	Chain	Res	Type
2	D	39	LYS
2	D	49	MET
2	D	78	ARG
2	D	92	LYS
2	D	129	THR
2	D	138	SER
2	D	164	VAL
2	D	177	LEU
2	D	179	GLU
2	D	201	THR
2	D	236	LEU
2	D	248	VAL
1	E	13	ILE
1	E	24	GLU
1	E	188	VAL
1	E	191	LEU
1	E	197	VAL
1	E	200	ILE
1	E	204	LYS
1	E	210	VAL
1	E	233	LEU
1	E	236	VAL
1	E	255	GLU
2	F	13	ILE
2	F	15	ASP
2	F	37	VAL
2	F	39	LYS
2	F	49	MET
2	F	78	ARG
2	F	83	MET
2	F	92	LYS
2	F	129	THR
2	F	138	SER
2	F	164	VAL
2	F	177	LEU
2	F	179	GLU
2	F	201	THR
2	F	202	LEU
2	F	248	VAL
1	G	13	ILE
1	G	24	GLU
1	G	188	VAL

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Mol	Chain	Res	Type
1	G	191	LEU
1	G	197	VAL
1	G	210	VAL
1	G	233	LEU
1	G	236	VAL
1	G	255	GLU
2	H	8	GLU
2	H	13	ILE
2	H	37	VAL
2	H	39	LYS
2	H	49	MET
2	H	74	ARG
2	H	78	ARG
2	H	83	MET
2	H	92	LYS
2	H	129	THR
2	H	138	SER
2	H	164	VAL
2	H	177	LEU
2	H	179	GLU
2	H	201	THR
2	H	202	LEU
2	H	236	LEU
2	H	248	VAL
1	I	13	ILE
1	I	24	GLU
1	I	188	VAL
1	I	191	LEU
1	I	197	VAL
1	I	210	VAL
1	I	233	LEU
1	I	236	VAL
1	I	255	GLU
2	J	13	ILE
2	J	15	ASP
2	J	37	VAL
2	J	39	LYS
2	J	78	ARG
2	J	83	MET
2	J	92	LYS
2	J	129	THR
2	J	138	SER

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Mol	Chain	Res	Type
2	J	164	VAL
2	J	177	LEU
2	J	179	GLU
2	J	201	THR
2	J	248	VAL
1	K	13	ILE
1	K	24	GLU
1	K	81	GLN
1	K	188	VAL
1	K	191	LEU
1	K	197	VAL
1	K	200	ILE
1	K	210	VAL
1	K	233	LEU
1	K	236	VAL
1	K	255	GLU
2	L	11	LYS
2	L	37	VAL
2	L	39	LYS
2	L	49	MET
2	L	78	ARG
2	L	92	LYS
2	L	129	THR
2	L	138	SER
2	L	164	VAL
2	L	173	ILE
2	L	177	LEU
2	L	179	GLU
2	L	201	THR
2	L	234	GLU
2	L	236	LEU
2	L	248	VAL
1	M	8	GLN
1	M	13	ILE
1	M	24	GLU
1	M	188	VAL
1	M	191	LEU
1	M	197	VAL
1	M	200	ILE
1	M	210	VAL
1	M	233	LEU
1	M	236	VAL

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Mol	Chain	Res	Type
1	M	255	GLU
2	N	13	ILE
2	N	16	ASP
2	N	37	VAL
2	N	39	LYS
2	N	78	ARG
2	N	83	MET
2	N	92	LYS
2	N	119	LEU
2	N	129	THR
2	N	138	SER
2	N	164	VAL
2	N	177	LEU
2	N	179	GLU
2	N	201	THR
2	N	236	LEU
2	N	248	VAL
1	O	13	ILE
1	O	24	GLU
1	O	188	VAL
1	O	191	LEU
1	O	197	VAL
1	O	210	VAL
1	O	233	LEU
1	O	236	VAL
1	O	255	GLU
2	P	11	LYS
2	P	37	VAL
2	P	39	LYS
2	P	49	MET
2	P	78	ARG
2	P	83	MET
2	P	92	LYS
2	P	119	LEU
2	P	129	THR
2	P	138	SER
2	P	164	VAL
2	P	173	ILE
2	P	177	LEU
2	P	179	GLU
2	P	201	THR
2	P	236	LEU

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Mol	Chain	Res	Type
2	P	248	VAL
1	Q	13	ILE
1	Q	24	GLU
1	Q	80	ASN
1	Q	188	VAL
1	Q	191	LEU
1	Q	197	VAL
1	Q	200	ILE
1	Q	210	VAL
1	Q	233	LEU
1	Q	236	VAL
1	Q	243	LYS
1	Q	255	GLU
2	R	5	LEU
2	R	37	VAL
2	R	39	LYS
2	R	49	MET
2	R	78	ARG
2	R	92	LYS
2	R	129	THR
2	R	138	SER
2	R	164	VAL
2	R	173	ILE
2	R	177	LEU
2	R	179	GLU
2	R	201	THR
2	R	248	VAL
1	S	13	ILE
1	S	24	GLU
1	S	188	VAL
1	S	191	LEU
1	S	197	VAL
1	S	200	ILE
1	S	204	LYS
1	S	210	VAL
1	S	233	LEU
1	S	236	VAL
1	S	243	LYS
1	S	255	GLU
2	T	7	VAL
2	T	9	ARG
2	T	11	LYS

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Mol	Chain	Res	Type
2	T	37	VAL
2	T	39	LYS
2	T	49	MET
2	T	78	ARG
2	T	92	LYS
2	T	129	THR
2	T	138	SER
2	T	164	VAL
2	T	173	ILE
2	T	177	LEU
2	T	179	GLU
2	T	201	THR
2	T	248	VAL
1	U	8	GLN
1	U	13	ILE
1	U	24	GLU
1	U	188	VAL
1	U	191	LEU
1	U	197	VAL
1	U	200	ILE
1	U	204	LYS
1	U	210	VAL
1	U	233	LEU
1	U	236	VAL
1	U	255	GLU
2	V	37	VAL
2	V	39	LYS
2	V	49	MET
2	V	78	ARG
2	V	92	LYS
2	V	129	THR
2	V	138	SER
2	V	164	VAL
2	V	177	LEU
2	V	179	GLU
2	V	201	THR
2	V	234	GLU
2	V	248	VAL
1	W	13	ILE
1	W	24	GLU
1	W	188	VAL
1	W	191	LEU

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Mol	Chain	Res	Type
1	W	197	VAL
1	W	200	ILE
1	W	210	VAL
1	W	233	LEU
1	W	236	VAL
1	W	255	GLU
2	X	13	ILE
2	X	15	ASP
2	X	16	ASP
2	X	37	VAL
2	X	39	LYS
2	X	49	MET
2	X	78	ARG
2	X	83	MET
2	X	92	LYS
2	X	129	THR
2	X	138	SER
2	X	164	VAL
2	X	177	LEU
2	X	179	GLU
2	X	201	THR
2	X	248	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	183	ASN
1	A	253	GLN
1	A	272	HIS
2	B	178	ASN
2	B	199	GLN
2	B	216	GLN
1	C	83	ASN
1	C	183	ASN
1	C	272	HIS
2	D	178	ASN
2	D	216	GLN
1	E	80	ASN
1	E	183	ASN
2	F	178	ASN
2	F	216	GLN

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Mol	Chain	Res	Type
1	G	83	ASN
1	G	183	ASN
2	H	40	ASN
2	H	178	ASN
2	H	216	GLN
1	I	81	GLN
1	I	183	ASN
1	I	253	GLN
1	I	272	HIS
2	J	178	ASN
2	J	198	ASN
2	J	216	GLN
1	K	83	ASN
1	K	183	ASN
1	K	272	HIS
2	L	178	ASN
2	L	198	ASN
2	L	216	GLN
1	M	9	ASN
1	M	81	GLN
1	M	83	ASN
1	M	183	ASN
1	M	272	HIS
2	N	178	ASN
2	N	198	ASN
2	N	216	GLN
1	O	8	GLN
1	O	83	ASN
1	O	183	ASN
1	O	272	HIS
2	P	178	ASN
2	P	216	GLN
1	Q	83	ASN
1	Q	183	ASN
1	Q	253	GLN
2	R	178	ASN
2	R	216	GLN
1	S	81	GLN
1	S	83	ASN
1	S	183	ASN
2	T	178	ASN
2	T	198	ASN

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Mol	Chain	Res	Type
2	T	216	GLN
1	U	80	ASN
1	U	83	ASN
1	U	183	ASN
2	V	178	ASN
2	V	216	GLN
1	W	83	ASN
1	W	183	ASN
1	W	272	HIS
2	X	178	ASN
2	X	198	ASN
2	X	216	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/275 (94%)	0.38	21 (8%) 18 13	23, 32, 46, 60	0
1	C	260/275 (94%)	0.33	17 (6%) 25 18	24, 32, 46, 58	0
1	E	260/275 (94%)	0.24	15 (5%) 29 22	24, 32, 46, 57	0
1	G	260/275 (94%)	0.49	19 (7%) 21 15	24, 32, 46, 58	0
1	I	260/275 (94%)	0.26	16 (6%) 26 20	24, 32, 46, 57	0
1	K	260/275 (94%)	0.30	17 (6%) 25 18	24, 32, 46, 58	0
1	M	260/275 (94%)	0.26	17 (6%) 25 18	24, 32, 46, 58	0
1	O	260/275 (94%)	0.39	24 (9%) 14 10	24, 32, 46, 59	0
1	Q	260/275 (94%)	0.28	17 (6%) 25 18	24, 32, 46, 59	0
1	S	260/275 (94%)	0.28	15 (5%) 29 22	24, 32, 46, 57	0
1	U	260/275 (94%)	0.31	15 (5%) 29 22	24, 32, 46, 58	0
1	W	260/275 (94%)	0.31	17 (6%) 25 18	24, 32, 46, 57	0
2	B	241/248 (97%)	0.16	8 (3%) 49 39	25, 31, 46, 59	0
2	D	247/248 (99%)	0.26	9 (3%) 46 37	22, 30, 46, 59	0
2	F	241/248 (97%)	0.14	10 (4%) 41 33	25, 31, 47, 59	0
2	H	241/248 (97%)	0.25	8 (3%) 49 39	25, 31, 46, 59	0
2	J	241/248 (97%)	0.20	9 (3%) 45 36	25, 31, 46, 59	0
2	L	247/248 (99%)	0.27	12 (4%) 35 27	22, 31, 46, 59	0
2	N	241/248 (97%)	0.18	11 (4%) 37 29	25, 31, 46, 59	0
2	P	248/248 (100%)	0.18	6 (2%) 59 49	23, 30, 46, 59	0
2	R	245/248 (98%)	0.24	11 (4%) 38 30	23, 31, 46, 59	0
2	T	247/248 (99%)	0.16	11 (4%) 38 30	22, 31, 46, 59	0
2	V	244/248 (98%)	0.09	8 (3%) 49 39	25, 31, 46, 59	0
2	X	241/248 (97%)	0.12	5 (2%) 63 54	25, 31, 46, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	6044/6276 (96%)	0.26	318 (5%) 32 24	22, 31, 47, 60	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	175	GLN	5.6
1	S	181	SER	5.5
2	R	60	GLY	5.3
2	P	60	GLY	5.3
2	L	60	GLY	5.3
1	O	175	GLN	5.2
1	S	180	ILE	5.1
1	O	181	SER	5.0
1	G	8	GLN	4.9
2	F	246	GLU	4.8
1	K	175	GLN	4.7
1	S	174	GLU	4.6
1	M	180	ILE	4.4
2	D	248	VAL	4.4
1	Q	181	SER	4.3
1	O	8	GLN	4.3
2	L	65	HIS	4.2
2	B	65	HIS	4.2
1	A	180	ILE	4.2
2	T	65	HIS	4.1
1	C	175	GLN	4.1
1	W	180	ILE	4.1
1	W	175	GLN	4.1
2	L	169	ALA	4.0
1	Q	175	GLN	4.0
1	K	181	SER	3.9
1	K	92	PRO	3.9
1	K	8	GLN	3.9
1	O	180	ILE	3.9
1	G	77	ASP	3.9
2	F	65	HIS	3.9
1	W	76	GLU	3.9
1	E	175	GLN	3.9
1	C	92	PRO	3.9
1	G	175	GLN	3.8
2	H	60	GLY	3.8
2	L	90	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	174	GLU	3.8
1	C	10	ILE	3.8
1	Q	174	GLU	3.7
1	U	275	ILE	3.7
1	W	8	GLN	3.7
1	M	181	SER	3.7
1	O	9	ASN	3.7
1	A	181	SER	3.7
1	M	8	GLN	3.7
2	R	248	VAL	3.7
1	E	77	ASP	3.6
1	W	80	ASN	3.6
1	U	175	GLN	3.6
1	C	77	ASP	3.6
1	G	181	SER	3.5
2	D	246	GLU	3.5
1	G	275	ILE	3.5
1	I	8	GLN	3.5
1	E	180	ILE	3.5
1	Q	9	ASN	3.5
1	I	9	ASN	3.4
1	O	10	ILE	3.4
1	A	7	ASN	3.4
1	O	7	ASN	3.4
1	A	11	ILE	3.4
1	S	7	ASN	3.4
2	T	60	GLY	3.3
1	Q	10	ILE	3.3
1	W	10	ILE	3.3
1	I	175	GLN	3.3
1	E	173	VAL	3.3
2	N	15	ASP	3.3
2	D	60	GLY	3.3
2	R	65	HIS	3.3
2	T	246	GLU	3.3
1	E	181	SER	3.3
2	H	178	ASN	3.2
1	E	10	ILE	3.2
1	S	10	ILE	3.2
1	U	180	ILE	3.2
2	P	65	HIS	3.2
1	C	8	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	173	VAL	3.2
1	M	175	GLN	3.2
2	R	246	GLU	3.2
1	C	180	ILE	3.2
1	Q	8	GLN	3.2
1	U	8	GLN	3.2
1	Q	180	ILE	3.2
2	F	60	GLY	3.2
2	P	246	GLU	3.2
1	C	181	SER	3.2
1	G	11	ILE	3.2
1	I	77	ASP	3.1
2	D	65	HIS	3.1
2	L	248	VAL	3.1
2	P	1	MET	3.1
1	S	8	GLN	3.1
1	U	174	GLU	3.1
1	A	173	VAL	3.0
2	X	60	GLY	3.0
1	M	10	ILE	3.0
1	Q	11	ILE	3.0
1	W	275	ILE	3.0
1	I	92	PRO	3.0
1	G	130	VAL	3.0
1	I	7	ASN	3.0
1	I	10	ILE	3.0
1	A	80	ASN	3.0
1	M	174	GLU	3.0
2	J	15	ASP	3.0
2	D	243	PHE	3.0
2	L	74	ARG	2.9
2	N	184	TRP	2.9
1	U	10	ILE	2.9
1	W	7	ASN	2.9
1	Q	185	ASN	2.9
1	S	182	VAL	2.9
2	T	248	VAL	2.9
2	J	65	HIS	2.9
1	E	275	ILE	2.9
2	F	66	PRO	2.9
1	C	7	ASN	2.9
1	I	173	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	175	GLN	2.8
1	G	174	GLU	2.8
2	T	90	GLU	2.8
2	D	169	ALA	2.8
2	H	15	ASP	2.8
1	O	11	ILE	2.8
1	U	76	GLU	2.8
1	K	10	ILE	2.8
1	M	77	ASP	2.8
1	A	8	GLN	2.8
2	J	60	GLY	2.8
1	A	174	GLU	2.7
1	C	1	MET	2.7
1	W	181	SER	2.7
2	F	247	GLY	2.7
2	L	246	GLU	2.7
1	G	91	LEU	2.7
1	Q	171	TYR	2.7
1	C	9	ASN	2.7
2	R	247	GLY	2.7
2	F	63	GLU	2.7
2	J	246	GLU	2.7
1	S	275	ILE	2.7
1	E	92	PRO	2.7
1	A	10	ILE	2.7
2	X	65	HIS	2.7
2	V	60	GLY	2.7
1	O	186	GLU	2.7
1	M	75	TYR	2.6
1	K	7	ASN	2.6
1	S	9	ASN	2.6
2	H	40	ASN	2.6
2	N	9	ARG	2.6
1	U	92	PRO	2.6
1	I	185	ASN	2.6
2	V	246	GLU	2.6
1	U	75	TYR	2.6
1	Q	275	ILE	2.6
1	K	1	MET	2.6
1	K	149	TYR	2.6
1	G	76	GLU	2.6
2	N	8	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	X	178	ASN	2.6
1	O	131	ILE	2.5
1	U	1	MET	2.5
1	A	185	ASN	2.5
1	U	181	SER	2.5
2	R	4	MET	2.5
1	E	185	ASN	2.5
2	P	178	ASN	2.5
2	H	244	LYS	2.5
1	M	92	PRO	2.5
1	G	180	ILE	2.5
1	C	249	GLN	2.5
1	K	9	ASN	2.5
1	M	9	ASN	2.5
1	A	77	ASP	2.5
1	Q	92	PRO	2.5
2	B	63	GLU	2.5
1	E	8	GLN	2.5
2	N	68	HIS	2.5
1	M	185	ASN	2.5
2	D	89	ASP	2.4
1	W	174	GLU	2.4
1	A	75	TYR	2.4
1	O	172	LYS	2.4
2	H	240	TYR	2.4
1	K	180	ILE	2.4
1	C	174	GLU	2.4
2	J	11	LYS	2.4
2	R	243	PHE	2.4
1	O	171	TYR	2.4
2	V	68	HIS	2.4
1	O	92	PRO	2.4
2	F	73	ASP	2.4
2	F	248	VAL	2.4
1	O	174	GLU	2.4
2	R	63	GLU	2.4
1	C	149	TYR	2.4
1	M	275	ILE	2.4
1	G	185	ASN	2.4
1	S	134	GLY	2.4
1	Q	104	ASP	2.4
2	N	234	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	X	234	GLU	2.4
2	H	169	ALA	2.4
1	I	181	SER	2.4
1	I	275	ILE	2.4
1	E	104	ASP	2.3
1	O	77	ASP	2.3
2	P	243	PHE	2.3
1	K	267	GLU	2.3
2	B	246	GLU	2.3
2	J	8	GLU	2.3
2	R	8	GLU	2.3
1	W	79	PRO	2.3
2	T	66	PRO	2.3
1	O	173	VAL	2.3
1	Q	182	VAL	2.3
2	N	40	ASN	2.3
2	V	234	GLU	2.3
1	G	131	ILE	2.3
1	W	9	ASN	2.3
2	R	178	ASN	2.3
1	K	174	GLU	2.3
1	W	1	MET	2.3
1	A	29	GLN	2.3
2	F	68	HIS	2.3
1	A	92	PRO	2.3
1	K	185	ASN	2.3
1	I	174	GLU	2.3
1	O	1	MET	2.3
1	S	14	ILE	2.3
1	U	11	ILE	2.3
1	W	75	TYR	2.3
1	E	183	ASN	2.2
1	A	135	LYS	2.2
1	A	131	ILE	2.2
1	M	1	MET	2.2
1	K	80	ASN	2.2
1	I	11	ILE	2.2
1	C	104	ASP	2.2
2	B	68	HIS	2.2
1	W	92	PRO	2.2
2	N	240	TYR	2.2
2	T	4	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	267	GLU	2.2
1	O	185	ASN	2.2
1	A	13	ILE	2.2
1	G	10	ILE	2.2
1	K	14	ILE	2.2
1	W	77	ASP	2.2
2	T	247	GLY	2.2
2	F	8	GLU	2.2
1	G	7	ASN	2.2
2	J	40	ASN	2.2
2	V	65	HIS	2.2
1	C	130	VAL	2.2
1	M	104	ASP	2.2
2	N	60	GLY	2.2
1	I	37	TYR	2.2
2	T	243	PHE	2.2
1	S	185	ASN	2.1
2	D	68	HIS	2.1
1	Q	173	VAL	2.1
2	J	69	LEU	2.1
2	N	65	HIS	2.1
1	M	183	ASN	2.1
2	B	40	ASN	2.1
1	O	182	VAL	2.1
1	O	188	VAL	2.1
2	H	66	PRO	2.1
2	L	89	ASP	2.1
2	L	247	GLY	2.1
2	X	243	PHE	2.1
1	G	37	TYR	2.1
1	G	136	SER	2.1
1	O	14	ILE	2.1
1	O	275	ILE	2.1
1	Q	13	ILE	2.1
2	D	90	GLU	2.1
1	C	256	ASN	2.1
1	M	130	VAL	2.1
1	M	173	VAL	2.1
1	O	104	ASP	2.1
2	B	60	GLY	2.1
2	V	74	ARG	2.1
1	A	132	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	149	TYR	2.1
1	O	184	LYS	2.1
1	U	80	ASN	2.1
2	T	40	ASN	2.1
2	V	178	ASN	2.1
2	N	17	GLY	2.1
2	B	15	ASP	2.1
1	A	76	GLU	2.1
2	R	244	LYS	2.0
2	V	5	LEU	2.0
2	J	247	GLY	2.0
2	L	2	ARG	2.0
2	L	243	PHE	2.0
2	T	2	ARG	2.0
1	S	77	ASP	2.0
1	K	37	TYR	2.0
1	U	171	TYR	2.0
1	S	173	VAL	2.0
1	I	183	ASN	2.0
2	B	243	PHE	2.0
1	K	275	ILE	2.0
1	U	13	ILE	2.0
1	A	104	ASP	2.0
1	C	120	ASP	2.0
1	I	104	ASP	2.0
1	Q	77	ASP	2.0
1	W	132	GLU	2.0
1	E	1	MET	2.0
2	L	7	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	B	1249	1/1	0.88	0.14	67,67,67,67	0
3	CL	D	1249	1/1	0.90	0.11	49,49,49,49	0
3	CL	J	1249	1/1	0.90	0.10	47,47,47,47	0
3	CL	V	1249	1/1	0.90	0.11	52,52,52,52	0
3	CL	P	1249	1/1	0.91	0.12	59,59,59,59	0
3	CL	N	1249	1/1	0.91	0.14	56,56,56,56	0
3	CL	T	1249	1/1	0.92	0.10	50,50,50,50	0
3	CL	L	1249	1/1	0.93	0.07	45,45,45,45	0
3	CL	X	1249	1/1	0.94	0.10	43,43,43,43	0
3	CL	R	1249	1/1	0.95	0.07	46,46,46,46	0
3	CL	F	1249	1/1	0.95	0.08	48,48,48,48	0
3	CL	H	1249	1/1	0.97	0.05	52,52,52,52	0
3	CL	M	1276	1/1	0.97	0.08	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.