Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:17 pm BST

PDB ID	:	4RQP
Title	:	Crystal structure of the natually occurring empty particle of a clinical C4 strain EV71
Authors	:	Chen, R.; Lyu, K.
Deposited on	:	2014-11-04
Resolution	:	3.15 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 following versions of software and data (see references ①) were used in the production of this report:

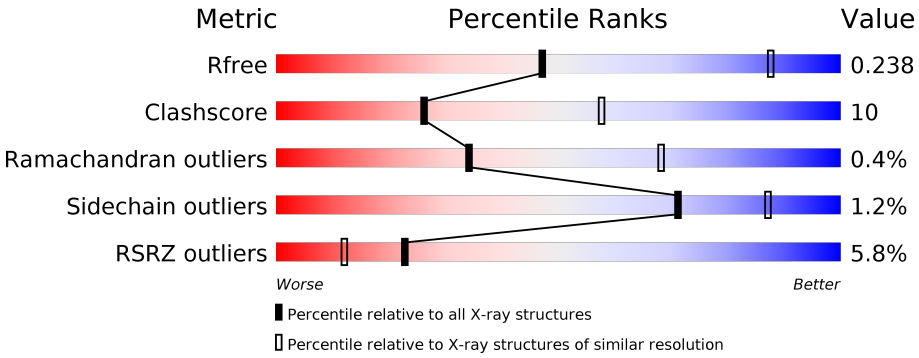
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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 <=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	297	3% 55% 19% • 25%
1	E	297	4% 57% 18% • 25%
1	I	297	4% 57% 18% • 25%
1	M	297	4% 56% 18% • 25%
1	Q	297	4% 57% 16% • 25%
2	B	242	2% 74% 18% • 7%

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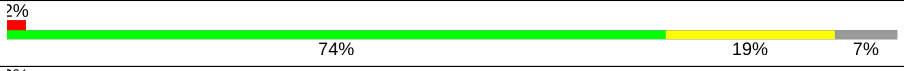
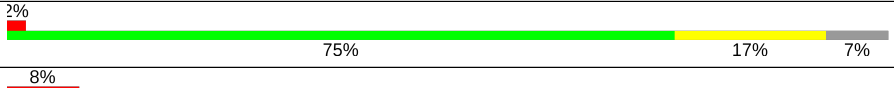
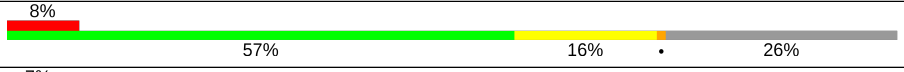
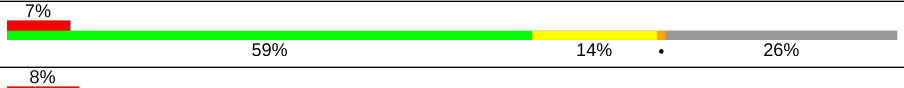
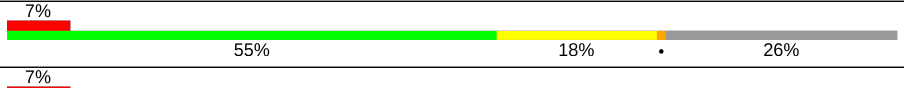
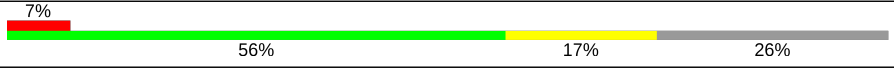
Mol	Chain	Length	Quality of chain
2	F	242	
2	J	242	
2	N	242	
2	R	242	
3	C	323	
3	G	323	
3	K	323	
3	O	323	
3	S	323	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26615 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	Q	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	I	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	M	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	A	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			

- Molecule 2 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	R	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	J	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	N	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	B	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	227	GLN	LYS	engineered mutation	UNP F6KTB0
R	227	GLN	LYS	engineered mutation	UNP F6KTB0
J	227	GLN	LYS	engineered mutation	UNP F6KTB0
N	227	GLN	LYS	engineered mutation	UNP F6KTB0
B	227	GLN	LYS	engineered mutation	UNP F6KTB0

- Molecule 3 is a protein called Capsid protein VP0.

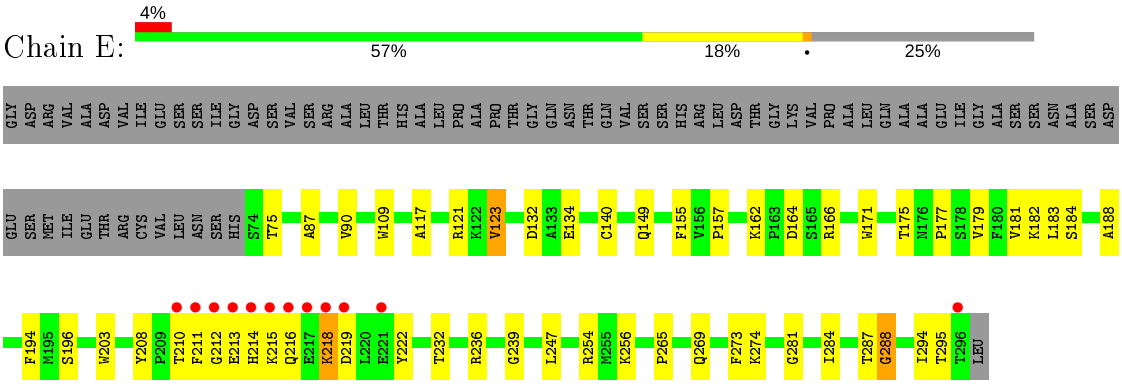
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	S	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	K	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	O	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	C	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			

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

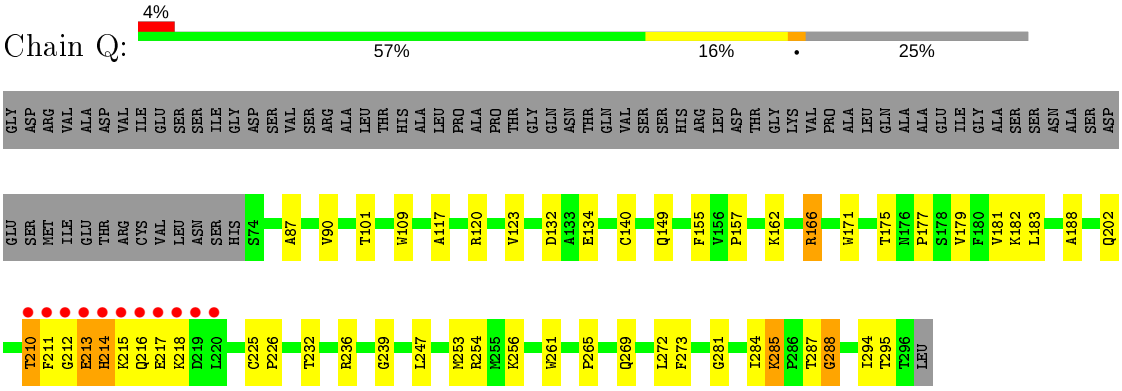
- Molecule 1: Capsid protein VP1

Chain E:



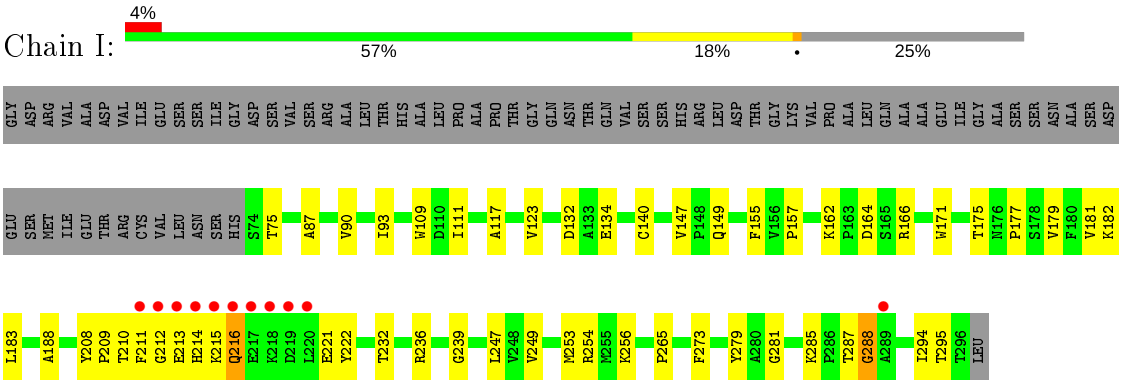
- Molecule 1: Capsid protein VP1

Chain Q:



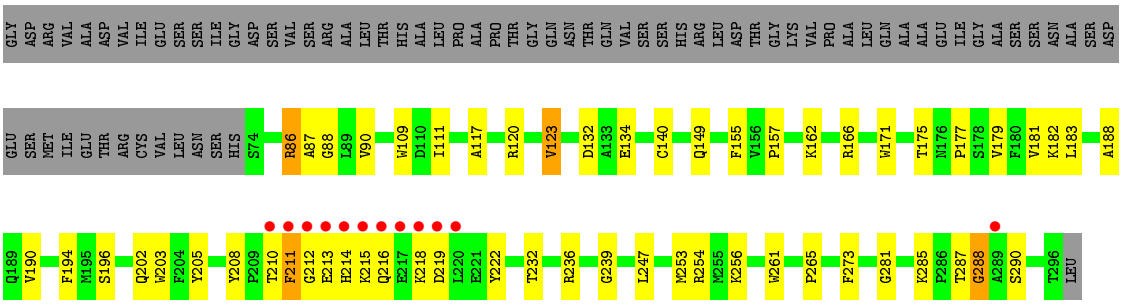
- Molecule 1: Capsid protein VP1

Chain I:



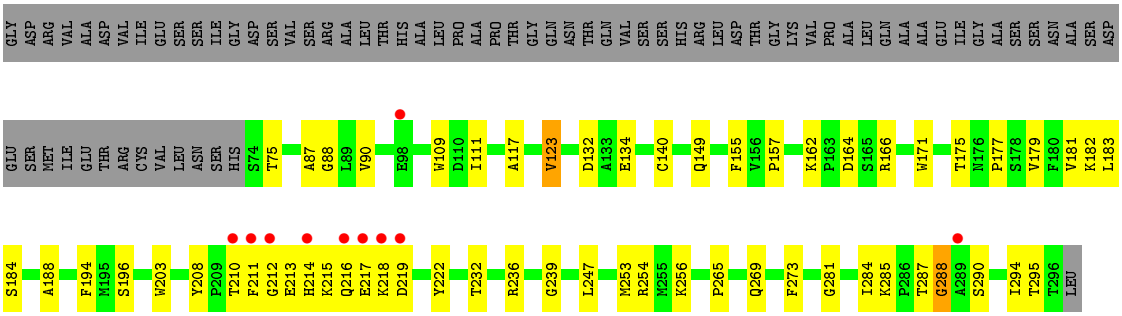
- Molecule 1: Capsid protein VP1

Chain M:



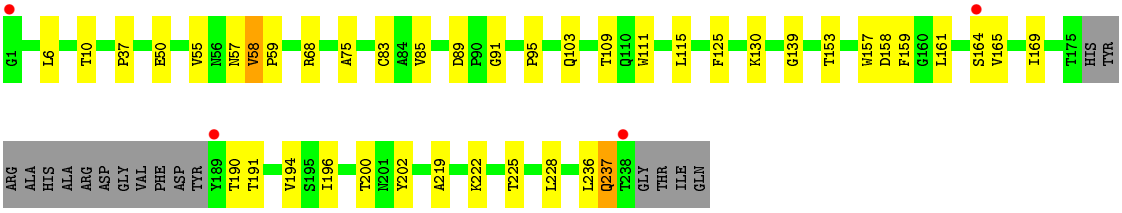
- Molecule 1: Capsid protein VP1

Chain A:



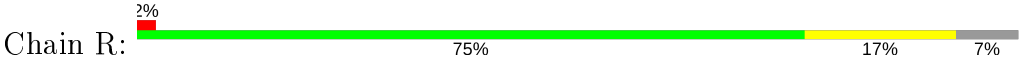
- Molecule 2: Capsid protein VP3

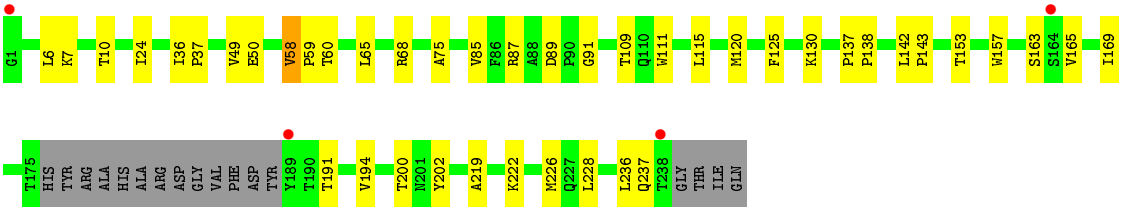
Chain F:



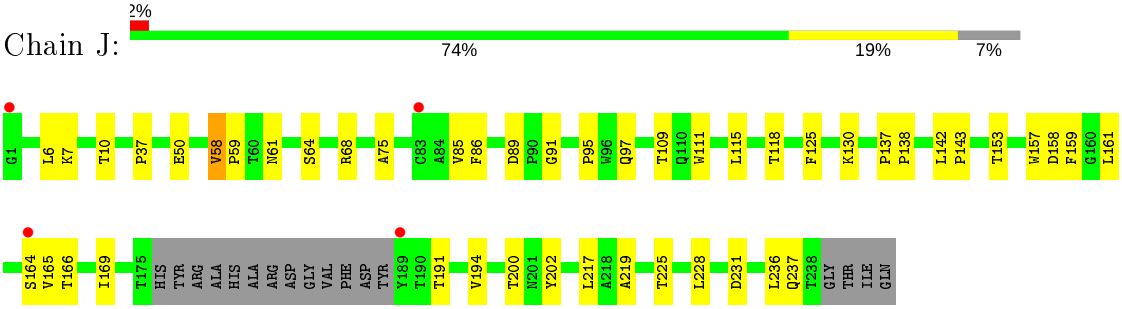
- Molecule 2: Capsid protein VP3

Chain R:

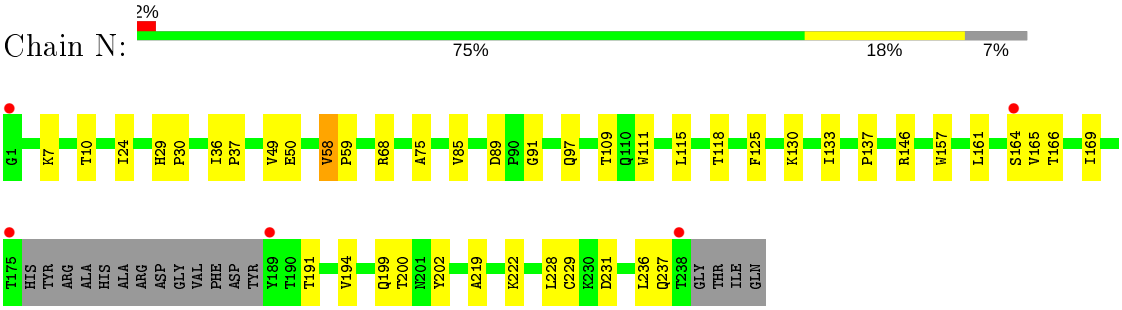




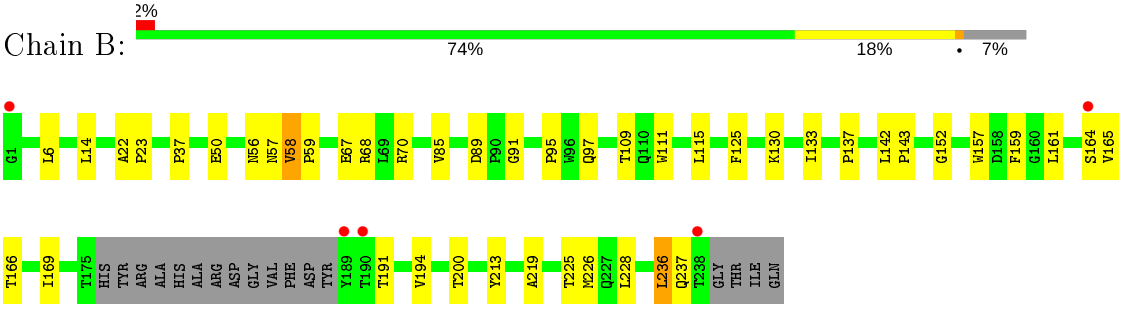
- Molecule 2: Capsid protein VP3



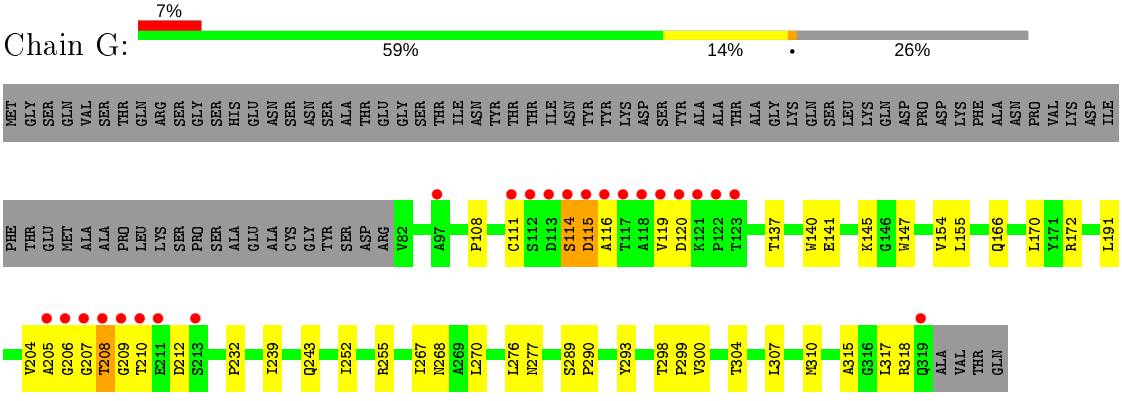
- Molecule 2: Capsid protein VP3



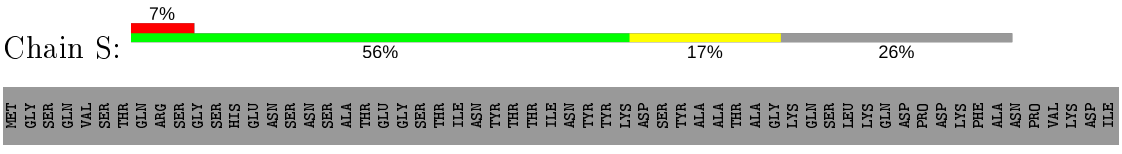
- Molecule 2: Capsid protein VP3

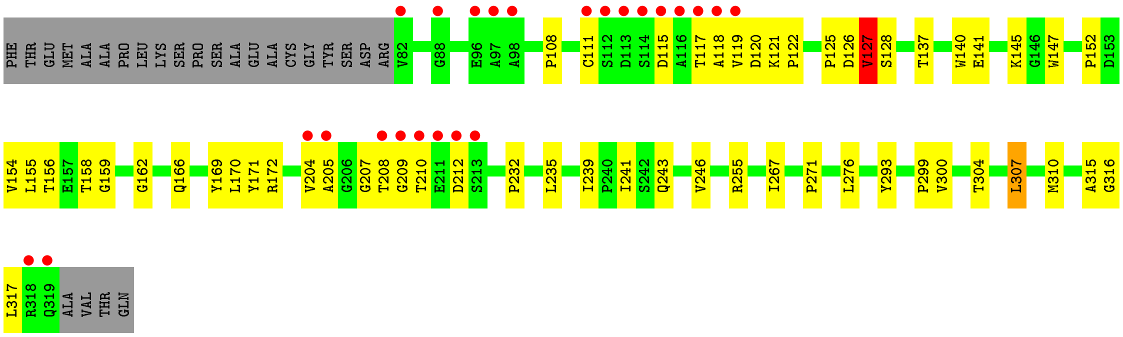


- Molecule 3: Capsid protein VP0



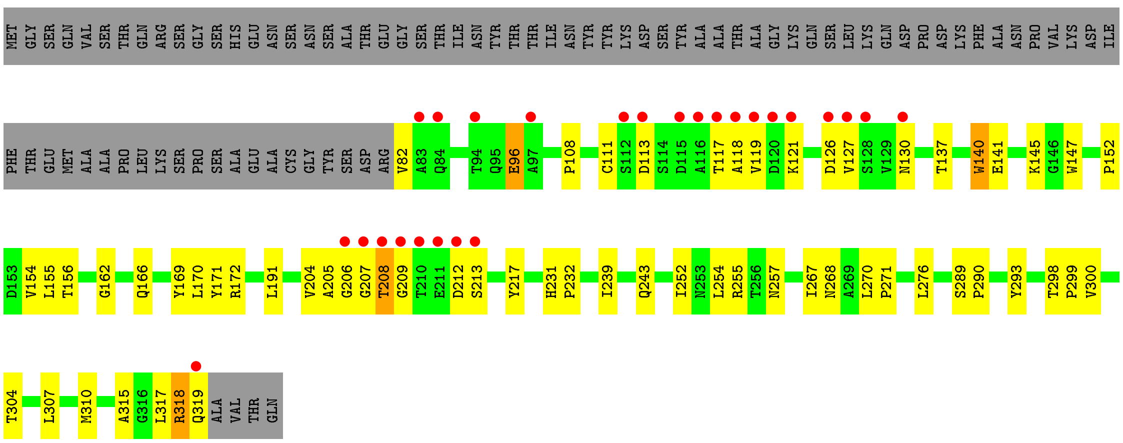
- Molecule 3: Capsid protein VP0





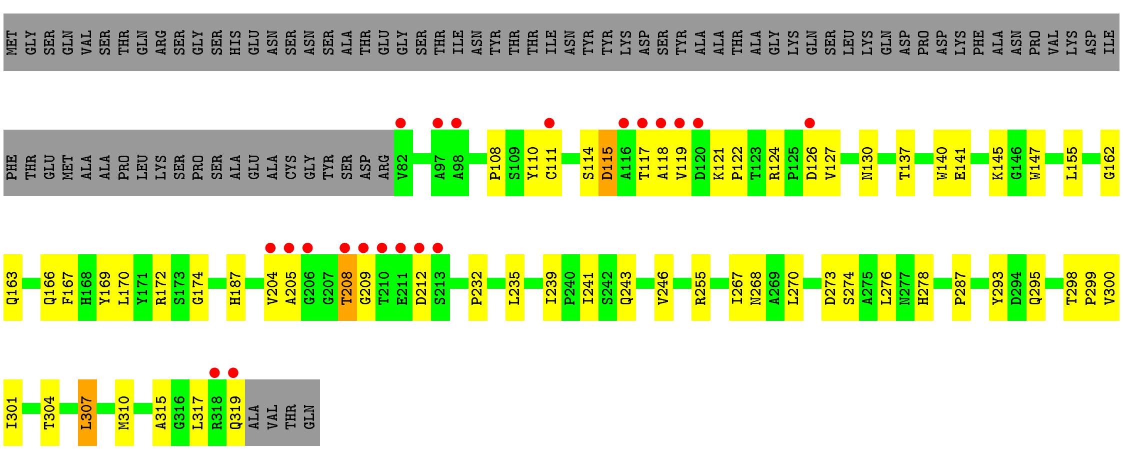
- Molecule 3: Capsid protein VP0

Chain K:



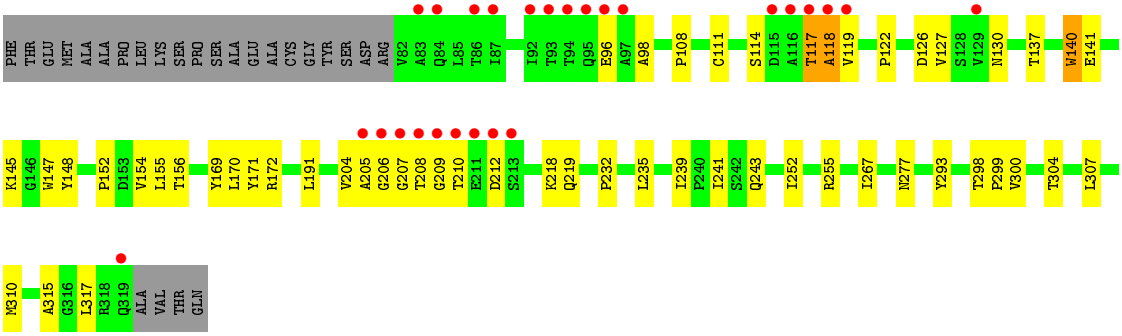
- Molecule 3: Capsid protein VP0

Chain O:



- Molecule 3: Capsid protein VP0

Chain C:


PHE THR GLU MET ALA ALA PRO LEU LYS SER PRO SER ALA GLU ALA CYS GLY TYR SER ASP ARG V82 A83 Q84 L85 T86 I87 I92 T93 T94 Q95 E96 A97 A98 P108 C111 S114 D115 A116 T117 A118 V119 P122 D126 V127 S128 V129 N130 T137 W140 E141
K145 G146 W147 Y148 P152 D153 V154 L155 T156 Y169 L170 Y171 R172 L191 V204 A205 G206 G207 T208 G209 T210 E211 D212 S213 K218 Q219 P232 L235 I239 P240 I241 S242 Q243 I252 R255 I267 N277 Y293 T298 P299 V300 T304 L307
M310 A315 G316 L317 R318 Q319 ALA VAL THR GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α, β, γ	352.98Å 352.98Å 352.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.15 49.92 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.92-3.15) 78.4 (49.92-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.216 , 0.234 0.216 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 20.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	26615	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.32	0/1818	0.51	0/2478
1	E	0.31	0/1818	0.50	0/2478
1	I	0.36	0/1818	0.53	0/2478
1	M	0.31	0/1818	0.50	0/2478
1	Q	0.35	0/1818	0.56	0/2478
2	B	0.31	0/1764	0.47	0/2415
2	F	0.27	0/1764	0.47	0/2415
2	J	0.30	0/1764	0.47	0/2415
2	N	0.29	0/1764	0.47	0/2415
2	R	0.28	0/1764	0.48	0/2415
3	C	0.31	0/1896	0.51	1/2602 (0.0%)
3	G	0.28	0/1896	0.50	1/2602 (0.0%)
3	K	0.30	0/1896	0.52	1/2602 (0.0%)
3	O	0.29	0/1896	0.51	1/2602 (0.0%)
3	S	0.32	0/1896	0.55	1/2602 (0.0%)
All	All	0.31	0/27390	0.50	5/37475 (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	I	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	115	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	115	ASP	N-CA-C	5.37	125.50	111.00
3	S	127	VAL	CG1-CB-CG2	-5.30	102.42	110.90
3	C	140	TRP	CA-CB-CG	5.02	123.23	113.70
3	K	140	TRP	CA-CB-CG	5.00	123.20	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	114	SER	Peptide
1	I	216	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1764	0	1712	54	0
1	E	1764	0	1712	47	0
1	I	1764	0	1712	44	0
1	M	1764	0	1712	55	0
1	Q	1764	0	1712	55	0
2	B	1718	0	1707	33	0
2	F	1718	0	1707	38	0
2	J	1718	0	1707	37	0
2	N	1718	0	1707	39	0
2	R	1718	0	1707	40	0
3	C	1841	0	1780	42	0
3	G	1841	0	1780	41	0
3	K	1841	0	1780	51	0
3	O	1841	0	1780	46	0
3	S	1841	0	1780	42	0
All	All	26615	0	25995	549	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 10.

All (549) 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:I:210:THR:HG22	1:I:211:PHE:HA	1.29	1.15
1:Q:213:GLU:HB2	1:Q:214:HIS:HA	1.34	1.05
1:A:215:LYS:H	1:A:216:GLN:HA	1.29	0.96
1:M:86:ARG:NH2	2:N:229:CYS:SG	2.42	0.92
1:Q:213:GLU:CB	1:Q:214:HIS:HA	2.03	0.88
1:I:287:THR:O	2:J:68:ARG:NH2	2.11	0.83
1:I:210:THR:CG2	1:I:211:PHE:HA	2.09	0.80
2:N:89:ASP:HB2	2:N:191:THR:HG21	1.63	0.80
1:M:181:VAL:HG21	1:M:188:ALA:HB2	1.64	0.79
1:M:287:THR:O	2:N:68:ARG:NH2	2.15	0.79
3:C:208:THR:OG1	3:C:209:GLY:N	2.13	0.79
2:R:89:ASP:HB2	2:R:191:THR:HG21	1.64	0.79
1:E:181:VAL:HG21	1:E:188:ALA:HB2	1.65	0.78
2:F:89:ASP:HB2	2:F:191:THR:HG21	1.66	0.78
3:S:119:VAL:HG13	3:S:120:ASP:HB3	1.65	0.77
1:A:181:VAL:HG21	1:A:188:ALA:HB2	1.67	0.76
2:B:89:ASP:HB2	2:B:191:THR:HG21	1.66	0.76
3:S:208:THR:HG22	3:S:209:GLY:N	2.00	0.76
1:E:287:THR:O	2:F:68:ARG:NH2	2.18	0.76
1:Q:215:LYS:H	1:Q:216:GLN:HA	1.52	0.75
1:A:218:LYS:HG2	1:A:219:ASP:H	1.51	0.75
1:A:215:LYS:N	1:A:216:GLN:HA	1.94	0.74
1:I:181:VAL:HG21	1:I:188:ALA:HB2	1.67	0.74
1:Q:210:THR:HG22	1:Q:211:PHE:HB3	1.68	0.74
3:K:318:ARG:HG2	3:K:319:GLN:N	2.01	0.74
2:J:109:THR:HB	2:J:228:LEU:HB3	1.69	0.74
1:A:287:THR:O	2:B:68:ARG:NH2	2.20	0.74
1:Q:287:THR:O	2:R:68:ARG:NH2	2.21	0.73
1:E:117:ALA:HA	2:F:236:LEU:HD22	1.70	0.73
3:G:317:LEU:HB2	2:B:137:PRO:HG3	1.68	0.73
1:Q:181:VAL:HG21	1:Q:188:ALA:HB2	1.69	0.73
1:E:213:GLU:HB2	1:E:214:HIS:HA	1.71	0.71
1:M:215:LYS:H	1:M:216:GLN:HA	1.53	0.71
1:A:117:ALA:HA	2:B:236:LEU:HD22	1.72	0.71
2:F:109:THR:HB	2:F:228:LEU:HB3	1.73	0.71
1:Q:117:ALA:HA	2:R:236:LEU:HD22	1.71	0.71
3:G:208:THR:OG1	3:G:209:GLY:N	2.22	0.70
2:F:236:LEU:HG	2:F:237:GLN:H	1.56	0.70
2:J:236:LEU:HG	2:J:237:GLN:H	1.57	0.70
1:Q:285:LYS:CD	1:Q:285:LYS:H	2.03	0.70
1:M:117:ALA:HA	2:N:236:LEU:HD22	1.73	0.70
3:K:140:TRP:HB2	3:K:147:TRP:HH2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:236:LEU:HG	2:R:237:GLN:H	1.56	0.69
3:O:140:TRP:HB2	3:O:147:TRP:HH2	1.55	0.69
1:E:216:GLN:HE21	3:G:277:ASN:HD21	1.40	0.69
3:G:140:TRP:HB2	3:G:147:TRP:HH2	1.56	0.69
2:N:109:THR:HB	2:N:228:LEU:HB3	1.73	0.69
3:S:140:TRP:HB2	3:S:147:TRP:HH2	1.55	0.69
2:N:236:LEU:HG	2:N:237:GLN:H	1.56	0.69
3:G:141:GLU:HG2	3:G:300:VAL:HG12	1.74	0.68
1:M:211:PHE:HE1	3:O:274:SER:HB2	1.57	0.68
3:C:140:TRP:HB2	3:C:147:TRP:HH2	1.56	0.68
2:J:89:ASP:HB2	2:J:191:THR:HG21	1.75	0.68
3:K:141:GLU:HG2	3:K:300:VAL:HG12	1.74	0.68
3:S:126:ASP:OD1	3:S:127:VAL:N	2.26	0.68
1:I:117:ALA:HA	2:J:236:LEU:HD22	1.76	0.68
2:B:85:VAL:HB	2:B:194:VAL:HB	1.75	0.67
3:K:208:THR:OG1	3:K:209:GLY:N	2.27	0.67
2:R:109:THR:HB	2:R:228:LEU:HB3	1.76	0.67
2:J:37:PRO:HG2	3:K:267:ILE:HG12	1.77	0.67
1:A:210:THR:OG1	1:A:211:PHE:HA	1.94	0.67
1:A:213:GLU:HG3	1:A:215:LYS:N	2.10	0.67
3:S:141:GLU:HG2	3:S:300:VAL:HG12	1.76	0.66
2:R:37:PRO:HG2	3:S:267:ILE:HG12	1.77	0.66
3:G:115:ASP:CG	3:G:116:ALA:H	1.99	0.65
1:E:213:GLU:HB2	1:E:214:HIS:CA	2.28	0.64
2:B:37:PRO:HG2	3:C:267:ILE:HG12	1.79	0.64
1:M:213:GLU:HB2	1:M:214:HIS:CA	2.29	0.63
1:Q:210:THR:HG22	1:Q:211:PHE:CB	2.28	0.63
3:C:141:GLU:HG2	3:C:300:VAL:HG12	1.80	0.62
1:I:265:PRO:HG2	3:K:239:ILE:HD12	1.81	0.62
2:N:85:VAL:HB	2:N:194:VAL:HB	1.80	0.62
1:E:162:LYS:HD3	1:E:232:THR:HG21	1.81	0.62
2:F:236:LEU:HG	2:F:237:GLN:HG3	1.82	0.62
2:J:161:LEU:HD23	2:J:164:SER:HB2	1.82	0.62
1:A:273:PHE:CE2	3:C:212:ASP:HB3	2.35	0.61
1:A:162:LYS:HD3	1:A:232:THR:HG21	1.81	0.61
1:E:215:LYS:H	1:E:216:GLN:HA	1.65	0.61
2:F:75:ALA:HA	2:F:202:TYR:HB3	1.83	0.61
1:M:134:GLU:HB2	1:M:256:LYS:HE3	1.81	0.61
2:R:130:LYS:HB2	2:R:200:THR:HG23	1.82	0.61
1:E:132:ASP:HB2	1:E:256:LYS:HB2	1.83	0.61
1:M:202:GLN:NE2	1:M:205:TYR:HD1	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:236:LEU:HG	2:F:237:GLN:CG	2.31	0.60
1:M:162:LYS:HD3	1:M:232:THR:HG21	1.83	0.60
1:Q:162:LYS:HD3	1:Q:232:THR:HG21	1.82	0.60
2:R:137:PRO:HD3	3:K:317:LEU:HD22	1.83	0.60
1:A:216:GLN:HG2	1:A:217:GLU:H	1.67	0.60
1:E:210:THR:HB	1:E:211:PHE:HA	1.83	0.60
1:E:218:LYS:HG3	1:E:219:ASP:H	1.66	0.60
2:B:50:GLU:HA	2:B:219:ALA:HB2	1.84	0.60
2:B:109:THR:HB	2:B:228:LEU:HB3	1.83	0.60
2:B:236:LEU:HG	2:B:237:GLN:H	1.65	0.60
3:K:204:VAL:HG12	3:K:206:GLY:H	1.68	0.59
1:Q:269:GLN:NE2	1:Q:284:ILE:O	2.33	0.59
1:I:166:ARG:NH2	1:I:239:GLY:O	2.34	0.59
1:I:281:GLY:N	3:K:204:VAL:HG11	2.18	0.59
2:R:115:LEU:HB2	2:R:169:ILE:HB	1.84	0.59
1:A:273:PHE:CZ	3:C:212:ASP:HB3	2.38	0.59
1:Q:217:GLU:O	1:Q:218:LYS:HG3	2.02	0.59
1:I:213:GLU:HB2	1:I:214:HIS:CA	2.33	0.59
3:K:82:VAL:N	3:K:96:GLU:OE2	2.35	0.59
3:O:208:THR:OG1	3:O:209:GLY:N	2.35	0.59
2:F:10:THR:HG23	2:B:6:LEU:H	1.68	0.58
2:N:50:GLU:HA	2:N:219:ALA:HB2	1.85	0.58
1:E:281:GLY:N	3:G:204:VAL:HG11	2.18	0.58
1:I:281:GLY:H	3:K:204:VAL:HG11	1.69	0.58
1:M:166:ARG:NH2	1:M:239:GLY:O	2.37	0.58
1:A:265:PRO:HB3	3:C:243:GLN:HB2	1.86	0.57
1:E:265:PRO:HG2	3:G:239:ILE:HD12	1.86	0.57
3:K:108:PRO:HG2	3:K:310:MET:HG3	1.86	0.57
2:N:161:LEU:HD13	2:N:164:SER:HB2	1.86	0.57
1:Q:213:GLU:HB2	1:Q:214:HIS:CA	2.23	0.57
1:M:211:PHE:CE1	3:O:274:SER:HB2	2.38	0.57
2:F:139:GLY:HA2	1:Q:211:PHE:HE1	1.67	0.57
2:B:115:LEU:HB2	2:B:169:ILE:HB	1.87	0.57
1:Q:273:PHE:CZ	3:S:212:ASP:HB3	2.39	0.57
2:J:137:PRO:HD3	3:O:317:LEU:HD22	1.85	0.57
2:R:85:VAL:HB	2:R:194:VAL:HB	1.87	0.57
1:E:273:PHE:CE2	3:G:212:ASP:HB3	2.40	0.56
2:J:85:VAL:HB	2:J:194:VAL:HB	1.86	0.56
1:E:166:ARG:NH2	1:E:239:GLY:O	2.38	0.56
2:F:190:THR:HB	1:Q:211:PHE:CZ	2.40	0.56
2:F:85:VAL:HB	2:F:194:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:91:GLY:HA3	2:J:111:TRP:CZ2	2.41	0.56
3:S:145:LYS:HB3	3:S:232:PRO:HG3	1.87	0.56
1:E:273:PHE:CZ	3:G:212:ASP:HB3	2.40	0.56
1:M:213:GLU:HB2	1:M:214:HIS:C	2.26	0.56
2:F:115:LEU:HB2	2:F:169:ILE:HB	1.87	0.56
1:A:281:GLY:N	3:C:204:VAL:HG11	2.21	0.56
2:N:137:PRO:HG3	3:C:317:LEU:HB2	1.88	0.56
1:A:166:ARG:NH2	1:A:239:GLY:O	2.39	0.56
3:C:126:ASP:OD1	3:C:127:VAL:N	2.38	0.56
3:O:141:GLU:HG2	3:O:300:VAL:HG12	1.87	0.56
1:I:294:ILE:HG13	1:I:295:THR:HG23	1.87	0.55
2:J:50:GLU:HA	2:J:219:ALA:HB2	1.87	0.55
2:N:130:LYS:HB2	2:N:200:THR:HG23	1.87	0.55
3:O:108:PRO:HG2	3:O:310:MET:HG3	1.87	0.55
1:Q:285:LYS:HD2	1:Q:285:LYS:H	1.69	0.55
1:I:287:THR:OG1	1:I:288:GLY:N	2.39	0.55
2:R:75:ALA:HA	2:R:202:TYR:HB3	1.87	0.55
3:S:108:PRO:HG2	3:S:310:MET:HG3	1.89	0.55
1:I:213:GLU:HB2	1:I:214:HIS:C	2.27	0.55
3:O:126:ASP:OD1	3:O:127:VAL:N	2.40	0.54
3:K:145:LYS:HB3	3:K:232:PRO:HG3	1.90	0.54
3:C:108:PRO:HG2	3:C:310:MET:HG3	1.88	0.54
2:J:130:LYS:HB2	2:J:200:THR:HG23	1.89	0.54
1:I:140:CYS:HA	1:I:183:LEU:HD21	1.90	0.54
2:B:157:TRP:CG	2:B:165:VAL:HG21	2.42	0.54
1:M:287:THR:OG1	1:M:288:GLY:N	2.41	0.54
1:Q:211:PHE:HD1	1:Q:212:GLY:O	1.89	0.54
1:A:140:CYS:HA	1:A:183:LEU:HD21	1.89	0.54
2:J:125:PHE:HA	3:K:255:ARG:HG3	1.90	0.54
2:R:143:PRO:HB3	3:K:318:ARG:NH2	2.23	0.54
1:Q:273:PHE:CE2	3:S:212:ASP:HB3	2.43	0.54
1:E:149:GLN:HG2	1:E:247:LEU:HD11	1.88	0.54
3:G:115:ASP:CG	3:G:116:ALA:N	2.60	0.54
1:M:213:GLU:HB2	1:M:214:HIS:HA	1.90	0.54
1:A:166:ARG:HG2	1:A:236:ARG:HH21	1.72	0.53
2:R:6:LEU:H	2:J:10:THR:HG23	1.73	0.53
2:F:37:PRO:HG2	3:G:267:ILE:HG12	1.89	0.53
2:R:143:PRO:HB3	3:K:318:ARG:HH22	1.74	0.53
1:E:182:LYS:HE2	1:A:184:SER:O	2.09	0.53
1:M:90:VAL:HG21	1:M:253:MET:HB3	1.89	0.53
1:A:265:PRO:HG2	3:C:239:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:LEU:HB2	3:C:252:ILE:HB	1.91	0.53
1:E:117:ALA:O	2:F:236:LEU:HD13	2.08	0.53
2:R:222:LYS:HD2	2:R:222:LYS:H	1.73	0.53
1:Q:285:LYS:HE2	2:R:60:THR:O	2.09	0.53
3:G:204:VAL:HG12	3:G:206:GLY:H	1.73	0.52
3:O:166:GLN:HG3	3:O:276:LEU:HD21	1.90	0.52
3:O:140:TRP:HB2	3:O:147:TRP:CH2	2.42	0.52
1:A:213:GLU:HG3	1:A:214:HIS:C	2.29	0.52
1:A:287:THR:OG1	1:A:288:GLY:N	2.40	0.52
1:I:162:LYS:HD3	1:I:232:THR:HG21	1.91	0.52
1:Q:294:ILE:HG13	1:Q:295:THR:HG23	1.90	0.52
2:B:125:PHE:HA	3:C:255:ARG:HG3	1.90	0.52
1:Q:90:VAL:HG12	1:Q:109:TRP:CZ2	2.45	0.52
2:N:125:PHE:HA	3:O:255:ARG:HG3	1.90	0.52
2:R:125:PHE:HA	3:S:255:ARG:HG3	1.92	0.52
2:R:50:GLU:HA	2:R:219:ALA:HB2	1.90	0.52
2:F:222:LYS:H	2:F:222:LYS:HD2	1.74	0.52
3:K:126:ASP:O	3:K:130:ASN:HB2	2.10	0.52
1:M:273:PHE:CZ	3:O:212:ASP:HB3	2.44	0.52
2:J:75:ALA:HA	2:J:202:TYR:HB3	1.91	0.52
2:J:115:LEU:HB2	2:J:169:ILE:HB	1.92	0.52
1:M:265:PRO:HB3	3:O:243:GLN:HB2	1.91	0.51
1:Q:287:THR:OG1	1:Q:288:GLY:N	2.43	0.51
2:R:120:MET:HA	2:R:163:SER:HB2	1.93	0.51
2:R:91:GLY:HA3	2:R:111:TRP:CZ2	2.44	0.51
2:F:190:THR:O	1:Q:211:PHE:HE2	1.93	0.51
1:M:86:ARG:HE	1:A:175:THR:HG22	1.74	0.51
3:K:204:VAL:HG12	3:K:205:ALA:H	1.75	0.51
1:M:273:PHE:CE2	3:O:212:ASP:HB3	2.46	0.51
2:F:6:LEU:H	2:R:10:THR:HG23	1.75	0.51
1:M:149:GLN:HG2	1:M:247:LEU:HD11	1.93	0.51
1:I:90:VAL:HG12	1:I:109:TRP:CZ2	2.45	0.51
1:A:181:VAL:HG12	1:A:182:LYS:O	2.11	0.51
3:C:111:CYS:SG	3:C:172:ARG:HD3	2.50	0.51
3:C:218:LYS:N	3:C:218:LYS:HD3	2.25	0.51
2:F:50:GLU:HA	2:F:219:ALA:HB2	1.91	0.51
3:S:170:LEU:HB2	3:S:315:ALA:HB3	1.93	0.51
2:N:91:GLY:HA3	2:N:111:TRP:CZ2	2.46	0.51
2:N:222:LYS:H	2:N:222:LYS:HD2	1.75	0.51
1:Q:272:LEU:HD22	3:S:208:THR:HG21	1.93	0.51
1:M:194:PHE:CZ	1:M:196:SER:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:117:THR:HG22	3:S:121:LYS:HG2	1.93	0.51
1:I:215:LYS:HB3	1:I:216:GLN:O	2.11	0.51
1:Q:281:GLY:N	3:S:204:VAL:HG11	2.26	0.50
2:F:130:LYS:HB2	2:F:200:THR:HG23	1.92	0.50
2:F:58:VAL:HG22	2:F:59:PRO:HD3	1.93	0.50
3:G:108:PRO:HG2	3:G:310:MET:HG3	1.92	0.50
2:N:75:ALA:HA	2:N:202:TYR:HB3	1.92	0.50
3:S:127:VAL:HG23	3:S:128:SER:H	1.76	0.50
1:A:269:GLN:NE2	1:A:284:ILE:O	2.41	0.50
1:A:213:GLU:OE1	3:C:277:ASN:ND2	2.43	0.50
2:B:130:LYS:HB2	2:B:200:THR:HG23	1.93	0.50
2:J:153:THR:H	3:O:317:LEU:CD2	2.24	0.50
1:I:273:PHE:CE2	3:K:212:ASP:HB3	2.46	0.50
3:O:163:GLN:OE1	3:O:167:PHE:HE2	1.94	0.50
2:J:58:VAL:HG22	2:J:59:PRO:HD3	1.94	0.50
2:J:7:LYS:O	2:J:10:THR:OG1	2.23	0.50
1:Q:179:VAL:HG12	1:Q:181:VAL:HG23	1.94	0.50
1:E:140:CYS:HA	1:E:183:LEU:HD21	1.94	0.49
3:C:152:PRO:O	3:C:156:THR:HG23	2.11	0.49
3:G:293:TYR:CZ	3:G:299:PRO:HA	2.47	0.49
1:I:90:VAL:HG21	1:I:253:MET:HB3	1.93	0.49
2:N:7:LYS:O	2:N:10:THR:OG1	2.21	0.49
2:J:118:THR:HG23	2:J:217:LEU:HB2	1.93	0.49
1:A:132:ASP:HB2	1:A:256:LYS:HB2	1.93	0.49
1:M:177:PRO:HB2	2:N:24:ILE:HG12	1.93	0.49
2:N:37:PRO:HG2	3:O:267:ILE:HG12	1.95	0.49
1:Q:90:VAL:HG12	1:Q:109:TRP:HZ2	1.78	0.49
1:Q:215:LYS:HB3	1:Q:216:GLN:O	2.12	0.49
2:F:59:PRO:HD2	2:F:68:ARG:HG2	1.95	0.49
1:Q:149:GLN:HG2	1:Q:247:LEU:HD11	1.95	0.49
2:B:111:TRP:HB3	2:B:226:MET:HG2	1.95	0.49
2:F:125:PHE:HA	3:G:255:ARG:HG3	1.94	0.49
3:C:204:VAL:HG12	3:C:205:ALA:H	1.77	0.48
2:F:157:TRP:CG	2:F:165:VAL:HG21	2.48	0.48
3:K:126:ASP:OD1	3:K:127:VAL:N	2.44	0.48
1:I:216:GLN:HG2	3:K:217:TYR:OH	2.13	0.48
2:R:137:PRO:HG3	3:K:317:LEU:HB2	1.95	0.48
2:R:142:LEU:HD12	2:R:143:PRO:HD2	1.93	0.48
1:E:265:PRO:HB3	3:G:243:GLN:HB2	1.93	0.48
3:C:235:LEU:HD21	3:C:241:ILE:HG13	1.95	0.48
3:K:117:THR:HG22	3:K:121:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:133:ILE:HD12	2:N:165:VAL:HG11	1.95	0.48
2:F:91:GLY:HA3	2:F:111:TRP:CZ2	2.48	0.48
1:Q:181:VAL:HG12	1:Q:182:LYS:O	2.14	0.48
3:S:207:GLY:HA2	3:S:208:THR:OG1	2.14	0.48
2:B:58:VAL:HG22	2:B:59:PRO:HD3	1.96	0.48
3:C:204:VAL:HG12	3:C:206:GLY:H	1.77	0.48
1:M:215:LYS:N	1:M:216:GLN:HA	2.22	0.48
1:M:285:LYS:HD2	1:M:287:THR:O	2.13	0.48
3:O:162:GLY:O	3:O:166:GLN:HB2	2.14	0.48
1:E:134:GLU:HB2	1:E:256:LYS:HE3	1.96	0.48
3:K:140:TRP:HB2	3:K:147:TRP:CH2	2.42	0.48
1:Q:272:LEU:HD13	3:S:208:THR:HG21	1.95	0.48
1:E:87:ALA:HB2	1:E:254:ARG:HB2	1.96	0.48
3:K:166:GLN:HG3	3:K:276:LEU:HD21	1.94	0.48
1:M:281:GLY:N	3:O:204:VAL:HG11	2.28	0.48
2:J:6:LEU:H	2:N:10:THR:HG23	1.78	0.48
3:S:204:VAL:HG12	3:S:205:ALA:H	1.78	0.48
3:C:126:ASP:O	3:C:130:ASN:HB2	2.13	0.48
3:G:145:LYS:HB3	3:G:232:PRO:HG3	1.96	0.48
3:G:204:VAL:HG12	3:G:205:ALA:H	1.78	0.48
3:K:204:VAL:HG12	3:K:205:ALA:N	2.29	0.47
2:N:58:VAL:HG22	2:N:59:PRO:HD3	1.96	0.47
1:Q:175:THR:O	1:Q:177:PRO:HD3	2.14	0.47
1:Q:265:PRO:HB3	3:S:243:GLN:HB2	1.95	0.47
3:S:293:TYR:CZ	3:S:299:PRO:HA	2.49	0.47
2:F:153:THR:H	3:S:317:LEU:CD1	2.26	0.47
3:O:204:VAL:HG12	3:O:205:ALA:H	1.78	0.47
1:M:265:PRO:HG2	3:O:239:ILE:HD12	1.97	0.47
1:Q:87:ALA:HB2	1:Q:254:ARG:HB2	1.95	0.47
1:A:90:VAL:HG21	1:A:253:MET:HB3	1.97	0.47
2:N:137:PRO:HD3	3:C:317:LEU:HD22	1.95	0.47
1:M:132:ASP:HB2	1:M:256:LYS:HB2	1.96	0.47
3:C:207:GLY:HA2	3:C:208:THR:HA	1.63	0.47
1:E:179:VAL:HG12	1:E:181:VAL:HG23	1.96	0.47
3:G:154:VAL:HG13	3:G:155:LEU:HG	1.95	0.47
3:G:207:GLY:HA2	3:G:208:THR:HA	1.69	0.47
1:I:213:GLU:HB2	1:I:214:HIS:HA	1.96	0.47
2:N:115:LEU:HB2	2:N:169:ILE:HB	1.97	0.47
3:O:117:THR:HG22	3:O:121:LYS:HG2	1.96	0.47
2:R:59:PRO:HD2	2:R:68:ARG:HG2	1.97	0.47
1:A:117:ALA:O	2:B:236:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:157:TRP:CG	2:J:165:VAL:HG21	2.49	0.47
2:R:153:THR:H	3:K:317:LEU:CD2	2.28	0.47
3:O:169:TYR:CD2	3:O:170:LEU:HG	2.49	0.47
2:B:161:LEU:HD13	2:B:164:SER:HB2	1.96	0.47
1:E:294:ILE:HG13	1:E:295:THR:HG23	1.97	0.47
3:K:111:CYS:SG	3:K:172:ARG:HD3	2.54	0.47
3:S:156:THR:HA	3:S:162:GLY:HA2	1.95	0.47
1:A:212:GLY:HA2	1:A:213:GLU:HA	1.47	0.47
3:C:122:PRO:HB3	3:C:315:ALA:HB2	1.96	0.47
1:E:90:VAL:HG12	1:E:109:TRP:CZ2	2.50	0.47
1:I:208:TYR:CE2	1:I:222:TYR:HB2	2.50	0.47
1:M:166:ARG:HG2	1:M:236:ARG:HH21	1.78	0.47
1:A:294:ILE:HG13	1:A:295:THR:HG23	1.96	0.47
3:K:191:LEU:HB2	3:K:252:ILE:HB	1.97	0.47
1:Q:212:GLY:HA2	1:Q:213:GLU:O	2.15	0.47
1:E:218:LYS:CG	1:E:219:ASP:H	2.29	0.46
3:G:209:GLY:HA3	3:G:210:THR:HA	1.74	0.46
1:I:175:THR:O	1:I:177:PRO:HD3	2.16	0.46
1:M:90:VAL:HG12	1:M:109:TRP:CZ2	2.49	0.46
2:R:49:VAL:HG11	3:S:246:VAL:HA	1.96	0.46
1:A:215:LYS:HB3	1:A:216:GLN:O	2.15	0.46
1:E:181:VAL:HG12	1:E:182:LYS:O	2.15	0.46
2:J:166:THR:O	2:J:166:THR:OG1	2.29	0.46
1:A:87:ALA:HB2	1:A:254:ARG:HB2	1.95	0.46
3:C:111:CYS:HB3	3:C:172:ARG:CZ	2.45	0.46
1:Q:140:CYS:HA	1:Q:183:LEU:HD21	1.96	0.46
1:A:90:VAL:HG12	1:A:109:TRP:CZ2	2.50	0.46
1:I:181:VAL:HG12	1:I:182:LYS:O	2.15	0.46
1:M:155:PHE:O	1:M:157:PRO:HD3	2.16	0.46
3:G:317:LEU:HD21	2:B:152:GLY:HA3	1.97	0.46
1:E:194:PHE:CZ	1:E:196:SER:HB3	2.51	0.46
3:O:111:CYS:SG	3:O:172:ARG:HD3	2.55	0.46
2:J:142:LEU:HD12	2:J:143:PRO:HD2	1.96	0.46
1:Q:155:PHE:O	1:Q:157:PRO:HD3	2.16	0.46
1:I:87:ALA:HB2	1:I:254:ARG:HB2	1.98	0.46
1:M:179:VAL:HG12	1:M:181:VAL:HG23	1.97	0.46
2:N:49:VAL:HG11	3:O:246:VAL:HA	1.98	0.46
1:A:194:PHE:CZ	1:A:196:SER:HB3	2.51	0.46
3:C:118:ALA:HA	3:C:119:VAL:HA	1.52	0.46
1:I:117:ALA:O	2:J:236:LEU:HD13	2.16	0.46
1:I:265:PRO:HB3	3:K:243:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:293:TYR:CZ	3:C:299:PRO:HA	2.51	0.46
3:C:96:GLU:O	3:C:98:ALA:N	2.45	0.46
1:E:287:THR:OG1	1:E:288:GLY:N	2.49	0.46
3:O:126:ASP:O	3:O:130:ASN:HB2	2.16	0.46
1:I:166:ARG:HG2	1:I:236:ARG:HH21	1.80	0.45
2:N:157:TRP:CG	2:N:165:VAL:HG21	2.51	0.45
3:G:170:LEU:HB2	3:G:315:ALA:HB3	1.97	0.45
1:A:149:GLN:HG2	1:A:247:LEU:HD11	1.97	0.45
1:I:134:GLU:HB2	1:I:256:LYS:HE3	1.98	0.45
2:J:138:PRO:HB3	2:J:191:THR:HA	1.97	0.45
2:J:86:PHE:HB3	2:J:95:PRO:HG2	1.98	0.45
1:M:109:TRP:CZ3	1:M:111:ILE:HA	2.52	0.45
1:M:87:ALA:HB2	1:M:254:ARG:HB2	1.99	0.45
3:O:268:ASN:HD22	3:O:270:LEU:H	1.63	0.45
2:R:222:LYS:CD	2:R:222:LYS:H	2.30	0.45
3:S:111:CYS:SG	3:S:172:ARG:HD3	2.56	0.45
1:A:285:LYS:HD2	1:A:287:THR:O	2.16	0.45
1:E:164:ASP:OD1	1:E:164:ASP:N	2.49	0.45
1:E:166:ARG:HG2	1:E:236:ARG:HH21	1.80	0.45
1:I:147:VAL:H	1:I:183:LEU:HD22	1.81	0.45
3:K:154:VAL:HG13	3:K:155:LEU:HG	1.98	0.45
3:O:122:PRO:HB3	3:O:315:ALA:HB2	1.99	0.45
1:Q:132:ASP:HB2	1:Q:256:LYS:HB2	1.99	0.45
2:R:58:VAL:HG22	2:R:59:PRO:HD3	1.99	0.45
1:A:109:TRP:CZ3	1:A:111:ILE:HA	2.51	0.45
1:E:212:GLY:HA2	1:E:213:GLU:HA	1.58	0.45
1:M:175:THR:HG21	2:J:231:ASP:H	1.82	0.45
1:M:211:PHE:CG	1:M:212:GLY:N	2.85	0.45
1:M:218:LYS:HG3	1:M:219:ASP:H	1.82	0.45
1:I:279:TYR:OH	3:K:231:HIS:ND1	2.35	0.45
1:M:88:GLY:O	1:M:90:VAL:HG23	2.17	0.45
1:Q:117:ALA:O	2:R:236:LEU:HD13	2.17	0.45
2:B:59:PRO:HD2	2:B:68:ARG:HG2	1.99	0.45
3:C:137:THR:HG22	3:C:304:THR:HG23	1.99	0.45
3:G:137:THR:HG22	3:G:304:THR:HG23	1.97	0.45
1:M:171:TRP:CE3	1:M:236:ARG:HD2	2.51	0.45
1:Q:210:THR:HA	1:Q:211:PHE:HA	1.44	0.45
3:S:122:PRO:HB3	3:S:315:ALA:HB2	1.98	0.45
2:B:166:THR:OG1	2:B:166:THR:O	2.35	0.45
1:E:208:TYR:CE2	1:E:222:TYR:HB2	2.52	0.45
3:G:111:CYS:SG	3:G:172:ARG:HD3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:169:TYR:CD2	3:S:170:LEU:HG	2.52	0.45
1:A:171:TRP:CE3	1:A:236:ARG:HD2	2.53	0.44
1:I:155:PHE:O	1:I:157:PRO:HD3	2.16	0.44
1:I:212:GLY:HA2	1:I:213:GLU:HA	1.51	0.44
2:J:118:THR:HA	2:J:166:THR:HA	1.98	0.44
1:Q:134:GLU:HB2	1:Q:256:LYS:HE3	1.99	0.44
3:S:152:PRO:HG3	3:S:171:TYR:CE2	2.52	0.44
1:E:274:LYS:HA	2:F:237:GLN:OE1	2.17	0.44
1:I:273:PHE:CZ	3:K:212:ASP:HB3	2.52	0.44
2:N:236:LEU:HG	2:N:237:GLN:N	2.30	0.44
3:K:172:ARG:HD2	3:K:271:PRO:O	2.18	0.44
1:M:212:GLY:HA2	1:M:213:GLU:HA	1.50	0.44
1:A:179:VAL:HG12	1:A:181:VAL:HG23	1.99	0.44
2:J:59:PRO:HD2	2:J:68:ARG:HG2	1.99	0.44
3:O:137:THR:HG22	3:O:304:THR:HG23	2.00	0.44
1:Q:225:CYS:HA	1:Q:226:PRO:HD3	1.87	0.44
3:C:209:GLY:HA3	3:C:210:THR:HA	1.63	0.44
1:E:215:LYS:HG2	1:E:216:GLN:O	2.18	0.44
1:M:285:LYS:NZ	1:M:288:GLY:HA3	2.32	0.44
3:S:209:GLY:HA3	3:S:210:THR:HA	1.89	0.44
3:S:316:GLY:O	3:S:317:LEU:HD23	2.17	0.44
2:F:161:LEU:HD13	2:F:164:SER:HB2	2.00	0.44
3:G:155:LEU:HD21	3:G:307:LEU:HD11	2.00	0.44
1:Q:90:VAL:HG21	1:Q:253:MET:HB3	2.00	0.44
1:M:210:THR:HA	1:M:211:PHE:HA	1.63	0.44
3:K:118:ALA:HA	3:K:119:VAL:HA	1.77	0.44
3:S:235:LEU:HD21	3:S:241:ILE:HG13	2.00	0.44
2:B:133:ILE:HD12	2:B:165:VAL:HG11	2.00	0.43
3:C:111:CYS:HB2	3:C:114:SER:OG	2.18	0.43
3:G:204:VAL:HG12	3:G:205:ALA:N	2.33	0.43
2:J:158:ASP:OD1	2:J:159:PHE:N	2.51	0.43
3:K:169:TYR:CD2	3:K:170:LEU:HG	2.53	0.43
1:M:208:TYR:CE2	1:M:222:TYR:HB2	2.53	0.43
1:Q:120:ARG:HH11	2:R:237:GLN:HG2	1.83	0.43
3:G:298:THR:HA	3:G:299:PRO:HD3	1.72	0.43
3:S:154:VAL:HG13	3:S:155:LEU:HG	2.00	0.43
1:A:164:ASP:OD1	1:A:164:ASP:N	2.50	0.43
3:G:268:ASN:HD22	3:G:270:LEU:H	1.65	0.43
1:I:179:VAL:HG12	1:I:181:VAL:HG23	2.00	0.43
1:M:117:ALA:O	2:N:236:LEU:HD13	2.18	0.43
3:O:293:TYR:CZ	3:O:299:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:171:TRP:CE3	1:Q:236:ARG:HD2	2.53	0.43
2:B:70:ARG:HB2	2:B:213:TYR:HB3	2.00	0.43
1:E:269:GLN:NE2	1:E:284:ILE:O	2.39	0.43
2:F:236:LEU:HG	2:F:237:GLN:HG2	1.99	0.43
2:F:55:VAL:HG13	2:F:85:VAL:HA	1.99	0.43
3:G:119:VAL:HA	3:G:120:ASP:HA	1.76	0.43
3:K:254:LEU:HD23	3:K:254:LEU:HA	1.88	0.43
1:M:140:CYS:HA	1:M:183:LEU:HD21	2.00	0.43
3:O:298:THR:HA	3:O:299:PRO:HD3	1.78	0.43
3:C:148:TYR:OH	3:C:219:GLN:O	2.25	0.43
3:K:155:LEU:HD21	3:K:307:LEU:HD11	2.01	0.43
1:A:175:THR:HG21	2:N:231:ASP:H	1.84	0.43
1:A:218:LYS:HG2	1:A:219:ASP:N	2.27	0.43
2:B:91:GLY:HA3	2:B:111:TRP:CZ2	2.54	0.43
3:G:166:GLN:HG3	3:G:276:LEU:HD21	1.99	0.43
1:I:75:THR:HG22	2:J:225:THR:HG22	2.01	0.43
2:J:153:THR:H	3:O:317:LEU:HD21	1.83	0.43
1:A:155:PHE:O	1:A:157:PRO:HD3	2.19	0.43
1:E:184:SER:O	1:Q:182:LYS:HE2	2.19	0.43
1:I:171:TRP:CE3	1:I:236:ARG:HD2	2.53	0.43
1:M:120:ARG:NH1	2:N:237:GLN:HG2	2.34	0.43
3:C:154:VAL:HG13	3:C:155:LEU:HG	2.01	0.43
1:E:123:VAL:HG13	1:E:203:TRP:NE1	2.33	0.43
2:F:139:GLY:HA2	1:Q:211:PHE:CE1	2.52	0.43
1:M:120:ARG:HH11	2:N:237:GLN:HG2	1.83	0.43
3:G:140:TRP:HB2	3:G:147:TRP:CH2	2.44	0.43
3:G:191:LEU:HB2	3:G:252:ILE:HB	2.00	0.43
3:K:155:LEU:HD11	3:K:307:LEU:HD13	2.00	0.43
1:M:181:VAL:HG12	1:M:182:LYS:O	2.18	0.43
1:Q:261:TRP:CD1	2:R:36:ILE:HB	2.54	0.43
1:I:209:PRO:HD2	1:I:221:GLU:HB3	2.01	0.42
3:K:137:THR:HG22	3:K:304:THR:HG23	2.01	0.42
3:K:207:GLY:HA2	3:K:208:THR:HA	1.74	0.42
3:O:187:HIS:CD2	3:O:301:ILE:HD11	2.54	0.42
1:E:171:TRP:CE3	1:E:236:ARG:HD2	2.54	0.42
3:K:156:THR:HA	3:K:162:GLY:HA2	2.00	0.42
2:B:159:PHE:HB3	3:C:255:ARG:NH2	2.33	0.42
3:C:298:THR:HA	3:C:299:PRO:HD3	1.74	0.42
1:E:281:GLY:H	3:G:204:VAL:HG11	1.81	0.42
2:N:222:LYS:H	2:N:222:LYS:CD	2.32	0.42
3:O:140:TRP:CZ3	3:O:287:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:166:GLN:HG3	3:S:276:LEU:HD21	2.01	0.42
1:A:208:TYR:CE2	1:A:222:TYR:HB2	2.54	0.42
3:C:145:LYS:HB3	3:C:232:PRO:HG3	2.00	0.42
2:F:222:LYS:H	2:F:222:LYS:CD	2.31	0.42
3:G:155:LEU:HD11	3:G:307:LEU:HD13	2.02	0.42
3:K:268:ASN:HD22	3:K:270:LEU:H	1.65	0.42
1:M:123:VAL:HG13	1:M:203:TRP:NE1	2.34	0.42
3:S:119:VAL:HA	3:S:120:ASP:HA	1.84	0.42
1:A:134:GLU:HB2	1:A:256:LYS:HE3	2.02	0.42
2:B:57:ASN:ND2	2:B:95:PRO:HD3	2.35	0.42
2:R:138:PRO:HB3	2:R:191:THR:HA	2.02	0.42
1:A:123:VAL:HG13	1:A:203:TRP:NE1	2.34	0.42
1:A:281:GLY:H	3:C:204:VAL:HG11	1.85	0.42
1:I:149:GLN:HG2	1:I:247:LEU:HD11	2.00	0.42
3:K:170:LEU:HB2	3:K:315:ALA:HB3	2.01	0.42
2:N:157:TRP:HB2	2:N:165:VAL:HG21	2.01	0.42
2:F:158:ASP:OD1	2:F:159:PHE:N	2.52	0.42
1:M:261:TRP:CD1	2:N:36:ILE:HB	2.55	0.42
3:O:115:ASP:O	3:O:117:THR:N	2.53	0.42
3:S:204:VAL:HG12	3:S:205:ALA:N	2.34	0.42
3:G:114:SER:HG	3:G:115:ASP:CG	2.23	0.42
1:M:190:VAL:HG21	2:N:24:ILE:HD12	2.01	0.42
1:M:211:PHE:CE2	3:O:169:TYR:CE1	3.07	0.42
3:S:155:LEU:HD11	3:S:307:LEU:HD13	2.02	0.42
2:F:57:ASN:ND2	2:F:95:PRO:HD3	2.35	0.42
1:I:171:TRP:CZ3	1:I:236:ARG:HD2	2.55	0.42
2:J:61:ASN:ND2	2:J:64:SER:OG	2.53	0.42
2:B:142:LEU:HD12	2:B:143:PRO:HD2	2.02	0.41
1:E:216:GLN:HE21	3:G:277:ASN:ND2	2.13	0.41
3:O:273:ASP:OD2	3:O:278:HIS:ND1	2.37	0.41
1:Q:265:PRO:HG2	3:S:239:ILE:HD12	2.02	0.41
1:A:287:THR:HG22	2:B:97:GLN:HB2	2.02	0.41
3:C:169:TYR:CD2	3:C:170:LEU:HG	2.54	0.41
1:E:155:PHE:O	1:E:157:PRO:HD3	2.19	0.41
3:G:289:SER:HA	3:G:290:PRO:HD3	1.82	0.41
3:K:293:TYR:CZ	3:K:299:PRO:HA	2.55	0.41
2:F:153:THR:OG1	3:S:317:LEU:HD11	2.20	0.41
3:G:317:LEU:HB3	3:G:318:ARG:H	1.45	0.41
2:J:137:PRO:HG3	3:O:317:LEU:HB2	2.03	0.41
1:Q:215:LYS:N	1:Q:216:GLN:HA	2.21	0.41
3:S:172:ARG:HD2	3:S:271:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:ASP:OD1	1:I:164:ASP:N	2.50	0.41
3:K:152:PRO:HG3	3:K:171:TYR:CE2	2.55	0.41
1:E:175:THR:O	1:E:177:PRO:HD3	2.20	0.41
1:E:121:ARG:NH2	2:F:103:GLN:OE1	2.52	0.41
3:K:257:ASN:OD1	3:K:257:ASN:N	2.53	0.41
1:M:175:THR:O	1:M:177:PRO:HD3	2.21	0.41
1:Q:166:ARG:NH2	1:Q:239:GLY:O	2.53	0.41
2:R:7:LYS:O	2:R:10:THR:OG1	2.29	0.41
1:A:88:GLY:O	1:A:90:VAL:HG23	2.20	0.41
3:C:204:VAL:HG12	3:C:205:ALA:N	2.34	0.41
1:E:75:THR:HG22	2:F:225:THR:HG22	2.01	0.41
1:I:132:ASP:HB2	1:I:256:LYS:HB2	2.02	0.41
3:O:108:PRO:HB3	3:O:174:GLY:HA3	2.02	0.41
3:S:115:ASP:N	3:S:115:ASP:OD1	2.52	0.41
1:A:175:THR:O	1:A:177:PRO:HD3	2.20	0.41
3:K:111:CYS:HB3	3:K:172:ARG:CZ	2.51	0.41
2:B:22:ALA:HA	2:B:23:PRO:HD2	1.94	0.41
3:K:289:SER:HA	3:K:290:PRO:HD3	1.89	0.41
2:N:97:GLN:HB3	2:N:97:GLN:HE21	1.74	0.41
3:O:111:CYS:HB3	3:O:172:ARG:CZ	2.51	0.41
3:O:145:LYS:HB3	3:O:232:PRO:HG3	2.03	0.41
2:R:111:TRP:HB3	2:R:226:MET:HG2	2.03	0.41
1:Q:120:ARG:NH1	2:R:237:GLN:HG2	2.36	0.41
2:N:29:HIS:HA	2:N:30:PRO:HD2	1.97	0.41
3:O:235:LEU:HD21	3:O:241:ILE:HG13	2.03	0.41
3:O:155:LEU:HD21	3:O:307:LEU:HD11	2.03	0.41
2:B:56:ASN:ND2	2:B:67:GLU:O	2.53	0.41
3:C:117:THR:O	3:C:118:ALA:C	2.58	0.41
1:M:215:LYS:HB3	1:M:216:GLN:O	2.21	0.41
1:A:285:LYS:NZ	1:A:288:GLY:HA3	2.36	0.41
1:A:75:THR:HG22	2:B:225:THR:HG22	2.03	0.41
3:C:210:THR:HG22	3:C:210:THR:O	2.21	0.41
2:F:83:CYS:SG	2:F:196:ILE:HD12	2.61	0.41
1:I:93:ILE:HB	1:I:249:VAL:HB	2.02	0.41
3:K:298:THR:HA	3:K:299:PRO:HD3	1.77	0.41
3:O:110:TYR:HB3	3:O:124:ARG:NH1	2.36	0.41
3:O:204:VAL:HG12	3:O:205:ALA:N	2.36	0.41
2:R:120:MET:HA	2:R:163:SER:CB	2.50	0.41
3:S:137:THR:HG22	3:S:304:THR:HG23	2.02	0.41
2:N:59:PRO:HD2	2:N:68:ARG:HG2	2.04	0.40
3:S:158:THR:HB	3:S:159:GLY:H	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:288:GLY:O	1:M:290:SER:N	2.54	0.40
2:N:146:ARG:NH1	2:N:199:GLN:OE1	2.53	0.40
2:R:157:TRP:CG	2:R:165:VAL:HG21	2.57	0.40
1:Q:177:PRO:HB2	2:R:24:ILE:HG12	2.02	0.40
2:R:87:ARG:H	2:R:87:ARG:HG3	1.65	0.40
1:A:288:GLY:O	1:A:290:SER:N	2.53	0.40
1:E:179:VAL:HG22	2:B:14:LEU:HD13	2.03	0.40
3:G:317:LEU:HB2	2:B:137:PRO:CG	2.45	0.40
2:J:159:PHE:HB3	3:K:255:ARG:NH2	2.37	0.40
2:N:118:THR:HA	2:N:166:THR:HA	2.03	0.40
1:Q:285:LYS:HG3	2:R:65:LEU:HD21	2.02	0.40
1:I:109:TRP:CZ3	1:I:111:ILE:HA	2.56	0.40
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.22	0.40
2:J:97:GLN:HE21	2:J:97:GLN:HB3	1.74	0.40
3:O:118:ALA:HA	3:O:119:VAL:HA	1.77	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	221/297 (74%)	207 (94%)	13 (6%)	1 (0%)	29	65
1	E	221/297 (74%)	206 (93%)	14 (6%)	1 (0%)	29	65
1	I	221/297 (74%)	208 (94%)	12 (5%)	1 (0%)	29	65
1	M	221/297 (74%)	207 (94%)	13 (6%)	1 (0%)	29	65
1	Q	221/297 (74%)	207 (94%)	12 (5%)	2 (1%)	17	53
2	B	221/242 (91%)	202 (91%)	18 (8%)	1 (0%)	29	65
2	F	221/242 (91%)	201 (91%)	20 (9%)	0	100	100
2	J	221/242 (91%)	201 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	221/242 (91%)	200 (90%)	21 (10%)	0	100	100
2	R	221/242 (91%)	201 (91%)	20 (9%)	0	100	100
3	C	236/323 (73%)	219 (93%)	16 (7%)	1 (0%)	34	68
3	G	236/323 (73%)	219 (93%)	17 (7%)	0	100	100
3	K	236/323 (73%)	220 (93%)	15 (6%)	1 (0%)	34	68
3	O	236/323 (73%)	219 (93%)	17 (7%)	0	100	100
3	S	236/323 (73%)	218 (92%)	15 (6%)	3 (1%)	12	44
All	All	3390/4310 (79%)	3135 (92%)	243 (7%)	12 (0%)	34	68

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	127	VAL
1	Q	288	GLY
1	M	288	GLY
1	A	288	GLY
3	K	113	ASP
3	C	118	ALA
1	E	288	GLY
2	B	236	LEU
3	S	118	ALA
1	Q	101	THR
1	I	288	GLY
3	S	125	PRO

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	191/251 (76%)	190 (100%)	1 (0%)	88	95
1	E	191/251 (76%)	189 (99%)	2 (1%)	76	89
1	I	191/251 (76%)	189 (99%)	2 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	191/251 (76%)	188 (98%)	3 (2%)	62 83
1	Q	191/251 (76%)	184 (96%)	7 (4%)	34 66
2	B	189/202 (94%)	188 (100%)	1 (0%)	88 95
2	F	189/202 (94%)	187 (99%)	2 (1%)	73 88
2	J	189/202 (94%)	188 (100%)	1 (0%)	88 95
2	N	189/202 (94%)	188 (100%)	1 (0%)	88 95
2	R	189/202 (94%)	188 (100%)	1 (0%)	88 95
3	C	202/272 (74%)	199 (98%)	3 (2%)	65 84
3	G	202/272 (74%)	201 (100%)	1 (0%)	88 95
3	K	202/272 (74%)	198 (98%)	4 (2%)	55 79
3	O	202/272 (74%)	197 (98%)	5 (2%)	47 75
3	S	202/272 (74%)	201 (100%)	1 (0%)	88 95
All	All	2910/3625 (80%)	2875 (99%)	35 (1%)	71 87

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	123	VAL
1	E	218	LYS
2	F	58	VAL
2	F	237	GLN
3	G	208	THR
1	Q	123	VAL
1	Q	166	ARG
1	Q	202	GLN
1	Q	210	THR
1	Q	213	GLU
1	Q	214	HIS
1	Q	285	LYS
1	I	123	VAL
1	I	285	LYS
1	M	86	ARG
1	M	123	VAL
1	M	211	PHE
1	A	123	VAL
2	R	58	VAL
2	J	58	VAL
2	N	58	VAL

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Mol	Chain	Res	Type
2	B	58	VAL
3	S	307	LEU
3	K	96	GLU
3	K	208	THR
3	K	213	SER
3	K	318	ARG
3	O	114	SER
3	O	208	THR
3	O	295	GLN
3	O	307	LEU
3	O	319	GLN
3	C	117	THR
3	C	171	TYR
3	C	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	277	ASN
1	I	189	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	223/297 (75%)	-0.32	10 (4%) 33 19	28, 37, 132, 220	0
1	E	223/297 (75%)	-0.25	12 (5%) 25 13	27, 37, 133, 222	0
1	I	223/297 (75%)	-0.30	11 (4%) 29 16	29, 38, 132, 219	0
1	M	223/297 (75%)	-0.31	12 (5%) 25 13	28, 38, 132, 219	0
1	Q	223/297 (75%)	-0.26	11 (4%) 29 16	28, 38, 133, 219	0
2	B	225/242 (92%)	-0.38	5 (2%) 62 47	30, 42, 79, 153	0
2	F	225/242 (92%)	-0.42	4 (1%) 68 55	30, 41, 77, 151	0
2	J	225/242 (92%)	-0.42	4 (1%) 68 55	30, 42, 79, 153	0
2	N	225/242 (92%)	-0.48	5 (2%) 62 47	30, 42, 81, 155	0
2	R	225/242 (92%)	-0.45	4 (1%) 68 55	30, 42, 79, 152	0
3	C	238/323 (73%)	0.18	26 (10%) 5 3	30, 50, 166, 220	0
3	G	238/323 (73%)	0.01	23 (9%) 7 4	30, 49, 161, 218	0
3	K	238/323 (73%)	0.24	26 (10%) 5 3	30, 50, 163, 218	0
3	O	238/323 (73%)	0.03	21 (8%) 10 5	31, 50, 163, 217	0
3	S	238/323 (73%)	0.22	24 (10%) 7 3	31, 52, 164, 221	0
All	All	3430/4310 (79%)	-0.19	198 (5%) 23 12	27, 42, 137, 222	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	210	THR	14.1
3	O	210	THR	10.7
3	S	210	THR	10.0
3	K	115	ASP	7.9
3	C	116	ALA	7.3
1	Q	212	GLY	7.1
1	Q	214	HIS	7.0

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Mol	Chain	Res	Type	RSRZ
3	K	210	THR	6.8
3	G	117	THR	6.7
1	M	212	GLY	6.4
3	G	116	ALA	6.4
3	G	210	THR	6.2
3	G	115	ASP	6.1
1	E	217	GLU	6.0
3	C	117	THR	5.8
2	B	164	SER	5.8
1	M	217	GLU	5.7
3	S	208	THR	5.7
3	S	118	ALA	5.7
1	A	212	GLY	5.7
1	Q	216	GLN	5.7
3	G	118	ALA	5.6
3	K	118	ALA	5.6
3	S	117	THR	5.6
2	J	189	TYR	5.5
1	E	219	ASP	5.5
1	E	216	GLN	5.4
1	A	217	GLU	5.4
3	S	209	GLY	5.3
3	K	120	ASP	5.3
3	C	115	ASP	5.2
3	G	208	THR	5.2
3	S	114	SER	5.2
1	E	215	LYS	5.2
1	M	214	HIS	5.2
3	C	208	THR	5.1
2	F	189	TYR	5.1
1	E	210	THR	5.1
1	E	214	HIS	5.0
3	G	319	GLN	5.0
3	O	211	GLU	5.0
3	S	112	SER	5.0
3	K	117	THR	5.0
1	E	212	GLY	5.0
1	I	212	GLY	4.9
3	S	211	GLU	4.9
3	K	209	GLY	4.8
1	A	216	GLN	4.8
1	I	213	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
3	K	319	GLN	4.7
3	G	206	GLY	4.7
1	Q	219	ASP	4.6
3	O	117	THR	4.5
3	C	119	VAL	4.5
3	G	121	LYS	4.5
3	K	208	THR	4.5
3	S	113	ASP	4.4
3	S	319	GLN	4.4
2	B	189	TYR	4.4
1	Q	213	GLU	4.4
3	O	97	ALA	4.4
1	Q	217	GLU	4.3
3	C	211	GLU	4.3
3	G	119	VAL	4.3
1	I	214	HIS	4.3
3	G	120	ASP	4.2
3	C	97	ALA	4.2
1	I	219	ASP	4.2
3	K	126	ASP	4.2
3	G	114	SER	4.2
1	Q	210	THR	4.1
3	O	126	ASP	4.1
3	S	116	ALA	4.0
1	E	213	GLU	4.0
3	G	207	GLY	4.0
1	E	211	PHE	4.0
3	K	116	ALA	3.9
3	G	111	CYS	3.9
3	O	119	VAL	3.8
3	C	212	ASP	3.8
3	C	319	GLN	3.8
3	S	97	ALA	3.8
2	R	164	SER	3.8
3	K	97	ALA	3.8
3	G	205	ALA	3.8
2	R	238	THR	3.8
1	M	219	ASP	3.7
1	A	219	ASP	3.7
3	O	208	THR	3.7
3	C	93	THR	3.7
2	F	164	SER	3.7

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Mol	Chain	Res	Type	RSRZ
3	K	207	GLY	3.7
3	K	94	THR	3.7
3	K	119	VAL	3.7
3	K	121	LYS	3.6
3	S	205	ALA	3.6
1	Q	218	LYS	3.6
3	S	119	VAL	3.6
3	K	213	SER	3.6
1	M	210	THR	3.5
3	G	209	GLY	3.5
1	E	218	LYS	3.5
3	K	113	ASP	3.5
1	M	213	GLU	3.5
2	N	189	TYR	3.5
3	O	116	ALA	3.5
3	K	127	VAL	3.5
3	G	113	ASP	3.4
3	O	118	ALA	3.4
1	M	218	LYS	3.4
1	M	216	GLN	3.4
1	A	214	HIS	3.4
3	S	82	VAL	3.4
1	I	218	LYS	3.4
3	K	211	GLU	3.4
1	I	220	LEU	3.3
2	J	164	SER	3.3
3	O	205	ALA	3.3
1	A	211	PHE	3.3
2	N	175	THR	3.2
3	C	83	ALA	3.2
3	C	118	ALA	3.2
2	R	189	TYR	3.2
3	K	83	ALA	3.2
3	G	122	PRO	3.1
3	O	318	ARG	3.0
1	A	218	LYS	3.0
3	C	205	ALA	3.0
3	S	115	ASP	2.9
3	G	213	SER	2.9
3	O	206	GLY	2.9
3	C	84	GLN	2.9
3	C	95	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	N	238	THR	2.9
3	C	209	GLY	2.9
3	G	97	ALA	2.9
3	G	123	THR	2.9
2	N	164	SER	2.8
3	S	98	ALA	2.8
3	C	207	GLY	2.8
3	O	209	GLY	2.8
3	S	96	GLU	2.8
3	O	98	ALA	2.8
1	A	289	ALA	2.7
3	O	111	CYS	2.7
3	O	120	ASP	2.7
3	O	319	GLN	2.6
1	M	211	PHE	2.6
3	K	84	GLN	2.6
3	K	128	SER	2.6
3	K	112	SER	2.5
2	B	1	GLY	2.5
1	I	215	LYS	2.5
3	K	130	ASN	2.5
3	O	82	VAL	2.5
1	E	221	GLU	2.5
1	Q	220	LEU	2.5
3	K	212	ASP	2.5
3	C	96	GLU	2.5
3	S	318	ARG	2.5
1	M	215	LYS	2.5
3	C	94	THR	2.5
1	Q	215	LYS	2.4
2	F	238	THR	2.4
3	C	213	SER	2.4
1	M	220	LEU	2.4
1	Q	211	PHE	2.4
3	O	204	VAL	2.4
3	S	111	CYS	2.4
3	C	87	ILE	2.4
1	A	210	THR	2.3
2	R	1	GLY	2.3
1	M	289	ALA	2.3
1	E	296	THR	2.3
2	F	1	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	S	204	VAL	2.3
3	O	212	ASP	2.3
2	N	1	GLY	2.3
3	S	212	ASP	2.3
2	J	83	CYS	2.3
3	G	211	GLU	2.3
3	C	129	VAL	2.3
3	O	213	SER	2.2
3	G	112	SER	2.2
1	I	217	GLU	2.2
3	S	213	SER	2.2
1	A	98	GLU	2.2
3	S	88	GLY	2.2
2	B	190	THR	2.1
2	J	1	GLY	2.1
1	I	211	PHE	2.1
3	K	206	GLY	2.1
3	C	86	THR	2.1
3	C	206	GLY	2.1
3	C	92	ILE	2.1
2	B	238	THR	2.0
1	I	289	ALA	2.0
1	I	216	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.