Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:52 AM GMT

PDB ID	:	2BR2
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
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:

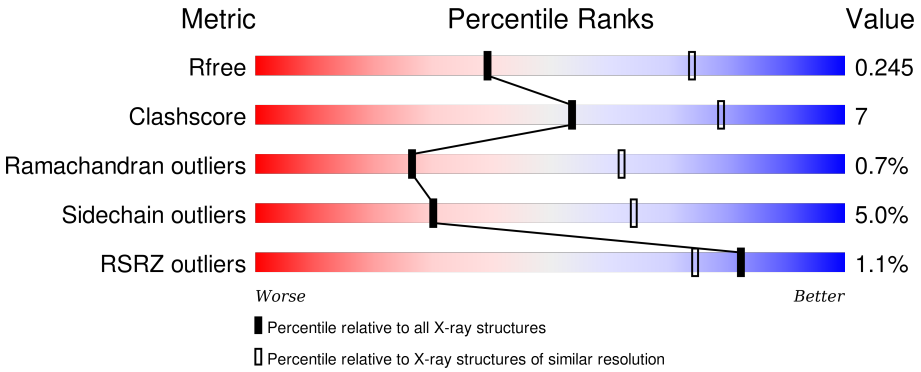
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	275	2% 82% 12% • 5%
1	C	275	81% 13% • 5%
1	E	275	% 82% 12% • 5%
1	G	275	3% 83% 11% 5%
1	I	275	81% 13% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	275	81% 13% • 5%
1	M	275	84% 10% 5%
1	O	275	2% 84% 11% 5%
1	Q	275	% 81% 13% 5%
1	S	275	% 83% 11% • 5%
1	U	275	% 83% 11% • 5%
1	W	275	% 83% 11% • 5%
2	B	248	75% 19% • •
2	D	248	% 81% 15% •
2	F	248	2% 76% 17% • •
2	H	248	% 74% 19% • •
2	J	248	75% 19% • •
2	L	248	3% 80% 17% •
2	N	248	77% 17% • •
2	P	248	% 76% 21% •
2	R	248	2% 76% 19% • ••
2	T	248	% 80% 16% •
2	V	248	% 75% 20% • •
2	X	248	77% 17% • •

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

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

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

Continued on next page...

Continued from previous page...

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 (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	V	1	Total	Cl	0	0
			1	1		
3	T	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		
3	X	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	M	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

Continued on next page...

Continued from previous page...

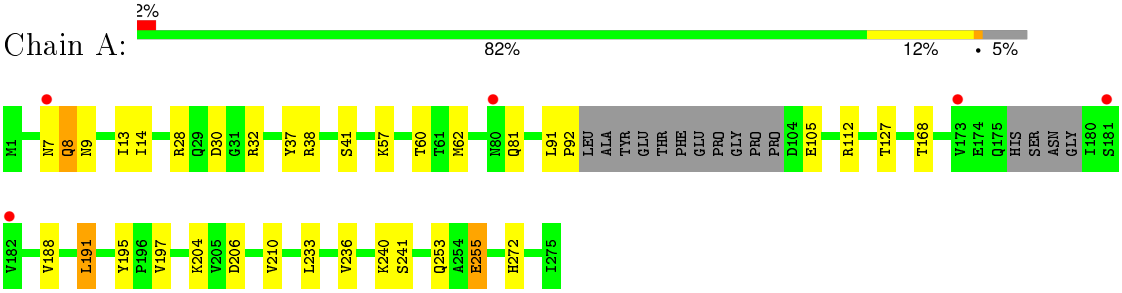
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	6	Total O 6 6	0	0
4	Q	4	Total O 4 4	0	0
4	R	5	Total O 5 5	0	0
4	S	6	Total O 6 6	0	0
4	T	4	Total O 4 4	0	0
4	U	3	Total O 3 3	0	0
4	V	3	Total O 3 3	0	0
4	W	2	Total O 2 2	0	0
4	X	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

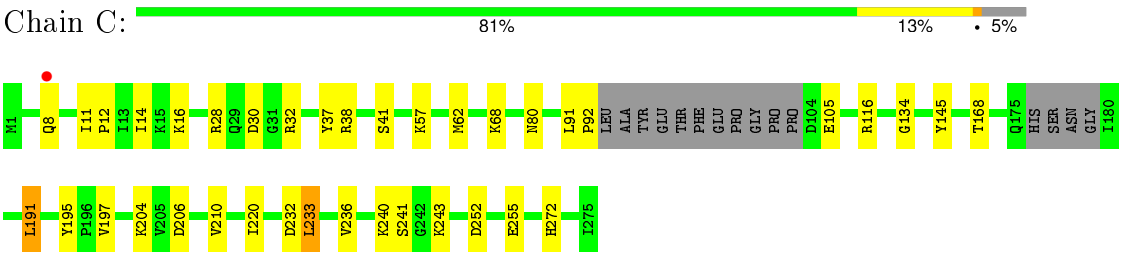
- Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain A:



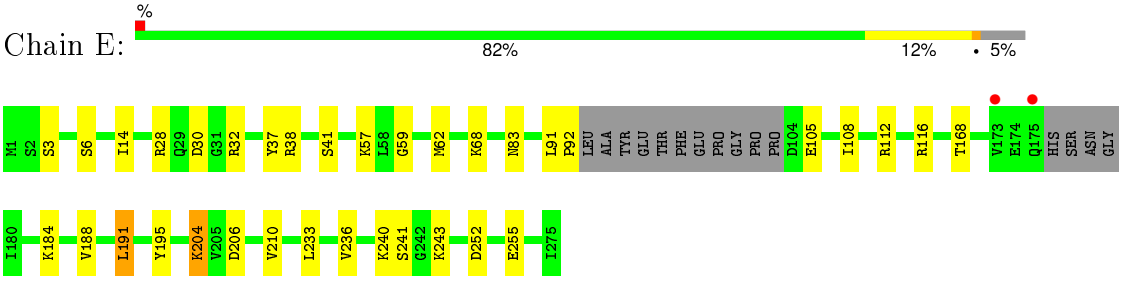
- Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain C:



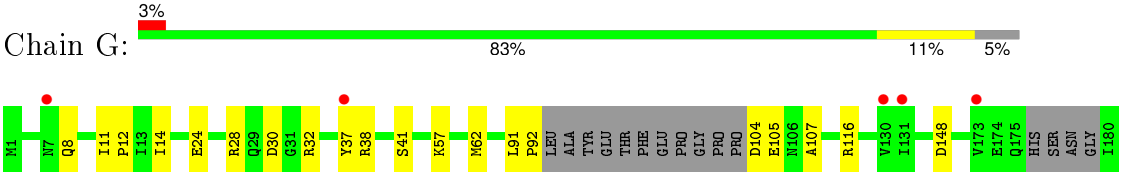
- Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain E:



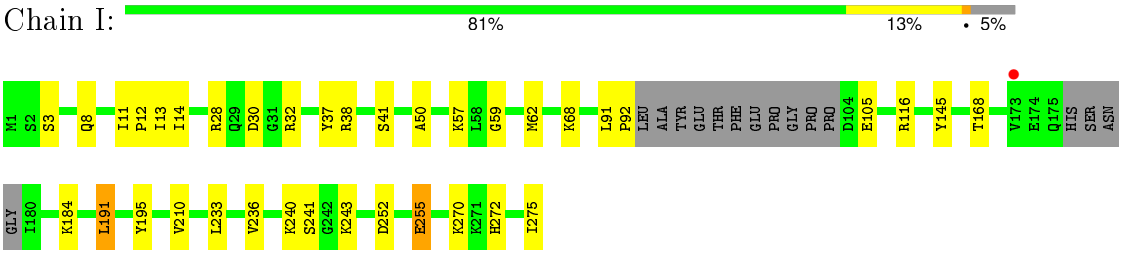
- Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain G:



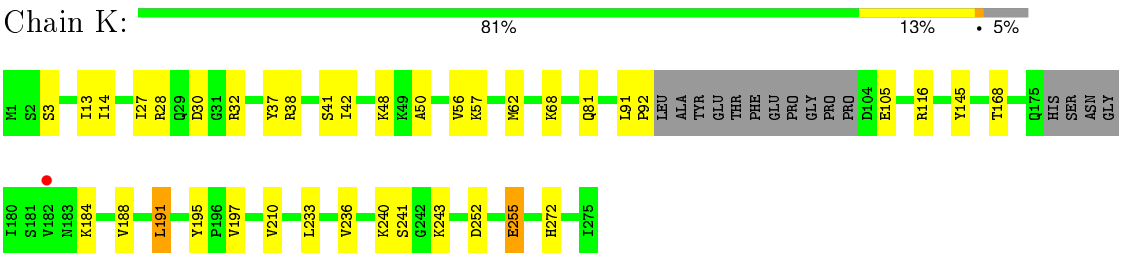
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain I:



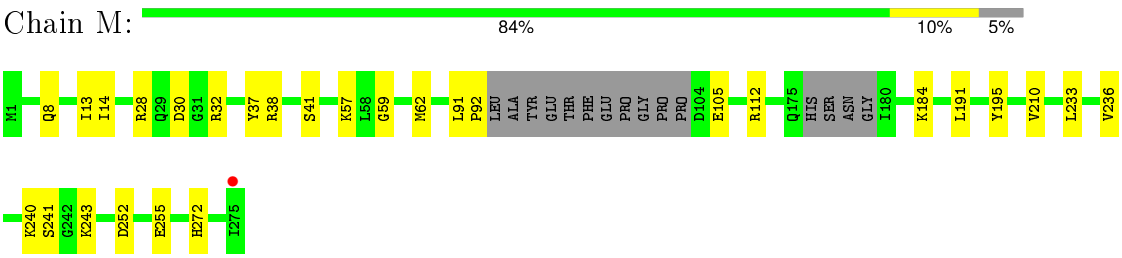
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain K:



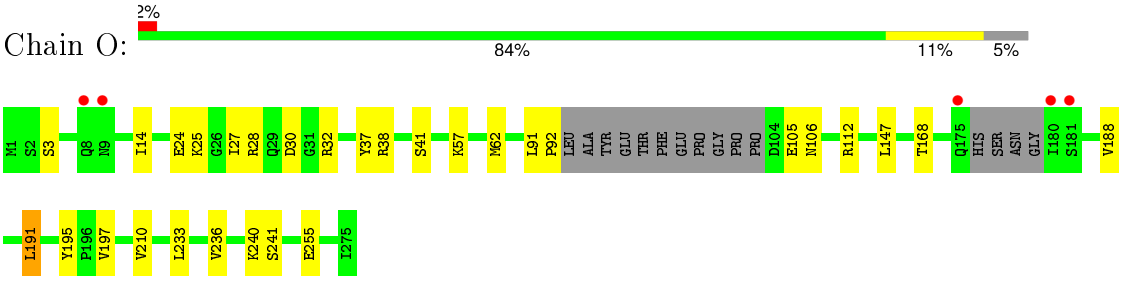
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain M:



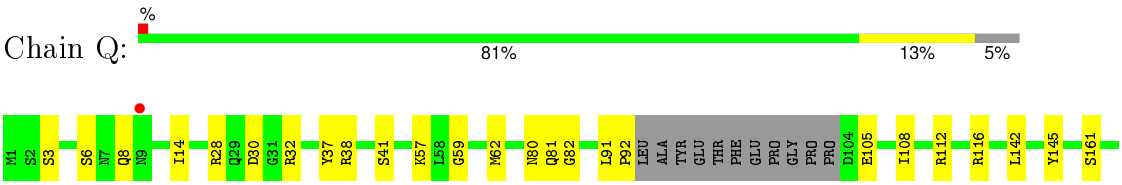
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

Chain O:



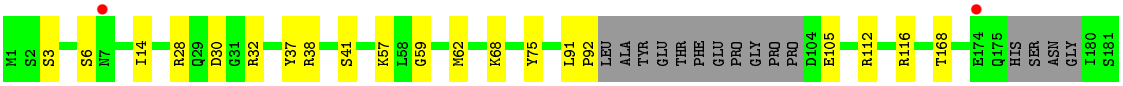
• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

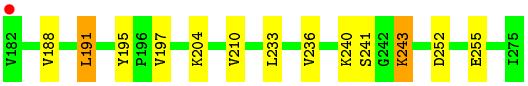
Chain Q:



• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

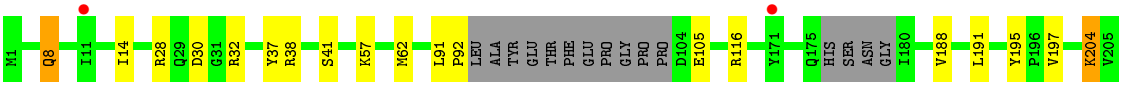
Chain S:

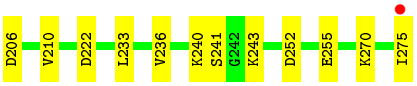




• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

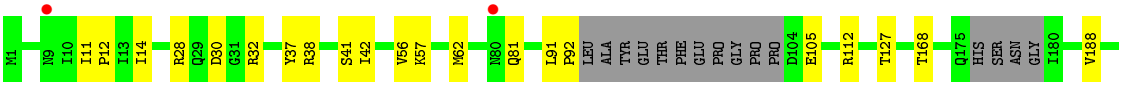
Chain U:

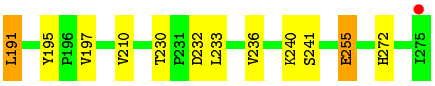




• Molecule 1: EXOSOME COMPLEX EXONUCLEASE 2

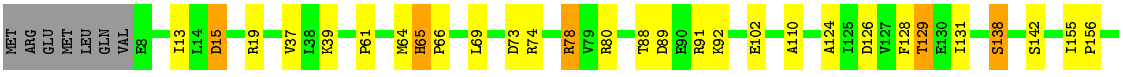
Chain W:





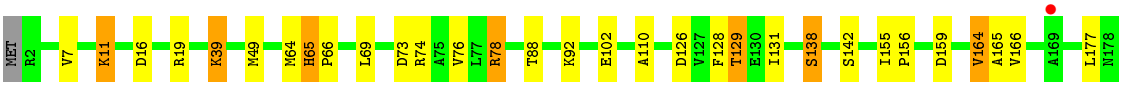
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

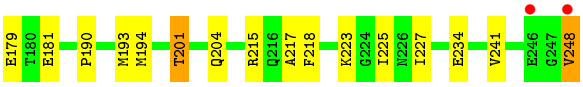
Chain B:



• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

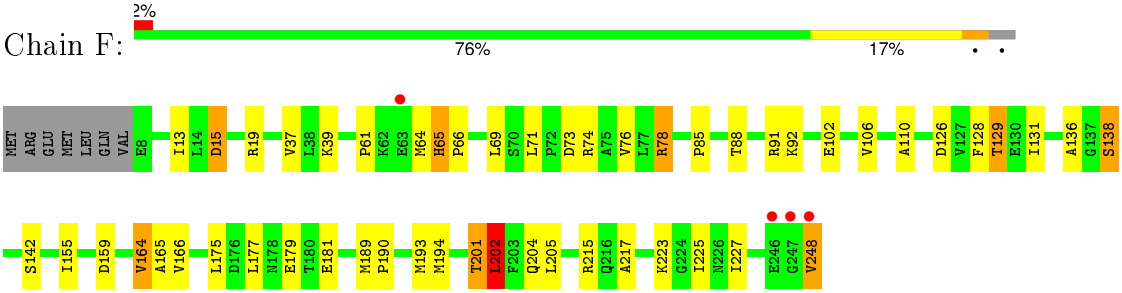
Chain D:





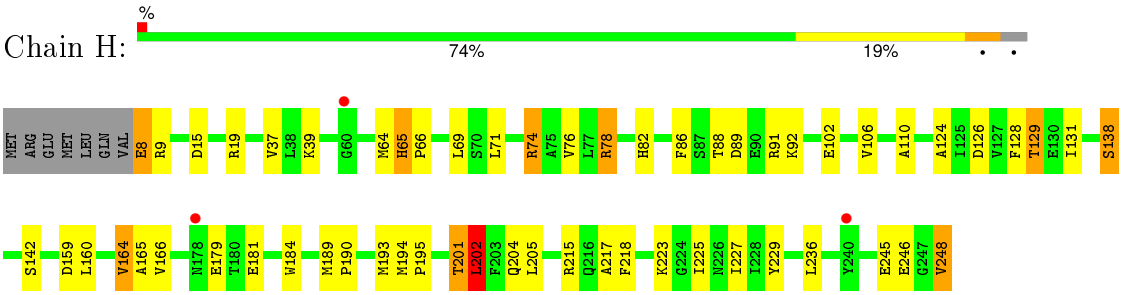
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain F:



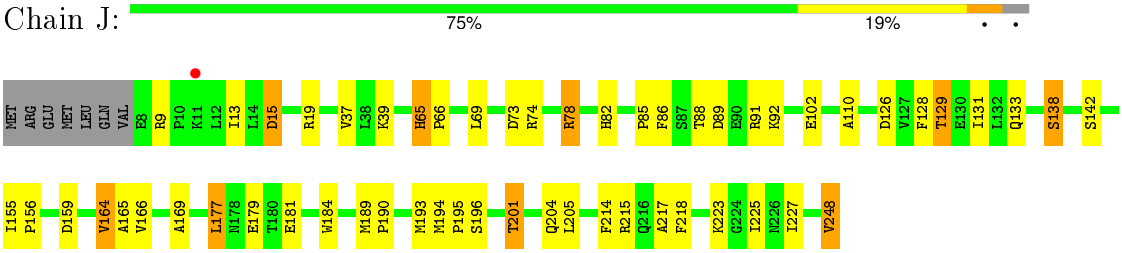
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain H:



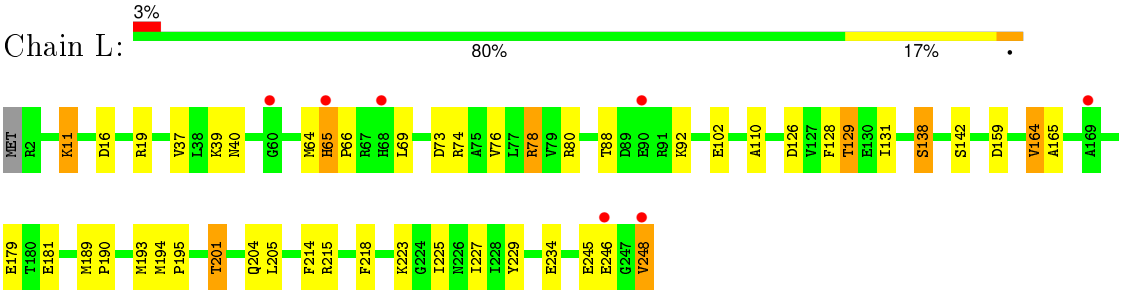
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain J:



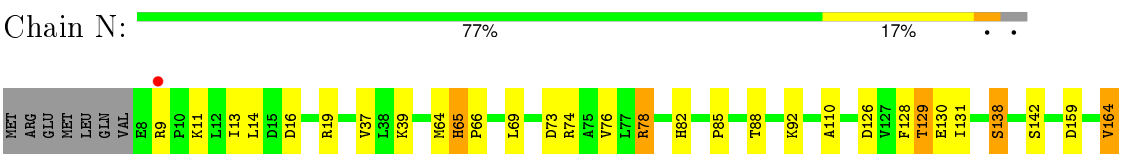
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

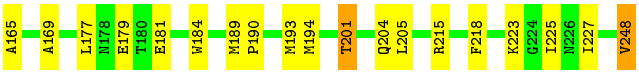
Chain L:



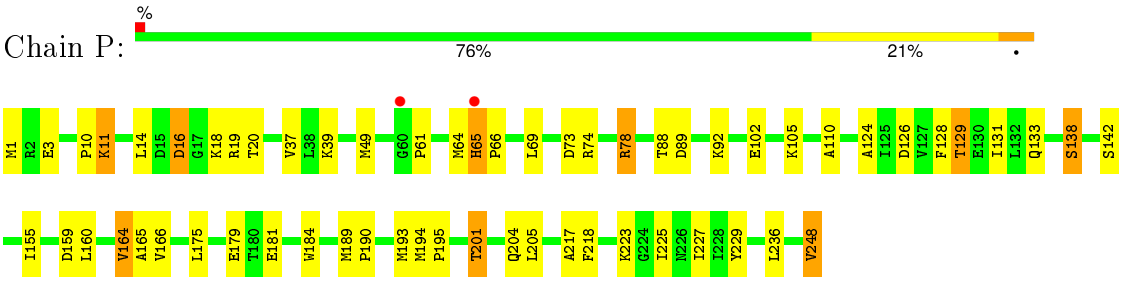
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

Chain N:

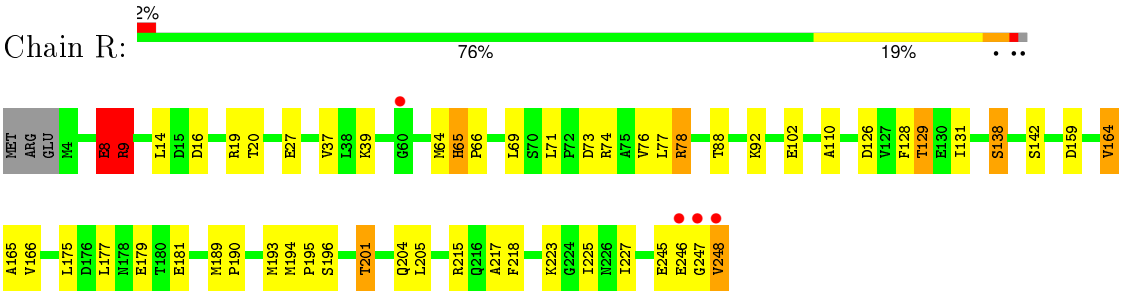




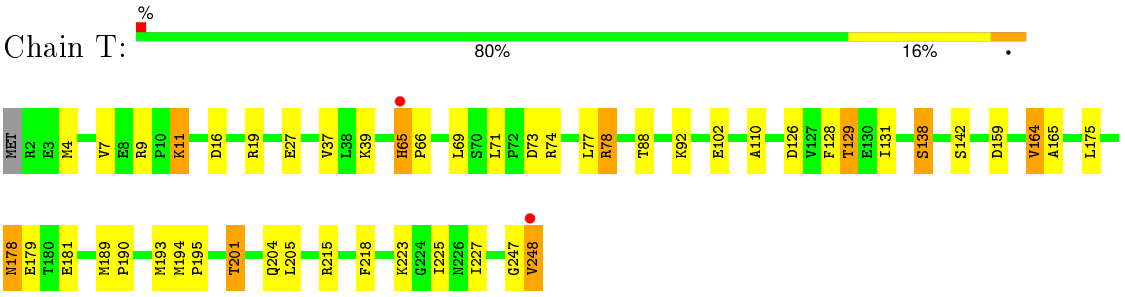
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



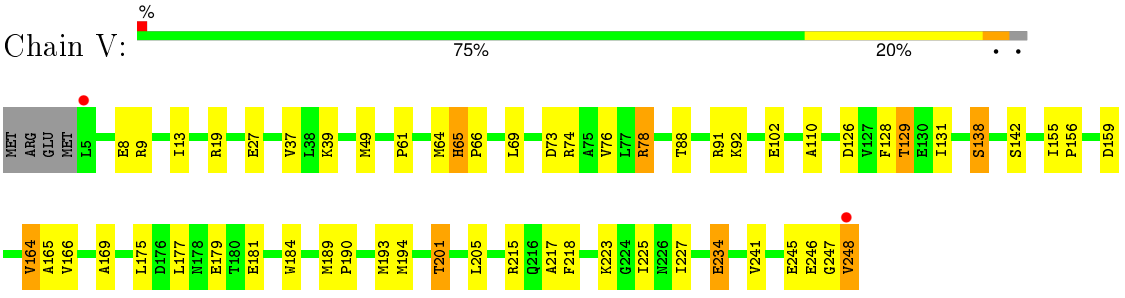
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



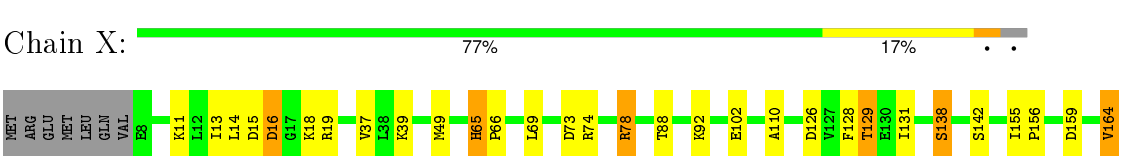
• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1

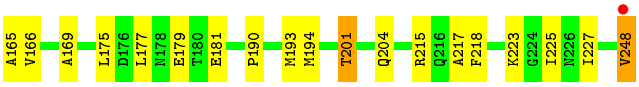


• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1



• Molecule 2: EXOSOME COMPLEX EXONUCLEASE 1




A165
V166
A169
L175
D176
L177
N178
E179
T180
E181
P190
M193
M194
T201
Q204
R215
Q216
A217
F218
K223
G224
I225
N226
I227
V248

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) 99.7 (217.03-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.237 0.227 , 0.245	Depositor DCC
R_{free} test set	7026 reflections (3.11%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.4	EDS
Estimated twinning fraction	0.033 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 233145 reflections (0.000%)	Xtriage
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

Xtriage'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.*

[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: 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	0.46	0/1985	0.57	0/2697
1	C	0.50	0/1997	0.58	0/2711
1	E	0.48	0/1993	0.58	0/2706
1	G	0.47	0/1989	0.59	0/2701
1	I	0.47	0/1986	0.60	0/2697
1	K	0.51	0/1989	0.59	0/2701
1	M	0.47	0/1997	0.58	0/2711
1	O	0.51	1/1993 (0.1%)	0.62	0/2706
1	Q	0.48	0/1993	0.59	0/2706
1	S	0.48	0/1992	0.60	0/2706
1	U	0.48	0/1993	0.58	0/2706
1	W	0.47	0/1993	0.57	0/2706
2	B	0.48	0/1891	0.65	0/2553
2	D	0.46	0/1933	0.64	0/2610
2	F	0.48	0/1891	0.66	1/2553 (0.0%)
2	H	0.46	0/1891	0.65	1/2553 (0.0%)
2	J	0.48	0/1891	0.64	1/2553 (0.0%)
2	L	0.48	0/1937	0.65	0/2615
2	N	0.48	0/1891	0.65	1/2553 (0.0%)
2	P	0.49	0/1935	0.65	0/2613
2	R	0.51	0/1917	0.69	3/2588 (0.1%)
2	T	0.49	0/1933	0.67	1/2610 (0.0%)
2	V	0.47	0/1911	0.64	0/2581
2	X	0.46	0/1891	0.63	0/2553
All	All	0.48	1/46812 (0.0%)	0.62	8/63389 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	25	LYS	C-N	5.08	1.42	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	202	LEU	CA-CB-CG	6.75	130.83	115.30
2	H	202	LEU	CA-CB-CG	6.36	129.93	115.30
2	R	9	ARG	N-CA-CB	5.46	120.44	110.60
2	R	177	LEU	CA-CB-CG	5.44	127.82	115.30
2	R	8	GLU	C-N-CA	5.36	135.09	121.70
2	J	177	LEU	CA-CB-CG	5.15	127.15	115.30
2	T	178	ASN	CB-CA-C	-5.09	100.22	110.40
2	N	177	LEU	CA-CB-CG	5.03	126.87	115.30

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	21	0
1	E	1968	0	2011	21	0
1	G	1964	0	2007	15	0
1	I	1961	0	2003	26	0
1	K	1964	0	2007	28	0
1	M	1972	0	2017	16	0
1	O	1968	0	2013	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1968	0	2013	25	0
1	S	1967	0	2011	22	0
1	U	1968	0	2013	15	0
1	W	1968	0	2011	16	0
2	B	1863	0	1895	36	0
2	D	1905	0	1936	33	0
2	F	1863	0	1895	35	0
2	H	1863	0	1895	39	0
2	J	1863	0	1895	47	0
2	L	1909	0	1940	36	0
2	N	1863	0	1895	34	0
2	P	1907	0	1937	41	0
2	R	1889	0	1921	40	0
2	T	1905	0	1936	37	0
2	V	1883	0	1917	36	0
2	X	1863	0	1895	28	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	4	0	0	0	0
4	O	9	0	0	3	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
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	610	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 (610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:62:MET:HE2	4:O:2003:HOH:O	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
2:H:19:ARG:HD2	2:H:181:GLU:OE2	1.92	0.70
1:O:62:MET:CE	4:O:2003:HOH:O	2.40	0.69
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
2:X:110:ALA:HB1	2:X:201:THR:CG2	2.24	0.68
1:O:57:LYS:HG2	1:O:62:MET:HG2	1.74	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
4:M:2002:HOH:O	2:P:133:GLN:HG2	1.93	0.67
2:F:65:HIS:CB	2:F:66:PRO:HD3	2.24	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:P:65:HIS:CB	2:P:66:PRO:HD3	2.24	0.67
2:H:65:HIS:CB	2:H: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
2:J:110:ALA:HB1	2:J:201:THR:CG2	2.26	0.66
1:I:243:LYS:HD3	2:J:74:ARG:HH12	1.60	0.66
2:B:110:ALA:HB1	2:B:201:THR:CG2	2.24	0.66
2:P:110:ALA:CB	2:P:201:THR:HG23	2.22	0.66
2:L:65:HIS:CB	2:L:66:PRO:HD3	2.25	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:L:66:PRO:HG2	2:L:69:LEU:HD12	1.78	0.65
2:J:19:ARG:HD2	2:J:181:GLU:OE2	1.96	0.65
2:V:65:HIS:CB	2:V:66:PRO:HD3	2.25	0.65
1:C:57:LYS:HG2	1:C:62:MET:HG2	1.77	0.65
1:G:57:LYS:HG2	1:G:62:MET:HG2	1.79	0.65
2:B:65:HIS:CB	2:B:66:PRO:HD3	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:110:ALA:CB	2:T:201:THR:HG23	2.26	0.65
2:R:8:GLU:CB	2:R:9:ARG:HB2	2.27	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
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:X:66:PRO:HG2	2:X:69:LEU:HD12	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: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:V:66:PRO:HG2	2:V:69:LEU:HD12	1.81	0.62
2:T:131:ILE:HG12	2:T:138:SER:HB3	1.81	0.62
1:Q:57:LYS:HG2	1:Q:62:MET:HG2	1.81	0.62
1:K:57:LYS:HG2	1:K:62:MET:HG2	1.81	0.62
2:L:131:ILE:HG12	2:L:138:SER:HB3	1.81	0.62
2:R:110:ALA:HB1	2:R:201:THR:CG2	2.28	0.62
2:H:227:ILE:HD12	2:H:248:VAL:HG22	1.82	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: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:X:110:ALA:CB	2:X:201:THR:HG23	2.30	0.62
2:P:223:LYS:HB3	2:P:248:VAL:HG13	1.81	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:110:ALA:CB	2:N:201:THR:HG23	2.27	0.61
2:J:110:ALA:CB	2:J:201:THR:HG23	2.28	0.61
2:D:78:ARG:HD3	2:D:126:ASP:OD1	2.01	0.61
2:R:110:ALA:CB	2:R:201:THR:HG23	2.31	0.61
2:R:66:PRO:HG2	2:R:69:LEU:HD12	1.82	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: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:N:129:THR:HG21	2:N:142:SER:OG	2.01	0.60
2:B:78:ARG:HD3	2:B:126:ASP:OD1	2.02	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:D:227:ILE:HD12	2:D:248:VAL:HG22	1.84	0.60
2:B:223:LYS:HB3	2:B:248:VAL:HG13	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:R:78:ARG:HD3	2:R:126:ASP:OD1	2.01	0.59
2:H:89:ASP:O	1:I:184:LYS:NZ	2.34	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:X:73:ASP:OD2	2:X:74:ARG:HG3	2.03	0.59
2:N:131:ILE:HG12	2:N:138:SER:HB3	1.82	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:F:66:PRO:HG2	2:F:69:LEU:HD12	1.83	0.59
2:B:89:ASP:O	1:E:184:LYS:NZ	2.35	0.59
2:V:131:ILE:HG12	2:V:138:SER:HB3	1.85	0.59
2:L:78:ARG:HD3	2:L:126:ASP:OD1	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:78:ARG:HD3	2:P:126:ASP:OD1	2.03	0.58
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:V:78:ARG:HD3	2:V: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:L:227:ILE:HD12	2:L:248:VAL:HG22	1.86	0.58
2:T:227:ILE:HD12	2:T:248:VAL:HG22	1.86	0.58
2:F:227:ILE:HD12	2:F: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:T:129:THR:HG21	2:T:142:SER:OG	2.04	0.57
2:H:78:ARG:HD3	2:H:126:ASP:OD1	2.04	0.57
2:P:131:ILE:HG12	2:P:138:SER:HB3	1.85	0.57
2:P:227:ILE:HD12	2:P:248:VAL:HG22	1.87	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:T:193:MET:HG3	2:T:225:ILE:HD13	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:B:164:VAL:HG22	2:B:225:ILE:HG13	1.86	0.57
2:H:131:ILE:HG12	2:H:138:SER:HB3	1.86	0.57
2:L:193:MET:HG3	2:L:225:ILE:HD13	1.87	0.57
1:I:252:ASP:OD1	2:J:215:ARG:NH1	2.36	0.57
2:R:73:ASP:OD2	2:R:74:ARG:HG3	2.04	0.57
2:F:129:THR:HG21	2:F:142:SER:OG	2.05	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:H:110:ALA:CB	2:H:201:THR:HG23	2.35	0.56
2:D:131:ILE:HG12	2:D:138:SER:HB3	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:R:193:MET:HG3	2:R:225:ILE:HD13	1.90	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: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
2:X:227:ILE:HD12	2:X:248:VAL:HG22	1.90	0.54
1:K:28:ARG:NH1	1:K:210:VAL:HG13	2.23	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
1:M:41:SER:HB2	1:M:57:LYS:HB2	1.91	0.53
2:J:227:ILE:HD12	2:J:248:VAL:HG22	1.89	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: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
1:W:30:ASP:OD1	1:W:32:ARG:HG2	2.09	0.53
2:N:85:PRO:HD3	1:Q:145:TYR:OH	2.08	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
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:D:159:ASP:HB3	2:D:194:MET:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:G:14:ILE:HD12	1:G:14:ILE:H	1.76	0.51
1:O:30:ASP:OD1	1:O:32:ARG:HG2	2.11	0.51
1:G:148:ASP:OD1	2:L:40:ASN:HB2	2.10	0.51
1:E:28:ARG:NH1	1:E:210:VAL:HG13	2.25	0.51
2:V:223:LYS:HB3	2:V:248:VAL:CG1	2.40	0.51
2:J:89:ASP:O	1:K:184:LYS:NZ	2.43	0.51
1:U:41:SER:HB2	1:U:57:LYS:HB2	1.91	0.51
1:S:28:ARG:NH1	1:S:210:VAL:HG13	2.25	0.51
2:D:88:THR:HG21	2:D:92:LYS:HE3	1.93	0.51
2:R:129:THR:HG21	2:R:142:SER:OG	2.09	0.51
1:K:252:ASP:OD1	2:L:215:ARG:NH1	2.41	0.51
1:E:240:LYS:HG2	1:E:241:SER:N	2.25	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
1:C:28:ARG:NH1	1:C:210:VAL:HG13	2.26	0.51
1:Q:3:SER:HA	2:R:77:LEU:O	2.11	0.51
2:D:164:VAL:HG22	2:D:225:ILE:HG13	1.93	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
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
1:M:30:ASP:OD1	1:M:32:ARG:HG2	2.12	0.50
2:J:133:GLN:NE2	1:K:48:LYS:HB2	2.27	0.50
1:Q:240:LYS:HG2	1:Q:241:SER:N	2.26	0.50
1:M:14:ILE:HD12	1:M:14:ILE:H	1.77	0.50
2:N:9:ARG:HG2	2:N:9:ARG:HH11	1.77	0.50
2:J:223:LYS:HB3	2:J:248:VAL:CG1	2.42	0.50
2:N:189:MET:HE3	2:N:205:LEU:HD13	1.93	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
2:V:193:MET:HG3	2:V:225:ILE:HD13	1.93	0.50
1:E:14:ILE:H	1:E:14:ILE:HD12	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:7:ASN:O	1:A:8:GLN:O	2.30	0.49
1:K:240:LYS:HG2	1:K:241:SER:N	2.28	0.49
2:D:126:ASP:HB3	2:D:128:PHE:CE1	2.48	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
1:U:14:ILE:HD12	1:U:14:ILE:H	1.77	0.49
2:P:190:PRO:HG2	2:P:204:GLN:HB2	1.95	0.49
2:V:126:ASP:HB3	2:V:128:PHE:CE1	2.48	0.48
1:C:204:LYS:HE2	1:C:206:ASP:O	2.13	0.48
2:H:88:THR:HG21	2:H:92:LYS:HE3	1.95	0.48
2:F:106:VAL:HG12	2:F:202:LEU:HD22	1.95	0.48
1:I:30:ASP:OD1	1:I:32:ARG:HG2	2.13	0.48
2:T:4:MET:HG3	2:T:4:MET:O	2.13	0.48
2:R:126:ASP:HB3	2:R:128:PHE:CE1	2.49	0.48
2:J:88:THR:HG21	2:J:92:LYS:HE3	1.94	0.48
1:Q:14:ILE:HD12	1:Q:14:ILE:H	1.77	0.48
1:Q:252:ASP:OD1	2:R:215:ARG:NH1	2.46	0.48
2:T:223:LYS:HB3	2:T:248:VAL:CG1	2.42	0.48
1:A:7:ASN:O	1:A:8:GLN:C	2.50	0.48
1:A:112:ARG:HD3	2:B:102:GLU:OE1	2.14	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:H	1:I:14:ILE:HD12	1.79	0.48
2:B:189:MET:HE3	2:B:205:LEU:HD13	1.94	0.48
2:F:15:ASP:OD1	2:F:15:ASP:N	2.47	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:X:126:ASP:HB3	2:X:128:PHE:CE1	2.49	0.48
1:Q:116:ARG:NH2	2:R:102:GLU:OE1	2.46	0.48
2:T:189:MET:HE3	2:T:205:LEU:HD13	1.96	0.48
2:J:159:ASP:HB3	2:J:194:MET:HB3	1.95	0.48
2:X:88:THR:HG21	2:X:92:LYS:HE3	1.94	0.48
1:W:14:ILE:H	1:W:14:ILE:HD12	1.79	0.48
1:I:240:LYS:HG2	1:I:241:SER:N	2.28	0.48
1:O:41:SER:HB2	1:O:57:LYS:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:64:MET:HE1	2:L:76:VAL:HB	1.96	0.47
2:H:82:HIS:HE1	1:I:145:TYR:OH	1.97	0.47
1:S:240:LYS:HG2	1:S:241:SER:N	2.29	0.47
1:O:240:LYS:HG2	1:O:241:SER:N	2.29	0.47
2:H:64:MET:HE1	2:H:76:VAL:HB	1.97	0.47
2:F:223:LYS:HB3	2:F:248:VAL:CG1	2.44	0.47
2:B:126:ASP:HB3	2:B:128:PHE:CE1	2.48	0.47
1:A:14:ILE:H	1:A:14:ILE:HD12	1.79	0.47
2:H:223:LYS:HB3	2:H:248:VAL:CG1	2.44	0.47
1:S:3:SER:HB3	2:T:78:ARG:CG	2.45	0.47
2:L:11:LYS:HD2	2:L:11:LYS:HA	1.68	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: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
2:J:189:MET:HE3	2:J:205:LEU:HD13	1.97	0.47
2:J:82:HIS:HE1	1:K:145:TYR:OH	1.98	0.47
1:U:243:LYS:HD3	2:V:74:ARG:HH12	1.80	0.47
1:O:28:ARG:CZ	1:O:210:VAL:HG13	2.45	0.47
2:V:189:MET:HE3	2:V:205:LEU:HD13	1.97	0.47
2:N:126:ASP:HB3	2:N:128:PHE:CE1	2.50	0.47
2:N:13:ILE:CD1	2:N:169:ALA:HB3	2.45	0.47
2:T:88:THR:HG21	2:T:92:LYS:HE3	1.97	0.47
1:C:14:ILE:H	1:C:14:ILE:HD12	1.80	0.47
2:P:159:ASP:HB3	2:P:194:MET:HB3	1.97	0.47
2:V:19:ARG:NH2	2:V:175:LEU:O	2.41	0.46
2:V:9:ARG:NH2	2:V:184:TRP:O	2.48	0.46
1:U:240:LYS:HG2	1:U:241:SER:N	2.29	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:S:112:ARG:HD3	2:T:102:GLU:OE1	2.15	0.46
1:G:28:ARG:CZ	1:G: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
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
2:F:126:ASP:HB3	2:F:128:PHE:CE1	2.51	0.46
1:Q:3:SER:HB3	2:R:78:ARG:HG3	1.97	0.46
2:P:189:MET:HE3	2:P:205:LEU:HD13	1.97	0.46
1:Q:41:SER:HB2	1:Q:57:LYS:HB2	1.96	0.46
1:K:243:LYS:HD3	2:L:74:ARG:HH12	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:28:ARG:NH1	1:W:210:VAL:HG13	2.30	0.46
2:P:126:ASP:HB3	2:P:128:PHE:CE1	2.50	0.46
1:G:240:LYS:HG2	1:G:241:SER:N	2.31	0.46
1:O:91:LEU:N	1:O:92:PRO:CD	2.79	0.46
1:G:30:ASP:OD1	1:G:32:ARG:HG2	2.15	0.46
1:Q:91:LEU:N	1:Q:92:PRO:CD	2.79	0.46
1:K:14:ILE:H	1:K:14:ILE:HD12	1.79	0.46
1:S:14:ILE:HD12	1:S:14:ILE:H	1.79	0.46
2:R:19:ARG:NH2	2:R:175:LEU:O	2.42	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:189:MET:HE3	2:R:205:LEU:HD13	1.96	0.46
2:F:189:MET:HE3	2:F:205:LEU:HD13	1.96	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
1:K:30:ASP:OD1	1:K:32:ARG:HG2	2.15	0.46
2:T:126:ASP:HB3	2:T:128:PHE:CE1	2.51	0.46
2:R:159:ASP:HB3	2:R:194:MET:HB3	1.98	0.46
1:W:42:ILE:HG12	1:W:56:VAL:HG22	1.98	0.46
2:P:16:ASP:C	2:P:18:LYS:H	2.19	0.46
1:I:13:ILE:H	1:I:13:ILE:HG13	1.58	0.46
2:F:190:PRO:HG2	2:F:204:GLN:HB2	1.98	0.46
2:F:19:ARG:NH2	2:F:175:LEU:O	2.41	0.45
1:K:91:LEU:N	1:K:92:PRO:CD	2.78	0.45
1:K:41:SER:HB2	1:K:57:LYS:HB2	1.96	0.45
2:B:138:SER:OG	4:B:2005:HOH:O	2.21	0.45
1:E:32:ARG:CZ	1:E:38:ARG:HG3	2.46	0.45
1:A:240:LYS:HG2	1:A:241:SER:N	2.31	0.45
2:X:165:ALA:HA	2:X:190:PRO:HA	1.97	0.45
2:T:159:ASP:HB3	2:T:194:MET:HB3	1.97	0.45
2:D:11:LYS:HA	2:D:11:LYS:HD2	1.71	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:H:15:ASP:OD1	2:H:15:ASP:N	2.45	0.45
2:X:11:LYS:HE3	2:X:14:LEU:HA	1.99	0.45
1:A:91:LEU:N	1:A:92:PRO:CD	2.80	0.45
2:F:165:ALA:HA	2:F:190:PRO:HA	1.99	0.45
2:D:165:ALA:HA	2:D:190:PRO:HA	1.99	0.45
1:C:91:LEU:N	1:C:92:PRO:CD	2.80	0.45
1:I:270:LYS:HB3	1:I:275:ILE:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:91:LEU:N	1:S:92:PRO:CD	2.80	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
1:G:91:LEU:N	1:G:92:PRO:CD	2.79	0.45
2:H:64:MET:HE2	2:H:124:ALA:HB2	1.98	0.45
2:L:189:MET:HE3	2:L:205:LEU:HD13	1.98	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
1:I:3:SER:HB3	2:J:78:ARG:HG3	1.99	0.45
1:C:145:TYR:OH	2:F:85:PRO:HD3	2.16	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:U:91:LEU:N	1:U:92:PRO:CD	2.80	0.45
2:J:126:ASP:HB3	2:J:128:PHE:CE1	2.52	0.45
1:Q:240:LYS:NZ	4:Q:2004:HOH:O	2.48	0.45
2:H:189:MET:HE3	2:H:205:LEU:HD13	1.99	0.45
1:O:168:THR:HB	1:O:191:LEU:HD22	1.99	0.45
2:F:159:ASP:HB3	2:F:194:MET:HB3	1.99	0.45
2:B:223:LYS:HB3	2:B:248:VAL:CG1	2.45	0.44
1:K:168:THR:HB	1:K:191:LEU:HD22	1.99	0.44
1:E:204:LYS:HE3	1:E:206:ASP:O	2.17	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
1:S:75:TYR:N	1:S:75:TYR:CD1	2.85	0.44
2:T:65:HIS:CB	2:T:66:PRO:CD	2.95	0.44
1:Q:168:THR:HB	1:Q:191:LEU:HD22	2.00	0.44
1:M:28:ARG:NH1	1:M:210:VAL:HG13	2.32	0.44
2:H:86:PHE:HB2	1:I:50:ALA:HB2	2.00	0.44
1:I:41:SER:HB2	1:I:57:LYS:HB2	1.98	0.44
1:S:168:THR:HB	1:S:191:LEU:HD22	1.99	0.44
2:N:159:ASP:HB3	2:N:194:MET:HB3	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
1:E:3:SER:HB3	2:F:78:ARG:CG	2.47	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:91:LEU:N	1:E:92:PRO:CD	2.80	0.44
1:E:243:LYS:HD3	2:F:74:ARG:HH12	1.82	0.44
1:M:184:LYS:NZ	2:P:89:ASP:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:88:THR:HG21	2:P:92:LYS:HE3	1.99	0.44
2:B:15:ASP:N	2:B:15:ASP:OD1	2.50	0.44
1:M:91:LEU:N	1:M:92:PRO:CD	2.80	0.44
1:A:41:SER:HB2	1:A:57:LYS:HB2	1.98	0.44
2:N:223:LYS:HB3	2:N:248:VAL:CG1	2.48	0.44
2:J:155:ILE:HA	2:J:156:PRO:HD3	1.86	0.44
2:P:73:ASP:CG	2:P:74:ARG:HG3	2.38	0.44
1:O:3:SER:HB3	2:P:78:ARG:CG	2.48	0.44
1:K:116:ARG:HH22	2:L:102:GLU:CD	2.21	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:L:88:THR:HG21	2:L:92:LYS:HE3	1.98	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
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
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
2:B:166:VAL:HG13	2:B:217:ALA:HB1	2.00	0.43
2:P:65:HIS:CB	2:P:66:PRO:CD	2.96	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
2:L:165:ALA:HA	2:L:190:PRO:HA	2.00	0.43
2:X:190:PRO:HG2	2:X:204:GLN:HB2	1.99	0.43
2:B:61:PRO:HD3	2:B:155:ILE:HD11	2.00	0.43
1:K:255:GLU:HG2	2:L:214:PHE:CE2	2.53	0.43
1:C:32:ARG:CZ	1:C:38:ARG:HG3	2.48	0.43
2:P:165:ALA:HA	2:P:190:PRO:HA	1.99	0.43
1:K:27:ILE:HG21	2:R:196:SER:HB3	2.00	0.43
1:O:62:MET:HE3	4:O:2003:HOH:O	2.11	0.43
1:C:41:SER:HB2	1:C:57:LYS:HB2	1.99	0.43
1:M:243:LYS:HD3	2:N:74:ARG:HH12	1.83	0.43
1:C:240:LYS:HG2	1:C:241:SER:N	2.33	0.43
2:J:165:ALA:HA	2:J:190:PRO:HA	2.00	0.43
2:T:11:LYS:HD2	2:T:11:LYS:HA	1.59	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
2:V:64:MET:HE1	2:V:76:VAL:HB	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:106:ASN:OD1	2:P:105:LYS:HE3	2.18	0.43
2:J:9:ARG:NH1	2:J:9:ARG:HB3	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:P:14:LEU:HD12	2:P:20:THR:HA	2.01	0.43
2:J:190:PRO:HG2	2:J:204:GLN:HB2	2.00	0.43
2:J:86:PHE:HB2	1:K:50:ALA:HB2	2.01	0.43
1:K:32:ARG:CZ	1:K:38:ARG:HG3	2.50	0.42
1:E:108:ILE:O	1:E:112:ARG:HG3	2.19	0.42
2:F:64:MET:HE1	2:F:76:VAL:HB	2.00	0.42
1:G:116:ARG:NH2	2:H:102:GLU:OE1	2.52	0.42
1:C:68:LYS:HG2	2:F:91:ARG:HB2	2.01	0.42
2:L:195:PRO:HG2	2:L:229:TYR:CD1	2.54	0.42
2:D:155:ILE:HA	2:D:156:PRO:HD3	1.87	0.42
1:U:32:ARG:CZ	1:U:38:ARG:HG3	2.49	0.42
2:R:190:PRO:HG2	2:R:204:GLN:HB2	2.00	0.42
1:I:168:THR:HB	1:I:191:LEU:HD22	2.02	0.42
1:A:204:LYS:HE3	1:A:206:ASP:O	2.19	0.42
1:K:13:ILE:H	1:K:13:ILE:HG13	1.59	0.42
2:F:65:HIS:CB	2:F:66:PRO:CD	2.96	0.42
1:U:204:LYS:HE2	1:U:206:ASP:O	2.18	0.42
1:C:11:ILE:HA	1:C:12:PRO:HD3	1.94	0.42
2:X:166:VAL:HG13	2:X:217:ALA:HB1	2.01	0.42
1:E:168:THR:HB	1:E:191:LEU:HD22	2.01	0.42
1:W:11:ILE:HA	1:W:12:PRO:HD3	1.93	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: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
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:N:65:HIS:CB	2:N:66:PRO:CD	2.97	0.42
2:R:193:MET:O	2:R:195:PRO:HD3	2.19	0.42
1:E:28:ARG:CZ	1:E:210:VAL:HG13	2.49	0.42
2:B:165:ALA:HA	2:B:190:PRO:HA	2.02	0.42
2:V:155:ILE:HA	2:V:156:PRO:HD3	1.87	0.42
1:M:13:ILE:H	1:M:13:ILE:HG13	1.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ILE:HA	2:B:156:PRO:HD3	1.84	0.42
1:S:41:SER:HB2	1:S:57:LYS:HB2	2.02	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
2:V:245:GLU:O	2:V:246:GLU:HB3	2.19	0.42
1:S:116:ARG:HH22	2:T:102:GLU:CD	2.23	0.42
1:U:28:ARG:CZ	1:U:210:VAL:HG13	2.50	0.42
2:D:64:MET:HE1	2:D:76:VAL:HB	2.01	0.42
2:P:160:LEU:HD11	2:P:236:LEU:HD22	2.02	0.42
2:V:27:GLU:HG2	2:V:247:GLY:HA2	2.02	0.42
2:R:65:HIS:CB	2:R:66:PRO:CD	2.95	0.41
1:O:32:ARG:CZ	1:O:38:ARG:HG3	2.50	0.41
2:J:13:ILE:CD1	2:J:169:ALA:HB3	2.50	0.41
1:I:32:ARG:CZ	1:I:38:ARG:HG3	2.50	0.41
1:C:16:LYS:HG3	1:C:220:ILE:HB	2.02	0.41
2:N:190:PRO:HG2	2:N:204:GLN:HB2	2.02	0.41
2:L:65:HIS:CB	2:L:66:PRO:CD	2.97	0.41
2:H:126:ASP:HB3	2:H:128:PHE:HE1	1.84	0.41
1:G:32:ARG:CZ	1:G:38:ARG:HG3	2.50	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:I:255:GLU:HG2	2:J:214:PHE:CE2	2.55	0.41
2:T:19:ARG:NH2	2:T:175:LEU:O	2.44	0.41
1:M:38:ARG:HD2	1:M:59:GLY:HA3	2.02	0.41
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
2:X:155:ILE:HA	2:X:156:PRO:HD3	1.86	0.41
2:R:64:MET:HE1	2:R:76:VAL:HB	2.02	0.41
2:P:195:PRO:HG2	2:P:229:TYR:CD1	2.55	0.41
2:L:73:ASP:CG	2:L:74:ARG:HG3	2.41	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:H:195:PRO:HG2	2:H:229:TYR:CD1	2.55	0.41
2:B:64:MET:HE2	2:B:124:ALA:HB2	2.03	0.41
2:J:65:HIS:CB	2:J:66:PRO:CD	2.97	0.41
1:S:243:LYS:HE2	2:T:74:ARG:HH12	1.85	0.41
2:N:165:ALA:HA	2:N:190:PRO:HA	2.02	0.41
1:A:30:ASP:OD1	1:A:32:ARG:HG2	2.21	0.41
1:U:270:LYS:HB3	1:U:275:ILE:HG12	2.03	0.41
2:N:64:MET:HE1	2:N:76:VAL:HB	2.03	0.41
2:P:16:ASP:O	2:P:18:LYS:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:GLU:OE2	2:H:215:ARG:NH2	2.52	0.41
2:V:73:ASP:CG	2:V:74:ARG:HG3	2.41	0.41
1:K:3:SER:HB3	2:L:78:ARG:HG3	2.01	0.41
1:C:116:ARG:HH22	2:D:102:GLU:CD	2.24	0.41
2:V:166:VAL:HG13	2:V:217:ALA:HB1	2.03	0.41
2:P:11:LYS:HD2	2:P:11:LYS:HA	1.60	0.41
2:J:166:VAL:CG1	2:J:217:ALA:HB1	2.51	0.41
1:I:38:ARG:HD2	1:I:59:GLY:HA3	2.02	0.41
1:A:168:THR:HB	1:A:191:LEU:HD22	2.02	0.41
2:P:64:MET:HE2	2:P:124:ALA:HB2	2.03	0.41
1:Q:142:LEU:HD21	1:Q:161:SER:HB3	2.02	0.41
1:A:13:ILE:H	1:A:13:ILE:HG13	1.62	0.41
2:T:178:ASN:HB2	2:T:181:GLU:H	1.86	0.41
2:D:65:HIS:CB	2:D:66:PRO:CD	2.98	0.41
1:W:168:THR:HB	1:W:191:LEU:HD22	2.03	0.41
1:U:252:ASP:OD1	2:V:215:ARG:NH1	2.52	0.41
1:Q:81:GLN:HG2	1:Q:82:GLY:O	2.21	0.41
2:L:245:GLU:O	2:L:246:GLU:HB3	2.20	0.41
2:F:166:VAL:HG13	2:F:217:ALA:HB1	2.02	0.41
2:B:19:ARG:NH2	2:B:175:LEU:O	2.45	0.41
2:N:82:HIS:HE1	1:Q:145:TYR:OH	2.04	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
2:P:61:PRO:HD3	2:P:155:ILE:HD11	2.03	0.41
1:A:60:THR:HG22	2:D:39:LYS:HG2	2.03	0.41
2:L:65:HIS:HA	4:L:2001:HOH:O	2.20	0.40
2:R:8:GLU:CB	2:R:9:ARG:CB	2.97	0.40
1:O:91:LEU:HD12	1:O:147:LEU:HD23	2.03	0.40
2:H:245:GLU:O	2:H:246:GLU:HB3	2.20	0.40
2:P:10:PRO:HD2	2:P:184:TRP:CD2	2.56	0.40
2:X:19:ARG:NH2	2:X:175:LEU:O	2.45	0.40
1:W:41:SER:HB2	1:W:57:LYS:HB2	2.03	0.40
1:I:116:ARG:HH22	2:J:102:GLU:CD	2.25	0.40
2:J:88:THR:O	1:K:68:LYS:CE	2.69	0.40
1:A:32:ARG:CZ	1:A:38:ARG:HG3	2.52	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
1:O:91:LEU:H	1:O:92:PRO:HD3	1.86	0.40
1:I:11:ILE:HA	1:I:12:PRO:HD3	1.92	0.40
1:G:104:ASP:HB3	1:G:107:ALA:HB3	2.02	0.40
2:D:234:GLU:HG3	2:D:241:VAL:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:32:ARG:CZ	1:W:38:ARG:HG3	2.51	0.40
1:Q:108:ILE:O	1:Q:112:ARG:HG3	2.21	0.40
1:E:6:SER:HA	2:F:71:LEU:HD21	2.04	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
1:G:270:LYS:HB3	1:G:275:ILE:HG12	2.02	0.40
2:T:27:GLU:HG2	2:T:247:GLY:HA2	2.03	0.40
2:V:234:GLU:HB3	2:V:241:VAL:HG21	2.03	0.40
1:E:83:ASN:HA	4:E:2003:HOH:O	2.20	0.40
2:D:73:ASP:CG	2:D:74:ARG:HG3	2.42	0.40
1:K:91:LEU:H	1:K:92:PRO:HD3	1.87	0.40
1:S:75:TYR:HD1	1:S:75:TYR:N	2.19	0.40
1:C:30:ASP:OD1	1:C:32:ARG:HG2	2.20	0.40
2:R:245:GLU:O	2:R:246:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

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	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	24	58
1	C	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	24	58
1	E	254/275 (92%)	247 (97%)	6 (2%)	1 (0%)	39	74
1	G	254/275 (92%)	247 (97%)	5 (2%)	2 (1%)	24	58
1	I	254/275 (92%)	243 (96%)	9 (4%)	2 (1%)	24	58
1	K	254/275 (92%)	245 (96%)	8 (3%)	1 (0%)	39	74
1	M	254/275 (92%)	244 (96%)	9 (4%)	1 (0%)	39	74
1	O	254/275 (92%)	245 (96%)	8 (3%)	1 (0%)	39	74
1	Q	254/275 (92%)	243 (96%)	9 (4%)	2 (1%)	24	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	254/275 (92%)	248 (98%)	5 (2%)	1 (0%)	39	74
1	U	254/275 (92%)	244 (96%)	8 (3%)	2 (1%)	24	58
1	W	254/275 (92%)	247 (97%)	6 (2%)	1 (0%)	39	74
2	B	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	39	74
2	D	245/248 (99%)	231 (94%)	12 (5%)	2 (1%)	24	58
2	F	239/248 (96%)	228 (95%)	9 (4%)	2 (1%)	24	58
2	H	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	39	74
2	J	239/248 (96%)	228 (95%)	10 (4%)	1 (0%)	39	74
2	L	245/248 (99%)	230 (94%)	13 (5%)	2 (1%)	24	58
2	N	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	39	74
2	P	246/248 (99%)	232 (94%)	12 (5%)	2 (1%)	24	58
2	R	243/248 (98%)	226 (93%)	13 (5%)	4 (2%)	12	38
2	T	245/248 (99%)	229 (94%)	14 (6%)	2 (1%)	24	58
2	V	242/248 (98%)	229 (95%)	11 (4%)	2 (1%)	24	58
2	X	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	39	74
All	All	5948/6276 (95%)	5684 (96%)	225 (4%)	39 (1%)	26	62

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	207 (96%)	9 (4%)	36	71
1	C	219/242 (90%)	210 (96%)	9 (4%)	37	72
1	E	218/242 (90%)	210 (96%)	8 (4%)	41	76
1	G	217/242 (90%)	208 (96%)	9 (4%)	37	72
1	I	216/242 (89%)	210 (97%)	6 (3%)	51	84
1	K	217/242 (90%)	208 (96%)	9 (4%)	37	72
1	M	219/242 (90%)	212 (97%)	7 (3%)	46	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	218/242 (90%)	210 (96%)	8 (4%)	41	76
1	Q	218/242 (90%)	208 (95%)	10 (5%)	33	67
1	S	218/242 (90%)	208 (95%)	10 (5%)	33	67
1	U	218/242 (90%)	208 (95%)	10 (5%)	33	67
1	W	218/242 (90%)	210 (96%)	8 (4%)	41	76
2	B	199/208 (96%)	188 (94%)	11 (6%)	27	59
2	D	203/208 (98%)	190 (94%)	13 (6%)	22	52
2	F	199/208 (96%)	186 (94%)	13 (6%)	21	52
2	H	199/208 (96%)	186 (94%)	13 (6%)	21	52
2	J	199/208 (96%)	187 (94%)	12 (6%)	24	56
2	L	204/208 (98%)	192 (94%)	12 (6%)	24	57
2	N	199/208 (96%)	188 (94%)	11 (6%)	27	59
2	P	203/208 (98%)	191 (94%)	12 (6%)	24	57
2	R	201/208 (97%)	191 (95%)	10 (5%)	30	64
2	T	203/208 (98%)	190 (94%)	13 (6%)	22	52
2	V	201/208 (97%)	188 (94%)	13 (6%)	21	52
2	X	199/208 (96%)	185 (93%)	14 (7%)	19	47
All	All	5021/5400 (93%)	4771 (95%)	250 (5%)	30	64

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	37	TYR
1	A	188	VAL
1	A	191	LEU
1	A	195	TYR
1	A	197	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	78	ARG
2	B	129	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	138	SER
2	B	164	VAL
2	B	179	GLU
2	B	201	THR
2	B	218	PHE
2	B	248	VAL
1	C	8	GLN
1	C	37	TYR
1	C	80	ASN
1	C	191	LEU
1	C	195	TYR
1	C	197	VAL
1	C	233	LEU
1	C	236	VAL
1	C	255	GLU
2	D	7	VAL
2	D	11	LYS
2	D	39	LYS
2	D	49	MET
2	D	78	ARG
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	218	PHE
2	D	248	VAL
1	E	37	TYR
1	E	188	VAL
1	E	191	LEU
1	E	195	TYR
1	E	204	LYS
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	78	ARG
2	F	129	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	24	GLU
1	G	37	TYR
1	G	188	VAL
1	G	191	LEU
1	G	195	TYR
1	G	197	VAL
1	G	233	LEU
1	G	236	VAL
1	G	255	GLU
2	H	8	GLU
2	H	37	VAL
2	H	39	LYS
2	H	74	ARG
2	H	78	ARG
2	H	129	THR
2	H	138	SER
2	H	164	VAL
2	H	179	GLU
2	H	201	THR
2	H	202	LEU
2	H	218	PHE
2	H	248	VAL
1	I	37	TYR
1	I	191	LEU
1	I	195	TYR
1	I	233	LEU
1	I	236	VAL
1	I	255	GLU
2	J	15	ASP
2	J	37	VAL
2	J	39	LYS
2	J	78	ARG
2	J	129	THR
2	J	138	SER
2	J	164	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	177	LEU
2	J	179	GLU
2	J	201	THR
2	J	218	PHE
2	J	248	VAL
1	K	37	TYR
1	K	81	GLN
1	K	188	VAL
1	K	191	LEU
1	K	195	TYR
1	K	197	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	78	ARG
2	L	129	THR
2	L	138	SER
2	L	164	VAL
2	L	179	GLU
2	L	201	THR
2	L	218	PHE
2	L	234	GLU
2	L	248	VAL
1	M	8	GLN
1	M	37	TYR
1	M	191	LEU
1	M	195	TYR
1	M	233	LEU
1	M	236	VAL
1	M	255	GLU
2	N	16	ASP
2	N	37	VAL
2	N	39	LYS
2	N	78	ARG
2	N	129	THR
2	N	138	SER
2	N	164	VAL
2	N	179	GLU
2	N	201	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	218	PHE
2	N	248	VAL
1	O	37	TYR
1	O	188	VAL
1	O	191	LEU
1	O	195	TYR
1	O	197	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	129	THR
2	P	138	SER
2	P	164	VAL
2	P	179	GLU
2	P	201	THR
2	P	218	PHE
2	P	248	VAL
1	Q	37	TYR
1	Q	80	ASN
1	Q	188	VAL
1	Q	191	LEU
1	Q	195	TYR
1	Q	197	VAL
1	Q	233	LEU
1	Q	236	VAL
1	Q	243	LYS
1	Q	255	GLU
2	R	37	VAL
2	R	39	LYS
2	R	78	ARG
2	R	129	THR
2	R	138	SER
2	R	164	VAL
2	R	179	GLU
2	R	201	THR
2	R	218	PHE
2	R	248	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	37	TYR
1	S	188	VAL
1	S	191	LEU
1	S	195	TYR
1	S	197	VAL
1	S	204	LYS
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
2	T	37	VAL
2	T	39	LYS
2	T	78	ARG
2	T	129	THR
2	T	138	SER
2	T	164	VAL
2	T	179	GLU
2	T	201	THR
2	T	218	PHE
2	T	248	VAL
1	U	8	GLN
1	U	37	TYR
1	U	188	VAL
1	U	191	LEU
1	U	195	TYR
1	U	197	VAL
1	U	204	LYS
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	129	THR
2	V	138	SER
2	V	164	VAL
2	V	177	LEU
2	V	179	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	201	THR
2	V	218	PHE
2	V	234	GLU
2	V	248	VAL
1	W	37	TYR
1	W	188	VAL
1	W	191	LEU
1	W	195	TYR
1	W	197	VAL
1	W	233	LEU
1	W	236	VAL
1	W	255	GLU
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	129	THR
2	X	138	SER
2	X	164	VAL
2	X	177	LEU
2	X	179	GLU
2	X	201	THR
2	X	218	PHE
2	X	248	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
2	B	178	ASN
1	C	272	HIS
2	D	178	ASN
1	E	80	ASN
2	F	178	ASN
2	H	178	ASN
1	I	272	HIS
2	J	178	ASN
2	J	198	ASN
1	K	272	HIS
2	L	178	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	9	ASN
1	M	81	GLN
1	M	272	HIS
2	N	178	ASN
1	O	8	GLN
1	O	29	GLN
1	O	272	HIS
2	P	40	ASN
2	P	178	ASN
2	R	178	ASN
1	U	29	GLN
2	V	178	ASN
1	W	272	HIS
2	X	178	ASN

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

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

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	260/275 (94%)	0.21	5 (1%)	70	59	23, 32, 46, 60	0
1	C	260/275 (94%)	0.20	1 (0%)	93	90	24, 32, 46, 58	0
1	E	260/275 (94%)	0.16	2 (0%)	87	81	24, 32, 46, 57	0
1	G	260/275 (94%)	0.24	8 (3%)	52	40	24, 32, 46, 58	0
1	I	260/275 (94%)	0.13	1 (0%)	93	90	24, 32, 46, 57	0
1	K	260/275 (94%)	0.22	1 (0%)	93	90	24, 32, 46, 58	0
1	M	260/275 (94%)	0.17	1 (0%)	93	90	24, 32, 46, 58	0
1	O	260/275 (94%)	0.28	5 (1%)	70	59	24, 32, 46, 59	0
1	Q	260/275 (94%)	0.20	3 (1%)	81	73	24, 32, 46, 59	0
1	S	260/275 (94%)	0.16	3 (1%)	81	73	24, 32, 46, 57	0
1	U	260/275 (94%)	0.16	3 (1%)	81	73	24, 32, 46, 58	0
1	W	260/275 (94%)	0.16	3 (1%)	81	73	24, 32, 46, 57	0
2	B	241/248 (97%)	0.18	0	100	100	25, 31, 46, 59	0
2	D	247/248 (99%)	0.21	3 (1%)	81	73	22, 30, 46, 59	0
2	F	241/248 (97%)	0.18	4 (1%)	73	63	25, 31, 47, 59	0
2	H	241/248 (97%)	0.18	3 (1%)	81	73	25, 31, 46, 59	0
2	J	241/248 (97%)	0.17	1 (0%)	93	90	25, 31, 46, 59	0
2	L	247/248 (99%)	0.22	7 (2%)	56	44	22, 31, 46, 59	0
2	N	241/248 (97%)	0.16	1 (0%)	93	90	25, 31, 46, 59	0
2	P	248/248 (100%)	0.20	2 (0%)	87	81	23, 30, 46, 59	0
2	R	245/248 (98%)	0.29	4 (1%)	74	66	23, 31, 46, 59	0
2	T	247/248 (99%)	0.21	2 (0%)	87	81	23, 31, 46, 59	0
2	V	244/248 (98%)	0.17	2 (0%)	87	81	25, 31, 46, 59	0
2	X	241/248 (97%)	0.17	1 (0%)	93	90	25, 31, 46, 59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	6044/6276 (96%)	0.19	66 (1%) 82 74	22, 31, 47, 60	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	248	VAL	4.6
2	F	247	GLY	3.9
1	G	181	SER	3.6
1	E	175	GLN	3.5
1	U	275	ILE	3.4
2	L	60	GLY	3.1
2	F	248	VAL	3.1
1	O	8	GLN	3.1
1	Q	9	ASN	3.1
2	F	246	GLU	3.1
2	P	60	GLY	3.0
1	A	173	VAL	3.0
1	O	180	ILE	3.0
1	O	181	SER	3.0
1	G	130	VAL	2.9
1	G	173	VAL	2.8
1	E	173	VAL	2.8
1	K	182	VAL	2.8
1	G	275	ILE	2.7
2	P	65	HIS	2.7
1	W	80	ASN	2.7
2	L	248	VAL	2.7
2	R	248	VAL	2.7
1	A	7	ASN	2.5
1	U	171	TYR	2.5
1	S	7	ASN	2.5
1	Q	182	VAL	2.5
1	A	181	SER	2.5
2	D	169	ALA	2.5
1	I	173	VAL	2.4
2	N	9	ARG	2.4
2	L	169	ALA	2.4
1	W	9	ASN	2.4
2	X	248	VAL	2.4
1	G	7	ASN	2.3
1	C	8	GLN	2.3
2	F	63	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	275	ILE	2.3
2	D	246	GLU	2.3
1	O	175	GLN	2.3
2	H	240	TYR	2.3
1	G	131	ILE	2.3
2	L	90	GLU	2.3
1	A	182	VAL	2.3
2	L	65	HIS	2.2
2	R	60	GLY	2.2
2	R	247	GLY	2.2
2	V	248	VAL	2.2
2	H	178	ASN	2.2
2	H	60	GLY	2.1
2	T	65	HIS	2.1
1	W	275	ILE	2.1
1	S	182	VAL	2.1
1	G	37	TYR	2.1
1	U	11	ILE	2.1
1	O	9	ASN	2.1
1	A	80	ASN	2.1
2	J	11	LYS	2.1
2	L	246	GLU	2.1
2	L	68	HIS	2.0
2	R	246	GLU	2.0
2	T	248	VAL	2.0
2	V	5	LEU	2.0
1	S	174	GLU	2.0
1	G	182	VAL	2.0
1	Q	185	ASN	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

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
3	CL	B	1249	1/1	0.86	0.20	0.08	67,67,67,67	0
3	CL	J	1249	1/1	0.95	0.17	-0.68	47,47,47,47	0
3	CL	V	1249	1/1	0.94	0.18	-0.72	52,52,52,52	0
3	CL	N	1249	1/1	0.85	0.19	-1.05	56,56,56,56	0
3	CL	L	1249	1/1	0.83	0.20	-1.31	45,45,45,45	0
3	CL	F	1249	1/1	0.90	0.17	-1.31	48,48,48,48	0
3	CL	H	1249	1/1	0.96	0.16	-1.32	52,52,52,52	0
3	CL	X	1249	1/1	0.90	0.16	-2.05	43,43,43,43	0
3	CL	T	1249	1/1	0.94	0.14	-2.27	50,50,50,50	0
3	CL	D	1249	1/1	0.77	0.15	-2.94	49,49,49,49	0
3	CL	R	1249	1/1	0.95	0.15	-3.14	46,46,46,46	0
3	CL	P	1249	1/1	0.93	0.09	-7.06	59,59,59,59	0
3	CL	M	1276	1/1	0.94	0.12	-	45,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.