Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 08:39 PM JST

PDB ID	:	4YVS
Title	:	crystal structure of the virus-like particle of a c4 strain EV71
Authors	:	Chen, R.; Lyu, K.
Deposited on	:	2015-03-20
Resolution	:	3.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

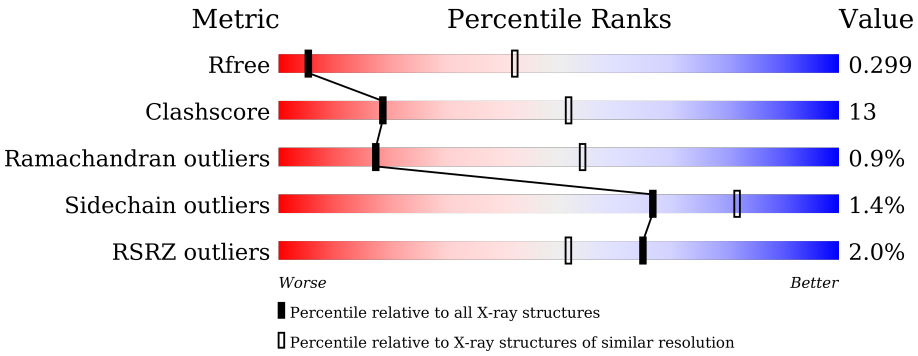
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.65 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	49% 26% 24%
1	D	297	4% 50% 26% 24%
1	G	297	51% 25% 24%
1	J	297	52% 23% 24%
1	M	297	2% 52% 24% 24%
2	B	242	63% 29% 7%

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Mol	Chain	Length	Quality of chain
2	E	242	64% 27% 7%
2	H	242	65% 27% 7%
2	K	242	63% 29% 7%
2	N	242	66% 26% 7%
3	C	323	2% 52% 19% 28%
3	F	323	2% 48% 23% 28%
3	I	323	2% 54% 17% 28%
3	L	323	4% 46% 25% 28%
3	O	323	2% 47% 23% 28%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26430 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	A	226	Total	C	N	O	S	0	0	0
			1789	1145	301	332	11			
1	D	226	Total	C	N	O	S	0	0	0
			1789	1145	301	332	11			
1	G	226	Total	C	N	O	S	0	0	0
			1789	1145	301	332	11			
1	J	226	Total	C	N	O	S	0	0	0
			1789	1145	301	332	11			
1	M	226	Total	C	N	O	S	0	0	0
			1789	1145	301	332	11			

- Molecule 2 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	224	Total	C	N	O	S	0	0	0
			1709	1099	282	317	11			
2	E	224	Total	C	N	O	S	0	0	0
			1709	1099	282	317	11			
2	H	224	Total	C	N	O	S	0	0	0
			1709	1099	282	317	11			
2	K	224	Total	C	N	O	S	0	0	0
			1709	1099	282	317	11			
2	N	224	Total	C	N	O	S	0	0	0
			1709	1099	282	317	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	227	GLN	LYS	engineered mutation	UNP F6KTB0
E	227	GLN	LYS	engineered mutation	UNP F6KTB0
H	227	GLN	LYS	engineered mutation	UNP F6KTB0
K	227	GLN	LYS	engineered mutation	UNP F6KTB0
N	227	GLN	LYS	engineered mutation	UNP F6KTB0

- Molecule 3 is a protein called Capsid protein VP0.

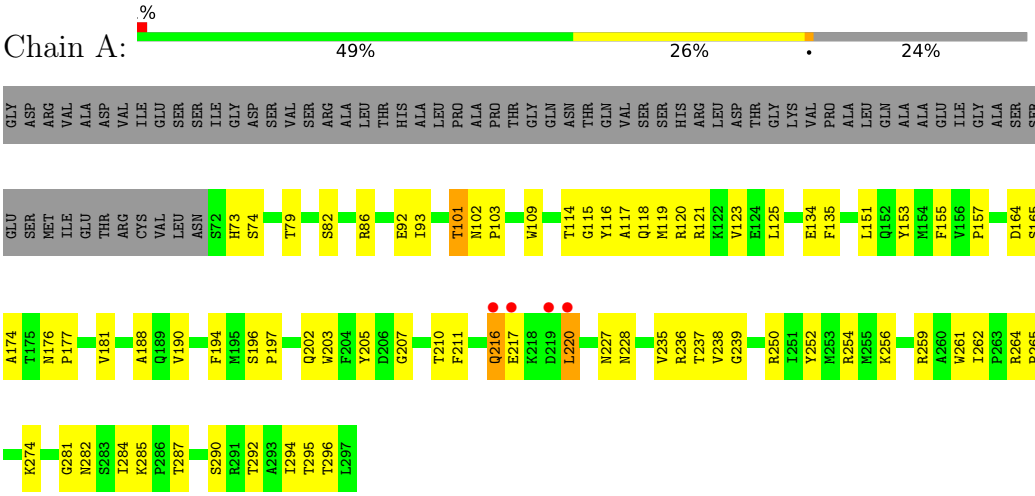
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	231	Total	C	N	O	S	0	0	0
			1788	1149	294	337	8			
3	F	231	Total	C	N	O	S	0	0	0
			1788	1149	294	337	8			
3	I	231	Total	C	N	O	S	0	0	0
			1788	1149	294	337	8			
3	L	231	Total	C	N	O	S	0	0	0
			1788	1149	294	337	8			
3	O	231	Total	C	N	O	S	0	0	0
			1788	1149	294	337	8			

3 Residue-property plots (i)

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

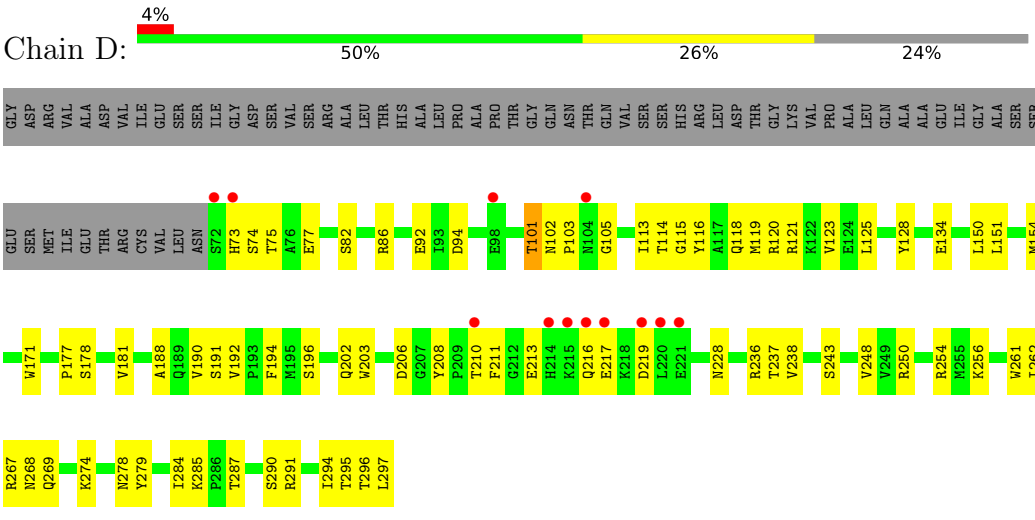
• Molecule 1: Capsid protein VP1

Chain A:



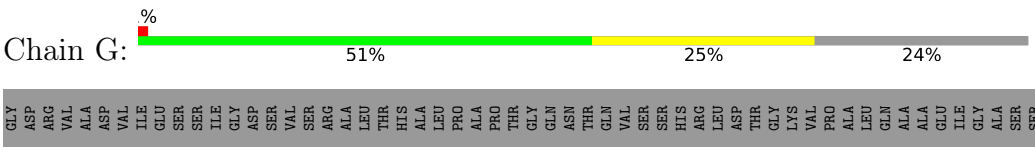
• Molecule 1: Capsid protein VP1

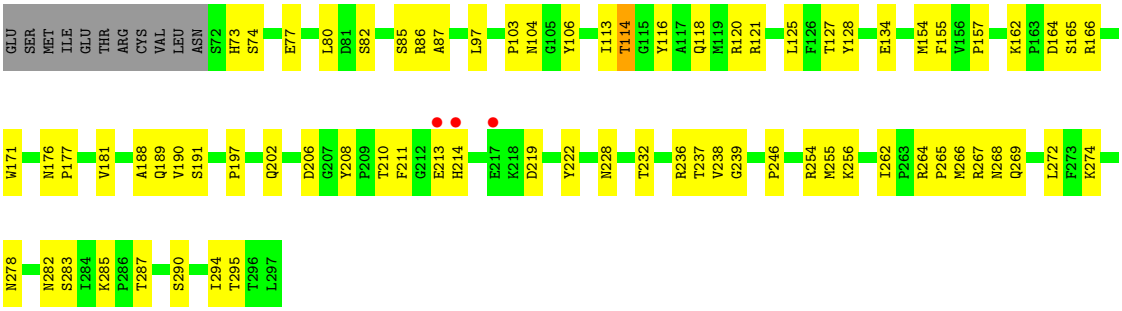
Chain D:



• Molecule 1: Capsid protein VP1

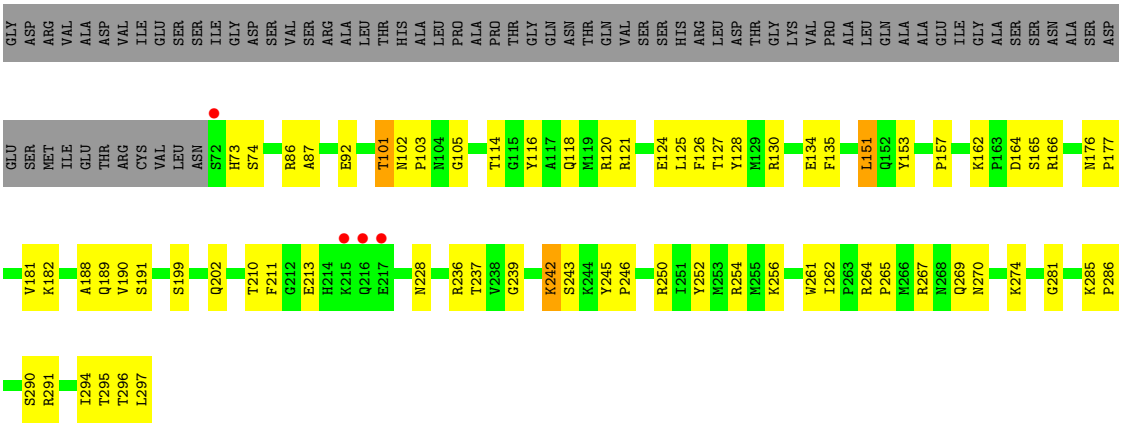
Chain G:





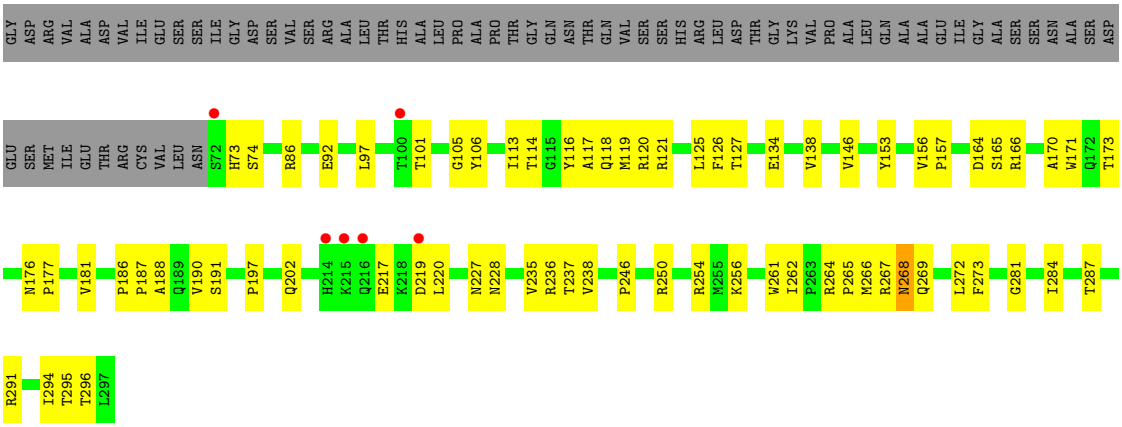
• Molecule 1: Capsid protein VP1

Chain J:



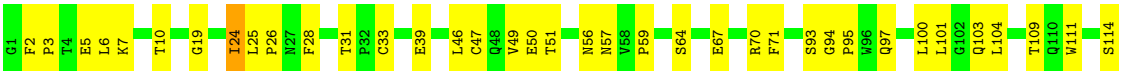
• Molecule 1: Capsid protein VP1

Chain M:



• Molecule 2: Capsid protein VP3

Chain B:

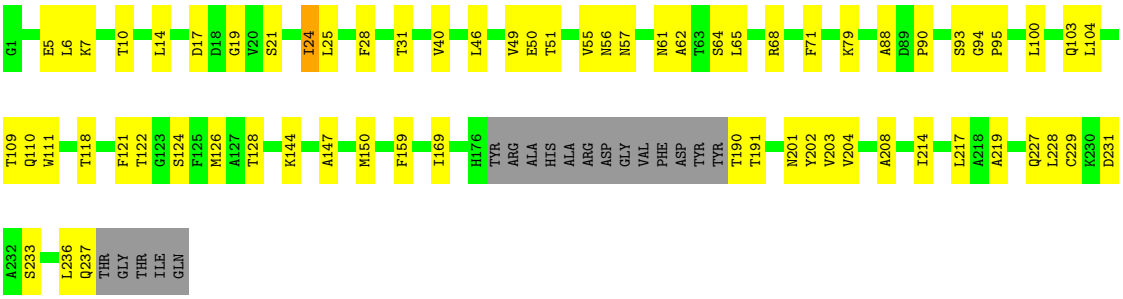


• Molecule 2: Capsid protein VP3

Chain E:

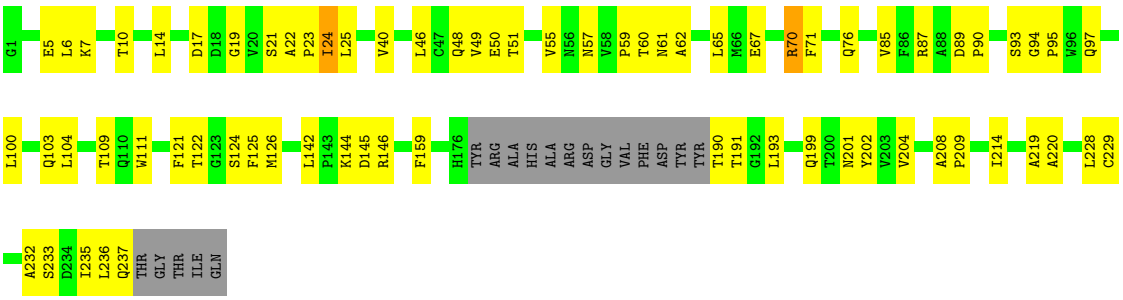
• Molecule 2: Capsid protein VP3

Chain H:



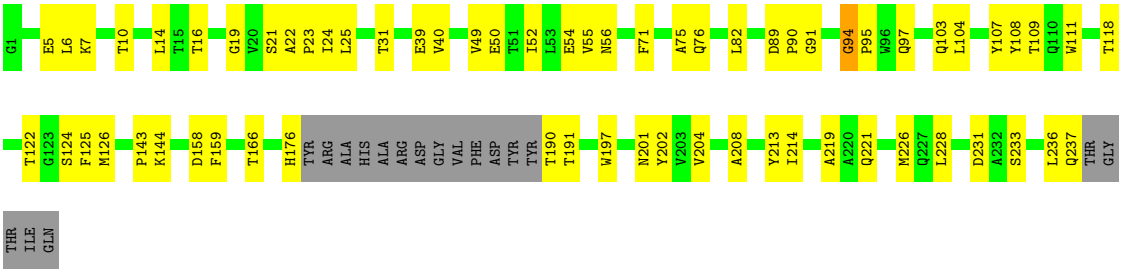
• Molecule 2: Capsid protein VP3

Chain K:

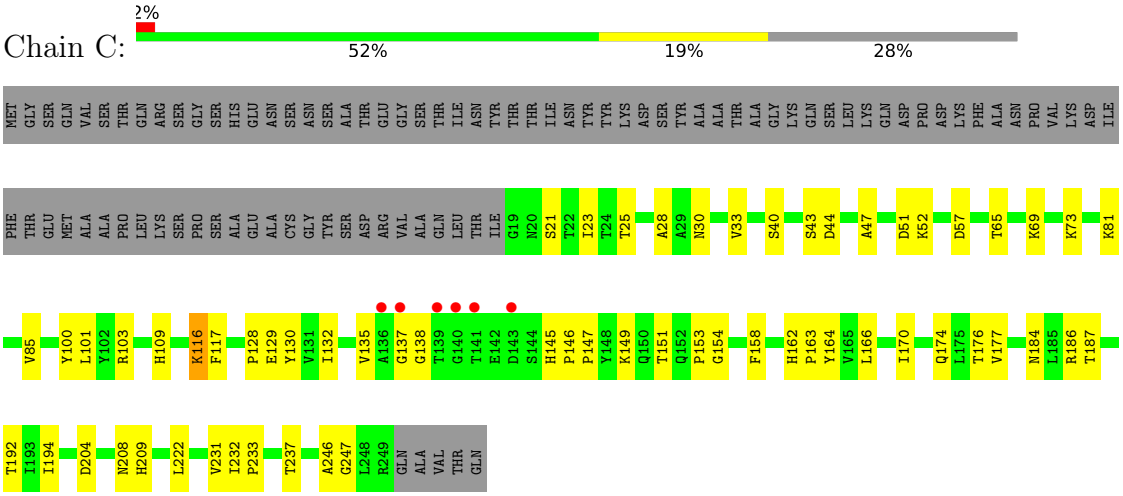


• Molecule 2: Capsid protein VP3

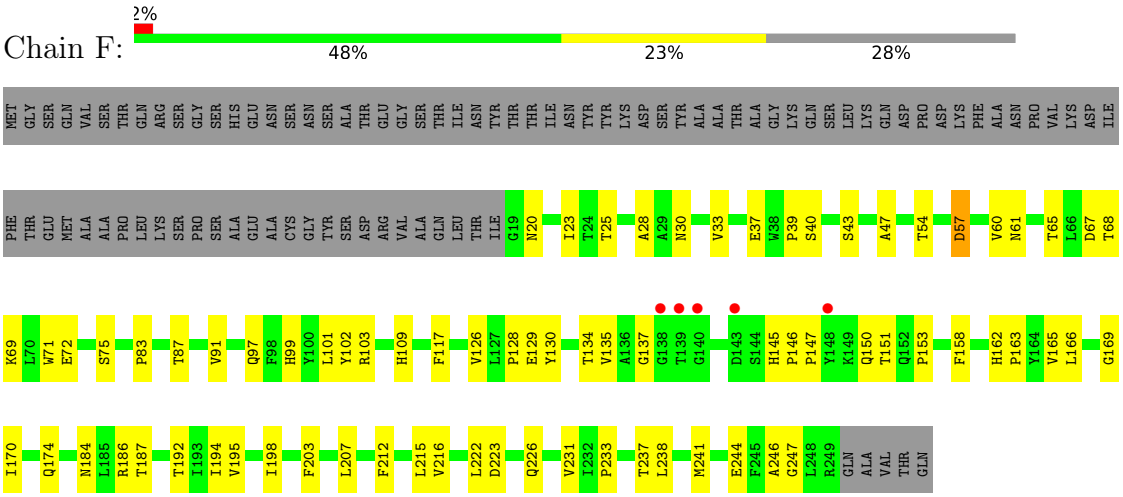
Chain N:



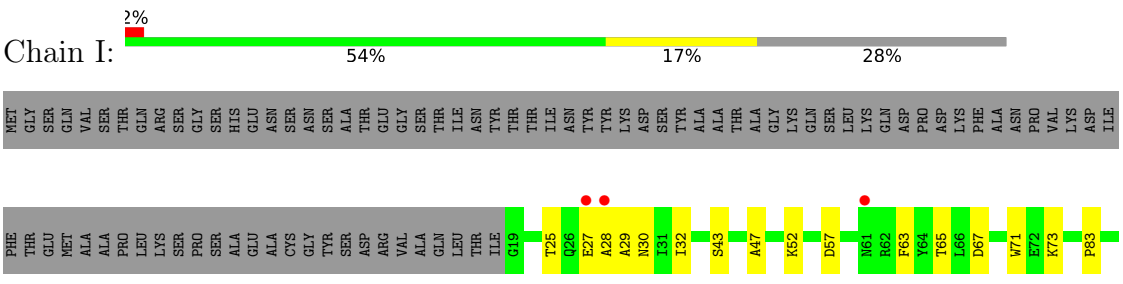
• Molecule 3: Capsid protein VP0

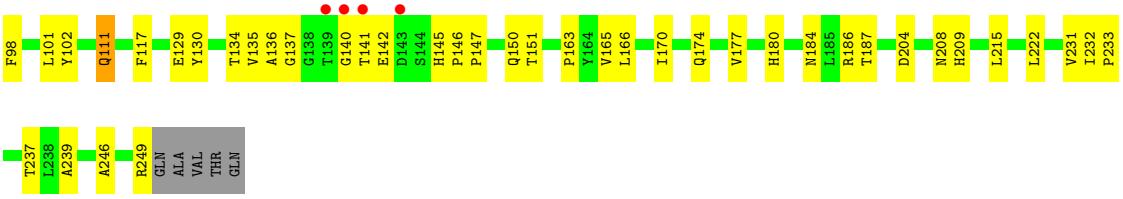


• Molecule 3: Capsid protein VP0

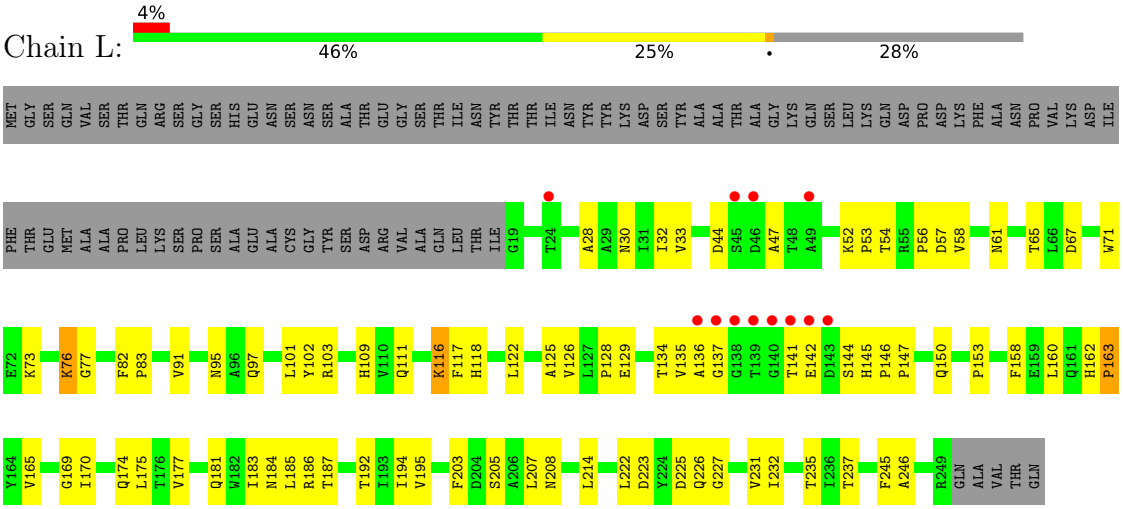


• Molecule 3: Capsid protein VP0

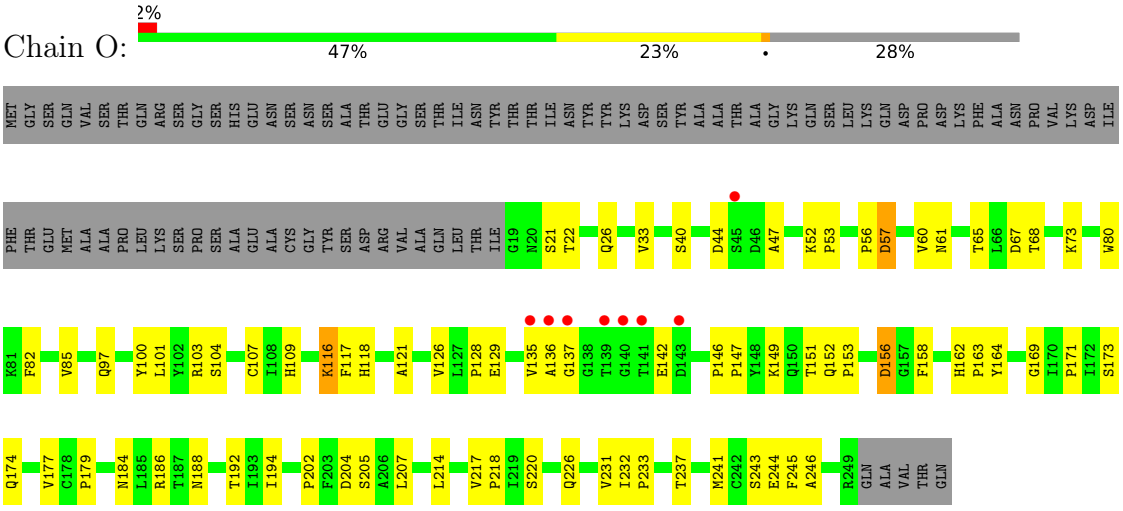




• Molecule 3: Capsid protein VP0



• Molecule 3: Capsid protein VP0



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α, β, γ	349.75Å 349.75Å 349.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 3.65 49.96 – 3.65	Depositor EDS
% Data completeness (in resolution range)	88.5 (49.96-3.65) 70.2 (49.96-3.65)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.271 , 0.300 0.271 , 0.299	Depositor DCC
R_{free} test set	2000 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å^2)	86.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 18.7	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	0.85	EDS
Total number of atoms	26430	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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	0.27	0/1844	0.49	0/2512
1	D	0.27	0/1844	0.49	0/2512
1	G	0.27	0/1844	0.49	0/2512
1	J	0.27	0/1844	0.48	0/2512
1	M	0.29	0/1844	0.51	0/2512
2	B	0.27	0/1755	0.54	0/2402
2	E	0.28	0/1755	0.52	0/2402
2	H	0.28	0/1755	0.53	0/2402
2	K	0.29	0/1755	0.55	0/2402
2	N	0.28	0/1755	0.54	0/2402
3	C	0.28	0/1843	0.50	0/2529
3	F	0.29	0/1843	0.51	0/2529
3	I	0.28	0/1843	0.52	0/2529
3	L	0.29	0/1843	0.51	0/2529
3	O	0.27	0/1843	0.51	0/2529
All	All	0.28	0/27210	0.51	0/37215

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1789	0	1735	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1789	0	1735	63	0
1	G	1789	0	1735	65	0
1	J	1789	0	1735	58	0
1	M	1789	0	1735	62	0
2	B	1709	0	1698	61	0
2	E	1709	0	1698	60	1
2	H	1709	0	1698	62	0
2	K	1709	0	1698	63	0
2	N	1709	0	1698	58	0
3	C	1788	0	1721	46	0
3	F	1788	0	1721	56	0
3	I	1788	0	1721	43	1
3	L	1788	0	1721	59	0
3	O	1788	0	1721	52	0
All	All	26430	0	25770	689	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (689) 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:M:181:VAL:HG21	1:M:188:ALA:HB2	1.58	0.86
1:J:210:THR:O	3:L:208:ASN:ND2	2.10	0.85
1:M:268:ASN:OD1	1:M:269:GLN:HG2	1.77	0.84
1:G:134:GLU:OE2	1:G:189:GLN:NE2	2.10	0.84
3:F:40:SER:O	3:F:103:ARG:NH2	2.12	0.81
2:H:61:ASN:HD21	2:H:64:SER:HB2	1.46	0.79
1:A:118:GLN:HE22	1:M:173:THR:HG22	1.49	0.78
1:A:202:GLN:O	1:A:228:ASN:ND2	2.19	0.76
3:C:40:SER:O	3:C:103:ARG:NH2	2.18	0.76
1:M:268:ASN:HD22	3:O:171:PRO:HB3	1.51	0.76
1:M:202:GLN:O	1:M:228:ASN:ND2	2.19	0.75
1:J:269:GLN:NE2	1:J:285:LYS:O	2.18	0.75
3:O:44:ASP:HA	3:O:47:ALA:HB3	1.67	0.75
2:N:109:THR:HB	2:N:228:LEU:HB3	1.68	0.75
2:B:236:LEU:HD23	2:B:237:GLN:HG2	1.69	0.75
1:J:182:LYS:HD3	1:M:146:VAL:HG11	1.69	0.75
1:G:181:VAL:HG21	1:G:188:ALA:HB2	1.70	0.74
1:G:210:THR:O	3:I:208:ASN:ND2	2.21	0.73
1:J:120:ARG:HH12	1:J:274:LYS:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:101:LEU:HB2	3:L:246:ALA:HB3	1.68	0.73
1:M:264:ARG:NH2	3:O:129:GLU:O	2.20	0.73
1:G:134:GLU:OE1	1:G:254:ARG:NH2	2.22	0.73
1:J:265:PRO:HB3	3:L:174:GLN:HB2	1.71	0.73
1:A:181:VAL:HG21	1:A:188:ALA:HB2	1.71	0.73
1:J:286:PRO:HG3	2:K:59:PRO:HB3	1.70	0.72
1:J:181:VAL:HG21	1:J:188:ALA:HB2	1.68	0.72
1:D:262:ILE:HG21	3:F:128:PRO:HG2	1.70	0.72
1:G:202:GLN:O	1:G:228:ASN:ND2	2.22	0.72
2:E:10:THR:HG22	2:K:5:GLU:HA	1.72	0.72
2:B:126:MET:HG3	3:C:117:PHE:HE1	1.56	0.71
1:A:259:ARG:NH2	2:B:33:CYS:SG	2.62	0.71
1:D:134:GLU:OE1	1:D:254:ARG:NH2	2.23	0.71
2:N:124:SER:O	3:O:186:ARG:NH1	2.24	0.71
1:D:92:GLU:OE2	1:D:250:ARG:NH1	2.24	0.70
1:D:177:PRO:HG2	2:E:24:ILE:HG23	1.74	0.70
2:B:10:THR:HG22	2:H:5:GLU:HA	1.74	0.69
1:A:134:GLU:OE1	1:A:254:ARG:NH2	2.25	0.69
1:A:269:GLN:NE2	1:A:285:LYS:O	2.24	0.69
2:B:124:SER:O	3:C:186:ARG:NH1	2.24	0.69
1:M:156:VAL:HA	1:M:176:ASN:HD22	1.58	0.69
1:A:92:GLU:OE2	1:A:250:ARG:NH1	2.25	0.69
1:G:121:ARG:HH22	2:H:103:GLN:HG2	1.56	0.68
1:J:118:GLN:NE2	2:K:232:ALA:O	2.26	0.68
1:D:202:GLN:O	1:D:228:ASN:ND2	2.26	0.68
1:J:92:GLU:OE2	1:J:250:ARG:NH1	2.26	0.68
1:M:92:GLU:OE2	1:M:250:ARG:NH1	2.27	0.68
2:K:124:SER:O	3:L:186:ARG:NH1	2.27	0.68
2:K:236:LEU:HD23	2:K:237:GLN:HG3	1.76	0.68
1:G:82:SER:O	1:G:86:ARG:NH2	2.27	0.68
1:J:290:SER:HB3	2:K:57:ASN:HB3	1.75	0.68
1:J:121:ARG:NH1	1:J:267:ARG:O	2.26	0.68
2:E:35:HIS:NE2	3:F:37:GLU:OE1	2.25	0.68
3:O:40:SER:O	3:O:103:ARG:NH2	2.28	0.67
1:J:86:ARG:NH2	2:K:229:CYS:SG	2.68	0.67
2:N:49:VAL:HG21	3:O:177:VAL:HG23	1.77	0.67
2:K:24:ILE:HG22	2:K:25:LEU:HG	1.76	0.66
1:M:268:ASN:HB3	3:O:171:PRO:HD3	1.76	0.66
1:D:105:GLY:HA3	1:D:166:ARG:HH21	1.59	0.66
1:A:121:ARG:HG3	1:A:267:ARG:HB3	1.77	0.65
3:L:141:THR:HG22	3:L:142:GLU:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:177:PRO:HG2	2:N:24:ILE:HG23	1.78	0.65
2:K:142:LEU:HB3	2:K:193:LEU:HD13	1.77	0.65
2:E:71:PHE:HB2	2:E:214:ILE:HB	1.79	0.65
2:K:204:VAL:HG13	2:K:208:ALA:HB3	1.77	0.65
2:E:236:LEU:HD23	2:E:237:GLN:HG2	1.78	0.65
1:A:281:GLY:HA3	3:C:135:VAL:HG22	1.77	0.65
3:O:156:ASP:OD1	3:O:156:ASP:N	2.30	0.65
1:D:181:VAL:HG21	1:D:188:ALA:HB2	1.79	0.65
1:G:265:PRO:HB3	3:I:174:GLN:HB2	1.78	0.64
1:G:290:SER:HA	2:H:57:ASN:HD22	1.62	0.64
1:A:290:SER:HA	2:B:57:ASN:HD22	1.62	0.64
3:F:65:THR:HG23	3:F:237:THR:HG22	1.80	0.64
1:D:269:GLN:NE2	1:D:285:LYS:O	2.31	0.64
2:H:24:ILE:HG22	2:H:25:LEU:HG	1.80	0.64
2:K:109:THR:HB	2:K:228:LEU:HB3	1.79	0.64
2:E:122:THR:HA	3:F:184:ASN:HD21	1.62	0.64
2:N:24:ILE:HG22	2:N:25:LEU:HG	1.79	0.64
1:M:134:GLU:OE1	1:M:254:ARG:NH2	2.28	0.64
1:A:82:SER:O	1:A:86:ARG:NH2	2.32	0.63
3:O:101:LEU:HB2	3:O:246:ALA:HB3	1.80	0.63
2:N:126:MET:HG3	3:O:117:PHE:CE1	2.33	0.63
3:I:135:VAL:HG12	3:I:137:GLY:H	1.64	0.63
1:J:294:ILE:HG23	1:J:295:THR:HG23	1.80	0.63
3:I:27:GLU:OE1	3:I:27:GLU:N	2.28	0.63
2:B:24:ILE:HG22	2:B:25:LEU:HG	1.79	0.63
3:C:153:PRO:HB3	3:C:158:PHE:HB2	1.81	0.62
1:J:134:GLU:OE1	1:J:254:ARG:NH2	2.33	0.62
2:K:10:THR:HG22	2:N:5:GLU:HA	1.81	0.62
3:F:101:LEU:HB2	3:F:246:ALA:HB3	1.80	0.62
1:A:121:ARG:HH22	2:B:103:GLN:HG2	1.65	0.62
1:G:190:VAL:HG21	2:H:24:ILE:HG13	1.81	0.62
2:N:109:THR:N	2:N:228:LEU:O	2.32	0.62
3:L:165:VAL:HG13	3:L:170:ILE:H	1.64	0.62
2:B:50:GLU:HA	2:B:219:ALA:HB2	1.82	0.62
1:M:125:LEU:HD11	2:N:104:LEU:HD21	1.82	0.62
3:I:130:TYR:OH	3:I:166:LEU:O	2.13	0.62
1:D:264:ARG:NH2	3:F:129:GLU:O	2.33	0.61
1:M:73:HIS:CG	1:M:74:SER:H	2.17	0.61
3:I:137:GLY:HA3	3:I:141:THR:HG22	1.82	0.61
2:K:71:PHE:HB2	2:K:214:ILE:HB	1.80	0.61
2:K:121:PHE:O	3:L:184:ASN:ND2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:236:ARG:HG2	1:J:237:THR:H	1.65	0.61
2:H:109:THR:HB	2:H:228:LEU:HB3	1.82	0.61
3:L:137:GLY:HA3	3:L:141:THR:H	1.65	0.61
1:G:121:ARG:NH1	1:G:267:ARG:O	2.32	0.61
3:F:186:ARG:HG3	3:F:187:THR:HG23	1.83	0.61
1:A:265:PRO:HB3	3:C:174:GLN:HB2	1.83	0.60
1:D:279:TYR:HE2	3:F:162:HIS:HD2	1.47	0.60
1:M:268:ASN:HB2	1:M:287:THR:HG22	1.83	0.60
1:A:166:ARG:HH22	1:A:237:THR:HG1	1.48	0.60
1:G:73:HIS:CG	1:G:74:SER:H	2.19	0.60
1:G:267:ARG:NH2	1:G:278:ASN:O	2.34	0.60
2:N:126:MET:HG3	3:O:117:PHE:HE1	1.66	0.60
2:B:5:GLU:HA	2:N:10:THR:HG22	1.82	0.60
2:H:118:THR:N	2:H:217:LEU:O	2.33	0.60
3:I:65:THR:HG23	3:I:237:THR:HG22	1.83	0.60
1:J:256:LYS:NZ	2:K:19:GLY:O	2.35	0.60
3:L:65:THR:HG23	3:L:237:THR:HG22	1.84	0.60
1:G:268:ASN:HB2	1:G:287:THR:HG22	1.84	0.59
3:O:33:VAL:HA	3:O:194:ILE:HD11	1.84	0.59
1:D:171:TRP:CE3	1:D:236:ARG:HD2	2.37	0.59
2:E:109:THR:HB	2:E:228:LEU:HB3	1.83	0.59
3:F:33:VAL:HG13	3:F:194:ILE:HD11	1.83	0.59
1:M:118:GLN:OE1	2:N:231:ASP:HB3	2.02	0.59
3:I:52:LYS:HD2	3:I:52:LYS:N	2.16	0.59
1:M:121:ARG:HH22	2:N:103:GLN:HG2	1.66	0.59
3:O:121:ALA:HB3	3:O:220:SER:HB3	1.83	0.59
3:L:186:ARG:HG3	3:L:187:THR:HG23	1.85	0.59
1:D:265:PRO:HB3	3:F:174:GLN:HB2	1.85	0.58
2:H:50:GLU:HA	2:H:219:ALA:HB2	1.86	0.58
1:D:73:HIS:CG	1:D:74:SER:H	2.21	0.58
2:E:12:GLN:HE21	2:E:14:LEU:HD23	1.69	0.58
2:B:126:MET:HG3	3:C:117:PHE:CE1	2.36	0.58
1:M:113:ILE:HG22	1:M:119:MET:HG2	1.84	0.58
1:J:191:SER:OG	2:K:21:SER:OG	2.19	0.58
2:H:121:PHE:O	3:I:184:ASN:ND2	2.36	0.58
2:N:14:LEU:HD12	2:N:16:THR:H	1.69	0.58
3:I:186:ARG:HG3	3:I:187:THR:HG23	1.85	0.58
1:G:294:ILE:HG23	1:G:295:THR:HG23	1.86	0.58
2:H:51:THR:HG21	2:H:100:LEU:HB2	1.86	0.58
3:L:97:GLN:HA	3:L:207:LEU:HD21	1.85	0.58
1:A:294:ILE:HG23	1:A:295:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:ARG:NH2	2:H:229:CYS:SG	2.77	0.58
1:M:197:PRO:HA	2:N:31:THR:HG21	1.86	0.58
2:K:87:ARG:HD3	2:K:191:THR:HG21	1.86	0.58
1:J:105:GLY:HA3	1:J:166:ARG:HH21	1.69	0.57
2:H:71:PHE:HB2	2:H:214:ILE:HB	1.85	0.57
2:B:109:THR:HB	2:B:228:LEU:HB3	1.85	0.57
2:B:227:GLN:HE22	2:N:31:THR:HG22	1.69	0.57
2:K:55:VAL:HB	2:K:71:PHE:HE1	1.69	0.57
1:G:116:TYR:OH	2:H:231:ASP:OD2	2.12	0.57
1:D:294:ILE:HG23	1:D:295:THR:HG23	1.86	0.57
2:K:126:MET:HG3	3:L:117:PHE:HE1	1.69	0.57
3:F:103:ARG:O	3:F:244:GLU:N	2.38	0.57
1:D:128:TYR:HB2	1:D:261:TRP:HB2	1.84	0.57
1:G:85:SER:O	1:G:85:SER:OG	2.19	0.57
1:G:106:TYR:OH	1:G:164:ASP:O	2.18	0.57
3:L:109:HIS:CD2	3:L:192:THR:HG22	2.40	0.57
1:A:121:ARG:NH1	1:A:267:ARG:O	2.36	0.57
2:H:126:MET:HG3	3:I:117:PHE:HE1	1.70	0.57
3:F:165:VAL:HG13	3:F:170:ILE:H	1.69	0.57
1:M:114:THR:O	1:M:116:TYR:N	2.38	0.57
1:D:166:ARG:NH2	1:D:237:THR:OG1	2.28	0.56
1:G:236:ARG:HG2	1:G:237:THR:H	1.70	0.56
1:G:264:ARG:NH2	3:I:129:GLU:O	2.38	0.56
1:J:202:GLN:O	1:J:228:ASN:ND2	2.38	0.56
3:F:57:ASP:O	3:F:61:ASN:ND2	2.38	0.56
1:A:120:ARG:HH12	1:A:274:LYS:HA	1.69	0.56
2:B:122:THR:HA	3:C:184:ASN:HD21	1.70	0.56
1:D:166:ARG:HH12	1:D:237:THR:HB	1.70	0.56
2:N:50:GLU:HA	2:N:219:ALA:HB2	1.88	0.56
3:F:83:PRO:HG3	3:F:102:TYR:CE2	2.40	0.56
2:N:75:ALA:HA	2:N:202:TYR:HB3	1.86	0.56
3:C:186:ARG:HG3	3:C:187:THR:HG23	1.86	0.56
1:J:242:LYS:HG3	1:J:243:SER:H	1.71	0.56
1:J:290:SER:HA	2:K:57:ASN:HD22	1.71	0.56
2:H:49:VAL:HG21	3:I:177:VAL:HG23	1.87	0.56
2:B:204:VAL:HG13	2:B:208:ALA:HB3	1.88	0.56
3:C:129:GLU:OE2	3:C:209:HIS:NE2	2.39	0.56
1:G:219:ASP:HB3	3:I:145:HIS:HB2	1.86	0.56
1:J:270:ASN:HB3	2:K:235:ILE:HD11	1.87	0.56
1:D:118:GLN:OE1	2:E:231:ASP:HB3	2.05	0.56
1:M:294:ILE:HG23	1:M:295:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:ILE:HG22	2:E:25:LEU:HG	1.87	0.56
3:C:65:THR:HA	3:C:237:THR:HA	1.87	0.56
1:G:166:ARG:NH2	1:G:237:THR:OG1	2.26	0.56
1:A:264:ARG:NH2	3:C:129:GLU:O	2.38	0.55
3:F:135:VAL:HG12	3:F:137:GLY:H	1.70	0.55
1:D:291:ARG:NH2	1:D:296:THR:O	2.39	0.55
2:E:121:PHE:O	3:F:184:ASN:ND2	2.38	0.55
2:K:60:THR:O	2:K:62:ALA:N	2.39	0.55
2:H:61:ASN:ND2	2:H:64:SER:HB2	2.18	0.55
2:E:138:PRO:HB3	2:E:190:THR:N	2.21	0.55
2:K:61:ASN:O	2:K:65:LEU:N	2.39	0.55
1:G:236:ARG:NH1	1:G:239:GLY:H	2.05	0.55
1:M:265:PRO:HB3	3:O:174:GLN:HB2	1.89	0.55
2:H:110:GLN:HG3	2:H:227:GLN:HE21	1.72	0.55
2:K:122:THR:HA	3:L:184:ASN:HD21	1.71	0.55
2:N:7:LYS:O	2:N:10:THR:HG23	2.07	0.55
1:D:284:ILE:HD11	3:F:162:HIS:CD2	2.42	0.54
1:A:166:ARG:HH12	1:A:237:THR:HB	1.72	0.54
3:O:136:ALA:O	3:O:142:GLU:N	2.38	0.54
3:C:135:VAL:HG12	3:C:137:GLY:H	1.71	0.54
2:H:110:GLN:HE21	2:H:227:GLN:NE2	2.05	0.54
1:D:262:ILE:HG13	3:F:198:ILE:HG21	1.90	0.54
2:H:159:PHE:O	3:I:186:ARG:NH2	2.40	0.54
2:H:204:VAL:HG13	2:H:208:ALA:HB3	1.89	0.54
2:N:236:LEU:HD23	2:N:237:GLN:HG3	1.90	0.54
2:H:90:PRO:HD2	2:H:111:TRP:CH2	2.43	0.54
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.30	0.54
1:A:174:ALA:H	1:G:116:TYR:HE1	1.56	0.54
2:K:94:GLY:H	2:K:95:PRO:CD	2.20	0.54
3:L:71:TRP:CD2	3:L:222:LEU:HD12	2.43	0.54
2:B:71:PHE:HB2	2:B:214:ILE:HB	1.90	0.54
3:L:77:GLY:HA3	3:L:160:LEU:HD12	1.88	0.54
1:M:191:SER:OG	2:N:21:SER:OG	2.27	0.53
1:D:268:ASN:HB2	1:D:287:THR:HG22	1.90	0.53
2:H:201:ASN:OD1	2:H:202:TYR:N	2.40	0.53
3:L:135:VAL:HG12	3:L:137:GLY:H	1.73	0.53
1:J:236:ARG:NH1	1:J:239:GLY:H	2.07	0.53
1:J:242:LYS:HG3	1:J:243:SER:N	2.24	0.53
1:M:157:PRO:HD2	1:M:176:ASN:ND2	2.24	0.53
2:N:233:SER:O	2:N:233:SER:OG	2.27	0.53
3:O:153:PRO:HB3	3:O:158:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:VAL:CG2	2:H:24:ILE:HG13	2.38	0.53
1:M:86:ARG:HG2	2:N:16:THR:HG22	1.91	0.53
2:K:51:THR:HG21	2:K:100:LEU:HB2	1.91	0.53
2:E:5:GLU:HA	2:H:10:THR:HG22	1.90	0.53
2:H:122:THR:HA	3:I:184:ASN:HD21	1.74	0.53
1:A:114:THR:O	1:A:116:TYR:N	2.41	0.53
1:D:297:LEU:HD21	2:E:85:VAL:HG22	1.91	0.53
2:H:236:LEU:HG	2:H:237:GLN:HG3	1.91	0.53
3:C:101:LEU:HB2	3:C:246:ALA:HB3	1.91	0.52
1:D:236:ARG:HG2	1:D:237:THR:H	1.74	0.52
3:O:109:HIS:HB3	3:O:237:THR:OG1	2.09	0.52
2:B:94:GLY:H	2:B:95:PRO:CD	2.22	0.52
1:A:197:PRO:HD2	1:A:227:ASN:HB3	1.92	0.52
1:A:290:SER:HB3	2:B:57:ASN:HB3	1.90	0.52
1:G:213:GLU:HG3	1:G:214:HIS:H	1.74	0.52
1:D:210:THR:HG22	1:D:211:PHE:H	1.74	0.52
1:G:118:GLN:OE1	2:H:231:ASP:HB3	2.10	0.52
1:G:191:SER:OG	2:H:21:SER:OG	2.25	0.52
1:J:264:ARG:NH2	3:L:129:GLU:O	2.43	0.52
1:M:236:ARG:HG2	1:M:237:THR:H	1.74	0.52
3:C:23:ILE:O	3:C:25:THR:HG23	2.10	0.52
2:K:10:THR:HB	2:N:6:LEU:HB2	1.92	0.52
1:A:116:TYR:HD2	1:A:119:MET:HB2	1.75	0.52
2:B:201:ASN:OD1	2:B:202:TYR:N	2.41	0.52
1:D:94:ASP:HA	1:D:248:VAL:HG22	1.90	0.52
1:J:291:ARG:NH2	1:J:296:THR:O	2.43	0.52
2:H:7:LYS:O	2:H:10:THR:HG23	2.09	0.52
2:E:204:VAL:HG13	2:E:208:ALA:HB3	1.92	0.52
1:M:164:ASP:OD1	1:M:165:SER:N	2.42	0.51
2:K:126:MET:HG3	3:L:117:PHE:CE1	2.45	0.51
3:F:72:GLU:O	3:F:75:SER:OG	2.24	0.51
1:A:261:TRP:HA	2:B:39:GLU:HA	1.92	0.51
1:A:86:ARG:NH2	2:B:229:CYS:SG	2.84	0.51
1:D:114:THR:O	1:D:116:TYR:N	2.44	0.51
3:F:97:GLN:HA	3:F:207:LEU:HD21	1.92	0.51
1:A:256:LYS:NZ	2:B:19:GLY:O	2.44	0.51
1:A:284:ILE:HD11	3:C:162:HIS:ND1	2.26	0.51
2:B:7:LYS:O	2:B:10:THR:HG23	2.10	0.51
1:J:267:ARG:NH1	3:L:169:GLY:HA3	2.26	0.51
2:E:124:SER:O	3:F:186:ARG:NH1	2.44	0.51
3:I:98:PHE:O	3:I:249:ARG:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:HIS:CG	1:A:74:SER:H	2.27	0.51
1:J:114:THR:O	1:J:116:TYR:N	2.43	0.50
2:N:143:PRO:HG2	2:N:197:TRP:HZ2	1.75	0.50
2:B:121:PHE:O	3:C:184:ASN:ND2	2.42	0.50
1:G:125:LEU:HD11	2:H:104:LEU:HD21	1.93	0.50
2:E:233:SER:O	2:E:233:SER:OG	2.29	0.50
2:N:94:GLY:H	2:N:95:PRO:CD	2.24	0.50
1:D:166:ARG:HH22	1:D:237:THR:HG1	1.54	0.50
1:M:291:ARG:NH2	1:M:296:THR:O	2.44	0.50
2:E:126:MET:HG3	3:F:117:PHE:CE1	2.46	0.50
2:E:157:TRP:NE1	2:E:162:GLN:O	2.39	0.50
2:H:124:SER:O	3:I:186:ARG:NH1	2.43	0.50
1:G:155:PHE:O	1:G:176:ASN:HB2	2.11	0.50
2:E:50:GLU:HA	2:E:219:ALA:HB2	1.91	0.50
1:A:125:LEU:HD11	2:B:104:LEU:HD21	1.92	0.50
2:N:118:THR:HG23	2:N:166:THR:HB	1.94	0.50
1:G:211:PHE:HA	3:I:208:ASN:HD21	1.77	0.50
1:M:256:LYS:NZ	2:N:19:GLY:O	2.44	0.50
3:I:165:VAL:HG13	3:I:170:ILE:H	1.76	0.50
1:A:207:GLY:HA3	3:C:208:ASN:O	2.12	0.50
1:A:262:ILE:HG21	3:C:128:PRO:HG2	1.93	0.49
1:G:127:THR:HB	1:G:262:ILE:HB	1.93	0.49
3:F:25:THR:HG21	3:F:109:HIS:CE1	2.46	0.49
3:I:63:PHE:HA	3:I:239:ALA:HB2	1.94	0.49
1:D:123:VAL:HG22	1:D:203:TRP:NE1	2.27	0.49
1:G:121:ARG:HG3	1:G:267:ARG:HB3	1.93	0.49
1:D:219:ASP:HB3	3:F:145:HIS:HB2	1.94	0.49
1:J:73:HIS:CG	1:J:74:SER:H	2.28	0.49
2:H:190:THR:HG23	2:H:191:THR:H	1.77	0.49
2:K:49:VAL:HG21	3:L:177:VAL:HG23	1.94	0.49
2:B:233:SER:O	2:B:233:SER:OG	2.29	0.49
3:C:43:SER:O	3:C:47:ALA:N	2.37	0.49
3:C:130:TYR:OH	3:C:166:LEU:O	2.21	0.49
1:G:269:GLN:NE2	1:G:285:LYS:O	2.45	0.49
1:J:130:ARG:NH1	1:J:199:SER:O	2.45	0.49
1:A:157:PRO:HD2	1:A:176:ASN:HB3	1.95	0.49
1:M:197:PRO:HD2	1:M:227:ASN:HB3	1.93	0.49
2:E:190:THR:HG23	2:E:191:THR:H	1.78	0.49
2:H:88:ALA:HB1	2:H:169:ILE:HD13	1.94	0.49
1:J:157:PRO:HD2	1:J:176:ASN:HB3	1.93	0.49
1:J:297:LEU:HD11	2:K:142:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:71:TRP:CD2	3:F:222:LEU:HD12	2.48	0.49
1:J:164:ASP:OD1	1:J:165:SER:N	2.45	0.49
3:I:83:PRO:HG3	3:I:102:TYR:CE2	2.48	0.49
1:G:120:ARG:HH12	1:G:274:LYS:HA	1.77	0.49
2:E:7:LYS:O	2:E:10:THR:HG23	2.12	0.49
2:E:94:GLY:H	2:E:95:PRO:CD	2.25	0.49
1:M:127:THR:N	1:M:262:ILE:O	2.45	0.49
3:C:109:HIS:CD2	3:C:192:THR:HG22	2.48	0.49
2:H:55:VAL:HB	2:H:71:PHE:HE1	1.77	0.49
2:K:109:THR:N	2:K:228:LEU:O	2.45	0.49
2:N:125:PHE:HB3	3:O:116:LYS:HG3	1.94	0.49
1:A:155:PHE:O	1:A:176:ASN:HB2	2.13	0.48
1:J:125:LEU:HD11	2:K:104:LEU:HD21	1.95	0.48
3:L:153:PRO:HB3	3:L:158:PHE:HB2	1.94	0.48
3:O:146:PRO:HA	3:O:147:PRO:HD3	1.70	0.48
2:E:94:GLY:O	2:E:97:GLN:HB2	2.12	0.48
1:G:219:ASP:HB3	3:I:145:HIS:CB	2.43	0.48
3:I:43:SER:O	3:I:47:ALA:N	2.39	0.48
3:O:57:ASP:O	3:O:61:ASN:ND2	2.46	0.48
2:K:46:LEU:O	2:K:49:VAL:HG22	2.14	0.48
2:N:190:THR:HG23	2:N:191:THR:H	1.78	0.48
1:D:113:ILE:HG22	1:D:119:MET:HG2	1.96	0.48
1:M:237:THR:H	1:M:238:VAL:HA	1.78	0.48
3:C:21:SER:OG	3:C:21:SER:O	2.21	0.48
1:M:97:LEU:HD11	1:M:246:PRO:HG3	1.95	0.48
1:A:118:GLN:OE1	2:B:231:ASP:HB3	2.13	0.48
1:G:113:ILE:HG21	1:G:255:MET:HE1	1.96	0.48
1:J:101:THR:HG23	1:J:102:ASN:H	1.79	0.48
2:E:75:ALA:HA	2:E:202:TYR:HB3	1.96	0.48
3:I:25:THR:H	3:I:27:GLU:CD	2.17	0.48
1:G:157:PRO:HD2	1:G:176:ASN:HB3	1.95	0.48
2:N:71:PHE:HB2	2:N:214:ILE:HB	1.96	0.48
2:N:108:TYR:HB2	2:N:226:MET:HE3	1.96	0.48
3:L:144:SER:OG	3:L:145:HIS:N	2.46	0.48
2:B:64:SER:O	2:B:64:SER:OG	2.29	0.47
2:B:125:PHE:HB3	3:C:116:LYS:HG3	1.95	0.47
2:B:190:THR:HG23	2:B:191:THR:H	1.78	0.47
1:J:177:PRO:HB2	2:K:24:ILE:HD12	1.96	0.47
2:K:85:VAL:HG21	2:K:142:LEU:HD22	1.96	0.47
1:A:220:LEU:HD23	3:C:145:HIS:CE1	2.49	0.47
1:G:282:ASN:OD1	1:G:283:SER:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:89:ASP:HA	2:K:90:PRO:HD3	1.61	0.47
2:B:51:THR:HG21	2:B:100:LEU:HB2	1.97	0.47
1:D:267:ARG:NH1	3:F:169:GLY:HA3	2.29	0.47
1:G:87:ALA:HB2	1:G:254:ARG:HB2	1.95	0.47
3:L:58:VAL:HA	3:L:61:ASN:HB3	1.95	0.47
2:E:6:LEU:HB2	2:H:10:THR:HB	1.96	0.47
2:N:91:GLY:HA3	2:N:111:TRP:CH2	2.49	0.47
3:O:65:THR:HA	3:O:237:THR:HA	1.97	0.47
1:A:190:VAL:HG21	2:B:24:ILE:HG13	1.95	0.47
2:E:35:HIS:HE2	3:F:37:GLU:CD	2.15	0.47
2:K:233:SER:O	2:K:233:SER:OG	2.32	0.47
2:N:201:ASN:OD1	2:N:202:TYR:N	2.47	0.47
3:O:21:SER:O	3:O:21:SER:OG	2.23	0.47
1:A:73:HIS:CE1	2:B:227:GLN:HE21	2.32	0.47
1:M:190:VAL:CG2	2:N:24:ILE:HG13	2.45	0.47
1:M:217:GLU:OE2	1:M:220:LEU:HG	2.15	0.47
1:M:237:THR:N	1:M:238:VAL:HA	2.30	0.47
3:L:122:LEU:HB2	3:L:183:ILE:HB	1.95	0.47
3:L:222:LEU:HD23	3:L:223:ASP:N	2.29	0.47
1:M:105:GLY:HA3	1:M:166:ARG:HH21	1.79	0.47
2:H:128:THR:HG23	2:H:203:VAL:HB	1.97	0.47
1:A:171:TRP:CD2	1:A:236:ARG:HD2	2.50	0.47
1:A:177:PRO:HG2	2:B:24:ILE:HG23	1.96	0.47
1:G:164:ASP:OD1	1:G:165:SER:N	2.48	0.47
2:E:14:LEU:HG	2:E:17:ASP:HB2	1.97	0.47
3:I:136:ALA:HB1	3:I:142:GLU:O	2.15	0.47
1:D:279:TYR:CE2	3:F:162:HIS:HD2	2.31	0.47
1:G:73:HIS:CG	1:G:74:SER:N	2.82	0.47
2:N:158:ASP:OD1	2:N:159:PHE:N	2.48	0.47
3:F:109:HIS:CD2	3:F:192:THR:HG22	2.49	0.47
3:I:166:LEU:HD22	3:I:215:LEU:HD21	1.95	0.47
1:A:236:ARG:HG2	1:A:237:THR:H	1.80	0.46
2:B:118:THR:HA	2:B:166:THR:HA	1.97	0.46
2:E:14:LEU:HD12	2:E:16:THR:H	1.80	0.46
1:G:197:PRO:HA	2:H:31:THR:HG21	1.97	0.46
2:H:46:LEU:O	2:H:49:VAL:HG22	2.15	0.46
2:K:50:GLU:HA	2:K:219:ALA:HB2	1.97	0.46
2:N:94:GLY:O	2:N:97:GLN:HB2	2.15	0.46
3:L:225:ASP:O	3:L:227:GLY:N	2.48	0.46
1:D:120:ARG:HH12	1:D:274:LYS:HA	1.80	0.46
2:E:201:ASN:OD1	2:E:202:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:101:LEU:HB2	3:I:246:ALA:HB3	1.96	0.46
3:C:73:LYS:HB3	3:C:222:LEU:O	2.16	0.46
1:M:284:ILE:HD11	3:O:162:HIS:ND1	2.31	0.46
3:F:23:ILE:O	3:F:25:THR:HG23	2.15	0.46
3:F:166:LEU:HD22	3:F:215:LEU:HD21	1.98	0.46
2:B:142:LEU:HB3	2:B:193:LEU:HD13	1.97	0.46
1:G:290:SER:HA	2:H:57:ASN:ND2	2.31	0.46
3:L:91:VAL:O	3:L:95:ASN:HB2	2.15	0.46
3:C:44:ASP:HA	3:C:47:ALA:HB3	1.98	0.46
3:C:132:ILE:HD12	3:C:151:THR:HA	1.98	0.46
1:D:73:HIS:CG	1:D:74:SER:N	2.83	0.46
2:N:118:THR:HA	2:N:166:THR:HA	1.97	0.46
3:O:151:THR:HG23	3:O:152:GLN:HG3	1.97	0.46
1:D:237:THR:HG23	1:D:243:SER:HB2	1.98	0.46
2:K:201:ASN:OD1	2:K:202:TYR:N	2.48	0.46
2:B:221:GLN:HG3	2:B:223:ASN:OD1	2.16	0.46
2:H:94:GLY:H	2:H:95:PRO:CD	2.28	0.46
2:K:7:LYS:O	2:K:10:THR:HG23	2.15	0.46
3:O:103:ARG:O	3:O:244:GLU:N	2.49	0.46
1:A:190:VAL:CG2	2:B:24:ILE:HG13	2.46	0.46
1:D:121:ARG:NH1	1:D:267:ARG:O	2.49	0.46
1:D:192:VAL:HG22	2:E:24:ILE:HD12	1.97	0.46
2:E:44:LEU:O	2:E:48:GLN:HG3	2.16	0.46
3:I:222:LEU:HD11	3:I:232:ILE:CG1	2.46	0.46
3:I:232:ILE:HA	3:I:233:PRO:HD3	1.74	0.46
3:L:65:THR:HA	3:L:237:THR:HA	1.97	0.46
3:L:82:PHE:HE1	3:L:214:LEU:HB2	1.81	0.46
1:D:294:ILE:HD13	2:E:56:ASN:HA	1.98	0.45
1:M:127:THR:HB	1:M:262:ILE:HB	1.98	0.45
3:L:33:VAL:HG13	3:L:194:ILE:HD11	1.99	0.45
3:O:82:PHE:HE1	3:O:214:LEU:HB2	1.81	0.45
3:O:104:SER:HB2	3:O:243:SER:HA	1.97	0.45
1:A:216:GLN:OE1	1:A:217:GLU:HG2	2.16	0.45
3:C:69:LYS:HA	3:C:69:LYS:HD2	1.79	0.45
2:B:114:SER:OG	2:B:221:GLN:NE2	2.47	0.45
3:L:103:ARG:HB2	3:L:203:PHE:CE2	2.51	0.45
1:A:101:THR:HG23	1:A:102:ASN:H	1.80	0.45
1:A:210:THR:HG22	1:A:211:PHE:H	1.80	0.45
1:D:101:THR:HG23	1:D:102:ASN:H	1.82	0.45
1:G:177:PRO:HG2	2:H:24:ILE:HG23	1.98	0.45
1:J:120:ARG:NE	1:J:124:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:262:ILE:HG21	3:L:128:PRO:HG2	1.97	0.45
3:F:43:SER:O	3:F:47:ALA:N	2.34	0.45
3:L:71:TRP:HZ3	3:L:185:LEU:HD21	1.82	0.45
2:B:93:SER:HA	2:B:94:GLY:HA2	1.73	0.45
1:G:114:THR:O	1:G:116:TYR:N	2.50	0.45
1:G:208:TYR:CE1	1:G:222:TYR:HB2	2.52	0.45
1:G:294:ILE:HD11	2:H:55:VAL:HG12	1.99	0.45
2:E:22:ALA:HA	2:E:23:PRO:HD3	1.85	0.45
3:F:134:THR:HG21	3:F:150:GLN:OE1	2.16	0.45
1:A:294:ILE:HD13	2:B:56:ASN:HA	1.99	0.45
1:D:290:SER:CB	2:E:59:PRO:HG3	2.47	0.45
1:G:294:ILE:HD13	2:H:56:ASN:HA	1.97	0.45
1:M:120:ARG:NH1	1:M:273:PHE:O	2.39	0.45
3:I:204:ASP:OD2	3:I:209:HIS:ND1	2.32	0.45
3:C:85:VAL:HA	3:C:154:GLY:HA2	1.99	0.45
2:E:89:ASP:HA	2:E:90:PRO:HD3	1.75	0.45
1:G:208:TYR:OH	3:I:151:THR:HG21	2.17	0.45
2:H:236:LEU:HG	2:H:237:GLN:N	2.32	0.45
2:K:10:THR:HG22	2:N:6:LEU:H	1.81	0.45
3:O:135:VAL:HG12	3:O:137:GLY:H	1.82	0.45
1:A:282:ASN:HB2	3:C:138:GLY:HA2	1.99	0.44
1:J:210:THR:OG1	1:J:211:PHE:N	2.50	0.44
2:K:67:GLU:O	2:K:70:ARG:HG3	2.18	0.44
2:K:190:THR:HG23	2:K:191:THR:H	1.82	0.44
2:N:122:THR:HA	3:O:184:ASN:HD21	1.82	0.44
3:F:39:PRO:HG3	3:F:241:MET:HG3	1.99	0.44
3:L:73:LYS:H	3:L:73:LYS:HG2	1.56	0.44
1:M:281:GLY:HA3	3:O:135:VAL:HG22	2.00	0.44
2:H:147:ALA:O	2:H:150:MET:HB3	2.17	0.44
1:A:268:ASN:HB2	1:A:287:THR:HG22	1.98	0.44
1:D:216:GLN:HG2	1:D:217:GLU:N	2.33	0.44
1:G:154:MET:SD	1:G:171:TRP:HA	2.57	0.44
1:J:127:THR:N	1:J:262:ILE:O	2.49	0.44
1:J:182:LYS:NZ	1:M:186:PRO:HA	2.32	0.44
3:C:100:TYR:HB3	3:C:247:GLY:HA3	1.98	0.44
2:H:93:SER:HA	2:H:94:GLY:HA2	1.64	0.44
1:A:153:TYR:HD1	1:A:235:VAL:HG12	1.81	0.44
1:D:82:SER:O	1:D:86:ARG:NH2	2.50	0.44
1:J:121:ARG:HG3	1:J:267:ARG:HB3	1.99	0.44
2:K:159:PHE:O	3:L:186:ARG:NH2	2.50	0.44
2:N:71:PHE:O	2:N:213:TYR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:ARG:HB2	3:F:203:PHE:CE2	2.52	0.44
3:F:126:VAL:HG13	3:F:212:PHE:CD2	2.52	0.44
3:I:28:ALA:C	3:I:30:ASN:H	2.20	0.44
1:A:292:THR:OG1	1:A:296:THR:HG21	2.17	0.44
1:G:237:THR:H	1:G:238:VAL:HA	1.82	0.44
2:E:10:THR:HB	2:K:6:LEU:HB2	1.99	0.44
2:K:14:LEU:HG	2:K:17:ASP:HB2	1.99	0.44
1:J:128:TYR:HB2	1:J:261:TRP:HB2	1.99	0.44
1:J:211:PHE:CZ	3:L:205:SER:HB2	2.53	0.44
2:E:16:THR:HG21	2:H:24:ILE:O	2.18	0.44
1:M:153:TYR:HD1	1:M:235:VAL:HG12	1.83	0.44
1:M:261:TRP:HA	2:N:39:GLU:HA	2.00	0.44
2:K:93:SER:HA	2:K:94:GLY:HA2	1.76	0.44
3:F:126:VAL:HG11	3:F:195:VAL:HG21	2.00	0.44
3:I:146:PRO:HA	3:I:147:PRO:HD3	1.71	0.44
1:A:237:THR:N	1:A:238:VAL:HA	2.33	0.44
3:C:146:PRO:HA	3:C:147:PRO:HD3	1.75	0.44
1:J:135:PHE:HA	1:J:252:TYR:O	2.18	0.44
1:M:73:HIS:CG	1:M:74:SER:N	2.83	0.44
2:E:2:PHE:HA	2:E:3:PRO:HD3	1.83	0.44
1:D:267:ARG:CZ	3:F:169:GLY:HA3	2.48	0.43
2:E:159:PHE:O	3:F:186:ARG:NH2	2.51	0.43
1:D:190:VAL:CG2	2:E:24:ILE:HG13	2.47	0.43
1:M:267:ARG:NH1	3:O:169:GLY:HA3	2.32	0.43
2:N:54:GLU:OE2	3:O:164:TYR:OH	2.21	0.43
1:A:236:ARG:NH1	1:A:239:GLY:H	2.16	0.43
2:B:67:GLU:HG2	2:B:70:ARG:NH2	2.33	0.43
2:E:91:GLY:HA3	2:E:111:TRP:CH2	2.54	0.43
2:N:104:LEU:HD23	2:N:104:LEU:HA	1.85	0.43
3:L:52:LYS:HA	3:L:53:PRO:HD3	1.86	0.43
1:A:116:TYR:CD2	1:A:119:MET:HB2	2.53	0.43
3:C:204:ASP:OD2	3:C:209:HIS:ND1	2.42	0.43
1:D:154:MET:HA	1:D:178:SER:HA	2.00	0.43
1:G:80:LEU:HD11	2:H:40:VAL:HG23	2.01	0.43
1:G:237:THR:N	1:G:238:VAL:HA	2.33	0.43
1:M:190:VAL:HG21	2:N:24:ILE:HG13	1.99	0.43
2:E:55:VAL:HB	2:E:71:PHE:HE1	1.83	0.43
2:E:109:THR:N	2:E:228:LEU:O	2.51	0.43
3:L:136:ALA:O	3:L:142:GLU:N	2.42	0.43
2:B:46:LEU:O	2:B:49:VAL:HG22	2.19	0.43
2:B:49:VAL:HG21	3:C:177:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:SER:HB3	2:B:170:PRO:O	2.18	0.43
1:G:256:LYS:NZ	2:H:19:GLY:O	2.52	0.43
1:G:290:SER:HB3	2:H:57:ASN:HB3	2.00	0.43
2:E:93:SER:HB2	2:E:97:GLN:HE22	1.83	0.43
2:K:90:PRO:HD2	2:K:111:TRP:CH2	2.53	0.43
3:L:134:THR:HG21	3:L:150:GLN:OE1	2.18	0.43
3:O:56:PRO:HG3	3:O:245:PHE:HE2	1.82	0.43
3:O:97:GLN:HG2	3:O:207:LEU:HD11	2.00	0.43
2:B:144:LYS:HG3	2:B:145:ASP:OD1	2.19	0.43
1:D:125:LEU:HD11	2:E:104:LEU:HD21	2.00	0.43
1:J:177:PRO:HG2	2:K:24:ILE:HG23	2.01	0.43
1:M:266:MET:HE3	2:N:107:TYR:HE2	1.83	0.43
2:H:62:ALA:HA	2:H:65:LEU:HG	2.00	0.43
3:L:44:ASP:HA	3:L:47:ALA:HB3	2.00	0.43
3:O:52:LYS:HA	3:O:53:PRO:HD3	1.70	0.43
1:A:93:ILE:HD11	1:A:109:TRP:HB2	2.00	0.43
1:A:117:ALA:HA	2:B:236:LEU:HD13	2.00	0.43
1:A:194:PHE:CZ	1:A:196:SER:HB3	2.53	0.43
1:J:189:GLN:OE1	2:K:21:SER:HB3	2.19	0.43
2:E:93:SER:HA	2:E:94:GLY:HA2	1.77	0.43
2:K:48:GLN:HA	2:K:220:ALA:O	2.18	0.43
1:D:77:GLU:OE2	2:H:28:PHE:HA	2.19	0.43
1:A:290:SER:CB	2:B:59:PRO:HG3	2.49	0.43
1:D:237:THR:H	1:D:238:VAL:HA	1.83	0.43
1:J:73:HIS:CG	1:J:74:SER:N	2.86	0.43
1:M:106:TYR:OH	1:M:164:ASP:O	2.30	0.43
1:M:171:TRP:CZ3	1:M:236:ARG:HB2	2.53	0.43
2:H:104:LEU:HD23	2:H:104:LEU:HA	1.87	0.43
2:N:52:ILE:HD12	3:O:173:SER:HA	2.01	0.43
2:B:10:THR:HB	2:H:6:LEU:HB2	2.00	0.43
1:D:269:GLN:HG3	3:F:165:VAL:HG21	2.01	0.43
1:D:278:ASN:OD1	3:F:134:THR:N	2.52	0.43
1:G:272:LEU:HD21	3:I:140:GLY:HA3	2.01	0.43
1:J:211:PHE:HA	3:L:208:ASN:HD21	1.83	0.43
2:E:126:MET:HG3	3:F:117:PHE:HE1	1.83	0.43
3:F:60:VAL:HG12	3:F:91:VAL:HG12	2.01	0.43
3:C:33:VAL:HG13	3:C:194:ILE:HD11	2.00	0.42
1:G:97:LEU:HD11	1:G:246:PRO:HG3	2.01	0.42
3:I:32:ILE:HD12	3:I:180:HIS:O	2.18	0.42
3:O:65:THR:HG23	3:O:237:THR:HG22	2.01	0.42
3:O:68:THR:HG21	3:O:233:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:LEU:N	3:C:170:ILE:O	2.42	0.42
1:J:87:ALA:HB2	1:J:254:ARG:HB2	2.01	0.42
2:K:144:LYS:HG3	2:K:145:ASP:OD1	2.19	0.42
2:N:143:PRO:HG2	2:N:197:TRP:CZ2	2.55	0.42
3:L:118:HIS:CE1	3:L:232:ILE:HD11	2.53	0.42
2:B:26:PRO:C	2:B:28:PHE:H	2.22	0.42
1:M:295:THR:HB	2:N:82:LEU:HD23	2.02	0.42
3:I:166:LEU:N	3:I:170:ILE:O	2.38	0.42
3:O:204:ASP:OD1	3:O:205:SER:N	2.45	0.42
2:B:158:ASP:OD1	2:B:159:PHE:N	2.52	0.42
1:D:237:THR:N	1:D:238:VAL:HA	2.34	0.42
1:M:294:ILE:HD13	2:N:56:ASN:HA	2.01	0.42
1:A:261:TRP:CD1	2:B:39:GLU:HB2	2.55	0.42
3:C:149:LYS:HE2	3:C:149:LYS:HB2	1.94	0.42
1:D:208:TYR:OH	3:F:151:THR:HG21	2.20	0.42
2:H:126:MET:HG3	3:I:117:PHE:CE1	2.50	0.42
2:K:94:GLY:O	2:K:97:GLN:HB2	2.20	0.42
3:F:99:HIS:HA	3:F:247:GLY:O	2.20	0.42
3:I:134:THR:HG21	3:I:150:GLN:OE1	2.20	0.42
1:A:114:THR:HG23	2:B:236:LEU:HD11	2.00	0.42
1:A:237:THR:H	1:A:238:VAL:HA	1.84	0.42
1:A:287:THR:HG1	3:C:164:TYR:HH	1.67	0.42
2:H:233:SER:O	2:H:233:SER:OG	2.32	0.42
1:A:120:ARG:NH1	1:A:274:LYS:HA	2.34	0.42
1:A:197:PRO:HA	2:B:31:THR:HG21	2.01	0.42
1:M:272:LEU:HD23	1:M:272:LEU:HA	1.77	0.42
3:L:54:THR:O	3:L:56:PRO:HD3	2.18	0.42
3:L:125:ALA:HB3	3:L:175:LEU:HD21	2.01	0.42
2:B:6:LEU:HB2	2:N:10:THR:HB	1.99	0.42
2:B:47:CYS:HB3	2:B:101:LEU:HD13	2.01	0.42
2:B:94:GLY:O	2:B:97:GLN:HB2	2.20	0.42
2:B:111:TRP:HB3	2:B:226:MET:HA	2.02	0.42
1:D:213:GLU:N	1:D:213:GLU:OE1	2.53	0.42
1:J:126:PHE:CE1	2:K:40:VAL:HG21	2.54	0.42
1:M:116:TYR:HD2	1:M:119:MET:HB2	1.85	0.42
2:E:6:LEU:H	2:H:10:THR:HG22	1.85	0.42
2:E:116:GLU:N	2:E:219:ALA:O	2.40	0.42
3:F:130:TYR:OH	3:F:166:LEU:O	2.18	0.42
1:J:281:GLY:HA3	3:L:135:VAL:HG22	2.02	0.42
3:F:222:LEU:HD23	3:F:223:ASP:N	2.35	0.42
3:L:76:LYS:HB2	3:L:163:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:103:ARG:HG3	3:O:202:PRO:O	2.20	0.42
3:O:149:LYS:HE3	3:O:149:LYS:HB3	1.81	0.42
1:A:164:ASP:OD1	1:A:165:SER:N	2.53	0.42
1:J:245:TYR:HA	1:J:246:PRO:HD3	1.90	0.42
2:N:25:LEU:HD23	2:N:25:LEU:HA	1.93	0.42
3:I:215:LEU:HD12	3:I:215:LEU:HA	1.90	0.42
3:L:83:PRO:HG3	3:L:102:TYR:CE2	2.54	0.42
3:C:65:THR:HG23	3:C:237:THR:HG22	2.02	0.41
1:D:256:LYS:NZ	2:E:19:GLY:O	2.53	0.41
1:J:190:VAL:CG2	2:K:24:ILE:HG12	2.50	0.41
3:L:111:GLN:O	3:L:235:THR:N	2.39	0.41
3:O:126:VAL:HB	3:O:179:PRO:HG2	2.01	0.41
1:D:164:ASP:OD1	1:D:165:SER:N	2.54	0.41
1:M:117:ALA:HA	2:N:236:LEU:HD13	2.02	0.41
3:L:162:HIS:HA	3:L:163:PRO:HD3	1.89	0.41
3:O:188:ASN:OD1	3:O:188:ASN:N	2.52	0.41
1:A:205:TYR:O	1:A:207:GLY:N	2.52	0.41
2:H:14:LEU:HG	2:H:17:ASP:HB2	2.03	0.41
2:N:55:VAL:HB	2:N:71:PHE:HE1	1.85	0.41
2:N:204:VAL:HG13	2:N:208:ALA:HB3	2.03	0.41
3:L:102:TYR:HD1	3:L:245:PHE:CE1	2.39	0.41
3:O:217:VAL:HA	3:O:218:PRO:HD2	1.88	0.41
3:C:232:ILE:HA	3:C:233:PRO:HD3	1.75	0.41
1:G:104:ASN:HD22	1:G:106:TYR:HE2	1.69	0.41
1:M:170:ALA:O	1:M:173:THR:OG1	2.39	0.41
1:M:262:ILE:HG21	3:O:128:PRO:HG2	2.01	0.41
1:M:268:ASN:OD1	1:M:268:ASN:C	2.59	0.41
2:N:22:ALA:HA	2:N:23:PRO:HD3	1.89	0.41
2:B:2:PHE:HA	2:B:3:PRO:HD3	1.81	0.41
1:J:151:LEU:HD13	1:J:153:TYR:CZ	2.55	0.41
2:E:54:GLU:OE1	2:E:68:ARG:NE	2.53	0.41
3:I:73:LYS:H	3:I:73:LYS:HG2	1.54	0.41
3:L:146:PRO:HA	3:L:147:PRO:HD3	1.81	0.41
1:G:266:MET:HE2	1:G:266:MET:HB3	1.72	0.41
1:J:166:ARG:HH12	1:J:237:THR:HB	1.84	0.41
1:M:126:PHE:CE1	2:N:40:VAL:HG21	2.56	0.41
2:H:79:LYS:H	2:H:79:LYS:HG3	1.59	0.41
3:L:97:GLN:HG2	3:L:207:LEU:HD11	2.01	0.41
3:L:126:VAL:HG21	3:L:195:VAL:HG21	2.03	0.41
3:L:165:VAL:HG13	3:L:170:ILE:N	2.32	0.41
1:A:79:THR:OG1	1:A:82:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG22	1:A:203:TRP:NE1	2.36	0.41
1:G:77:GLU:HA	1:G:82:SER:CB	2.50	0.41
2:E:131:MET:N	2:E:157:TRP:O	2.37	0.41
2:K:104:LEU:HD23	2:K:104:LEU:HA	1.86	0.41
2:N:89:ASP:HA	2:N:90:PRO:HD3	1.79	0.41
3:I:71:TRP:CD2	3:I:222:LEU:HD12	2.55	0.41
3:L:82:PHE:CE1	3:L:214:LEU:HB2	2.55	0.41
2:B:51:THR:HA	3:C:176:THR:HG21	2.03	0.41
1:D:75:THR:O	2:E:42:ASN:ND2	2.53	0.41
1:G:162:LYS:HE3	1:G:232:THR:HG21	2.01	0.41
1:G:166:ARG:HH12	1:G:237:THR:HB	1.86	0.41
1:M:138:VAL:HG22	1:M:187:PRO:HG3	2.03	0.41
1:M:266:MET:HE2	1:M:266:MET:HB3	1.90	0.41
2:H:150:MET:HE3	2:H:150:MET:HB2	1.69	0.41
2:K:24:ILE:HD13	2:K:24:ILE:HA	1.92	0.41
3:F:28:ALA:C	3:F:30:ASN:H	2.24	0.41
3:F:69:LYS:HA	3:F:69:LYS:HD2	1.81	0.41
3:F:146:PRO:HA	3:F:147:PRO:HD3	1.84	0.41
3:F:147:PRO:HD2	3:F:150:GLN:HB3	2.03	0.41
3:L:32:ILE:HD12	3:L:181:GLN:HG2	2.02	0.41
3:O:80:TRP:HB3	3:O:85:VAL:HG22	2.02	0.41
3:O:100:TYR:CD2	3:O:101:LEU:HG	2.56	0.41
1:A:135:PHE:HA	1:A:252:TYR:O	2.21	0.41
2:B:128:THR:HG23	2:B:203:VAL:HB	2.02	0.41
1:D:191:SER:OG	2:E:21:SER:OG	2.37	0.41
1:J:182:LYS:HZ3	1:M:186:PRO:HA	1.86	0.41
2:E:26:PRO:C	2:E:28:PHE:H	2.25	0.41
2:H:65:LEU:O	2:H:68:ARG:HG3	2.21	0.41
2:K:22:ALA:HA	2:K:23:PRO:HD3	1.88	0.41
2:K:190:THR:HG23	2:K:191:THR:N	2.36	0.41
3:F:83:PRO:O	3:F:87:THR:HG23	2.21	0.41
3:F:153:PRO:HB3	3:F:158:PHE:HB2	2.02	0.41
3:O:109:HIS:CD2	3:O:192:THR:HG22	2.56	0.41
3:C:51:ASP:OD1	3:C:52:LYS:N	2.53	0.41
2:E:104:LEU:HD23	2:E:104:LEU:HA	1.87	0.41
2:K:125:PHE:HB3	3:L:116:LYS:HG3	2.02	0.41
3:C:222:LEU:HD11	3:C:232:ILE:CG1	2.51	0.40
1:D:190:VAL:HG21	2:E:24:ILE:HG13	2.02	0.40
2:K:146:ARG:HD2	2:K:199:GLN:OE1	2.20	0.40
3:F:68:THR:CG2	3:F:233:PRO:HB3	2.51	0.40
3:O:56:PRO:O	3:O:60:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:107:CYS:HB2	3:O:241:MET:SD	2.62	0.40
1:D:150:LEU:O	1:D:238:VAL:HG13	2.21	0.40
1:J:121:ARG:HH22	2:K:103:GLN:HG2	1.86	0.40
3:O:73:LYS:H	3:O:73:LYS:HG2	1.54	0.40
3:O:118:HIS:CD2	3:O:232:ILE:HD11	2.56	0.40
3:C:28:ALA:C	3:C:30:ASN:H	2.25	0.40
1:D:75:THR:HB	2:E:44:LEU:HD12	2.02	0.40
1:D:194:PHE:CZ	1:D:196:SER:HB3	2.57	0.40
1:G:128:TYR:OH	3:I:129:GLU:OE2	2.40	0.40
3:L:28:ALA:C	3:L:30:ASN:H	2.25	0.40
3:C:81:LYS:O	3:C:85:VAL:HG23	2.21	0.40
2:E:173:SER:OG	2:E:174:ASN:N	2.54	0.40
2:K:208:ALA:HA	2:K:209:PRO:HD3	1.90	0.40
1:D:219:ASP:HB3	3:F:145:HIS:CB	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:LYS:NZ	3:I:111:GLN:OE1[4_555]	2.10	0.10

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	224/297 (75%)	200 (89%)	21 (9%)	3 (1%)	12	47
1	D	224/297 (75%)	198 (88%)	23 (10%)	3 (1%)	12	47
1	G	224/297 (75%)	198 (88%)	24 (11%)	2 (1%)	17	54
1	J	224/297 (75%)	199 (89%)	23 (10%)	2 (1%)	17	54
1	M	224/297 (75%)	199 (89%)	25 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	220/242 (91%)	203 (92%)	17 (8%)	0	100	100
2	E	220/242 (91%)	201 (91%)	18 (8%)	1 (0%)	29	66
2	H	220/242 (91%)	201 (91%)	19 (9%)	0	100	100
2	K	220/242 (91%)	202 (92%)	18 (8%)	0	100	100
2	N	220/242 (91%)	203 (92%)	16 (7%)	1 (0%)	29	66
3	C	229/323 (71%)	204 (89%)	23 (10%)	2 (1%)	17	54
3	F	229/323 (71%)	204 (89%)	21 (9%)	4 (2%)	9	42
3	I	229/323 (71%)	206 (90%)	19 (8%)	4 (2%)	9	42
3	L	229/323 (71%)	206 (90%)	19 (8%)	4 (2%)	9	42
3	O	229/323 (71%)	206 (90%)	18 (8%)	5 (2%)	6	37
All	All	3365/4310 (78%)	3030 (90%)	304 (9%)	31 (1%)	17	54

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
3	C	57	ASP
3	F	57	ASP
3	I	57	ASP
3	L	57	ASP
3	O	57	ASP
3	C	163	PRO
3	I	67	ASP
3	I	163	PRO
3	O	163	PRO
3	F	67	ASP
3	F	163	PRO
3	L	163	PRO
3	O	26	GLN
3	O	67	ASP
1	D	103	PRO
3	F	226	GLN
3	L	226	GLN
1	D	206	ASP
3	I	29	ALA
3	L	67	ASP
1	A	115	GLY
1	G	103	PRO

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Mol	Chain	Res	Type
1	G	206	ASP
1	J	103	PRO
1	J	213	GLU
3	O	226	GLN
1	A	103	PRO
1	D	115	GLY
2	E	94	GLY
2	N	94	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	194/251 (77%)	191 (98%)	3 (2%)	65	81
1	D	194/251 (77%)	192 (99%)	2 (1%)	76	86
1	G	194/251 (77%)	193 (100%)	1 (0%)	88	94
1	J	194/251 (77%)	190 (98%)	4 (2%)	53	73
1	M	194/251 (77%)	191 (98%)	3 (2%)	65	81
2	B	188/202 (93%)	187 (100%)	1 (0%)	88	94
2	E	188/202 (93%)	186 (99%)	2 (1%)	73	85
2	H	188/202 (93%)	186 (99%)	2 (1%)	73	85
2	K	188/202 (93%)	185 (98%)	3 (2%)	62	79
2	N	188/202 (93%)	184 (98%)	4 (2%)	53	73
3	C	196/272 (72%)	194 (99%)	2 (1%)	76	86
3	F	196/272 (72%)	191 (97%)	5 (3%)	46	68
3	I	196/272 (72%)	194 (99%)	2 (1%)	76	86
3	L	196/272 (72%)	193 (98%)	3 (2%)	65	81
3	O	196/272 (72%)	192 (98%)	4 (2%)	55	74
All	All	2890/3625 (80%)	2849 (99%)	41 (1%)	67	82

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	THR
1	A	151	LEU
1	A	220	LEU
2	B	24	ILE
3	C	116	LYS
3	C	231	VAL
1	D	101	THR
1	D	151	LEU
1	G	114	THR
1	J	101	THR
1	J	151	LEU
1	J	162	LYS
1	J	242	LYS
1	M	101	THR
1	M	219	ASP
1	M	268	ASN
2	E	24	ILE
2	E	222	LYS
2	H	24	ILE
2	H	144	LYS
2	K	24	ILE
2	K	70	ARG
2	K	76	GLN
2	N	76	GLN
2	N	144	LYS
2	N	176	HIS
2	N	221	GLN
3	F	20	ASN
3	F	54	THR
3	F	216	VAL
3	F	231	VAL
3	F	238	LEU
3	I	111	GLN
3	I	231	VAL
3	L	76	LYS
3	L	116	LYS
3	L	231	VAL
3	O	22	THR
3	O	116	LYS
3	O	156	ASP
3	O	231	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
2	B	221	GLN
2	B	227	GLN
3	C	111	GLN
1	M	176	ASN
2	H	227	GLN
2	K	237	GLN
3	F	61	ASN
3	F	162	HIS
3	F	208	ASN
3	O	61	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 monosaccharides in this entry.

5.6 Ligand geometry

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	226/297 (76%)	-0.24	4 (1%)	68	55	60, 81, 134, 274	0
1	D	226/297 (76%)	-0.11	12 (5%)	26	18	61, 82, 146, 274	0
1	G	226/297 (76%)	-0.17	3 (1%)	77	65	63, 85, 146, 274	0
1	J	226/297 (76%)	-0.31	4 (1%)	68	55	55, 78, 147, 274	0
1	M	226/297 (76%)	-0.23	6 (2%)	54	40	64, 83, 144, 274	0
2	B	224/242 (92%)	-0.33	0	100	100	60, 81, 113, 216	0
2	E	224/242 (92%)	-0.24	0	100	100	67, 84, 114, 217	0
2	H	224/242 (92%)	-0.36	0	100	100	65, 83, 112, 219	0
2	K	224/242 (92%)	-0.34	0	100	100	56, 76, 113, 216	0
2	N	224/242 (92%)	-0.40	0	100	100	59, 82, 112, 217	0
3	C	231/323 (71%)	-0.05	6 (2%)	56	42	63, 83, 151, 185	0
3	F	231/323 (71%)	-0.11	5 (2%)	62	48	60, 86, 152, 183	0
3	I	231/323 (71%)	-0.02	7 (3%)	50	36	66, 88, 154, 180	0
3	L	231/323 (71%)	-0.07	12 (5%)	27	19	58, 78, 154, 185	0
3	O	231/323 (71%)	-0.17	8 (3%)	44	31	63, 88, 154, 179	0
All	All	3405/4310 (79%)	-0.21	67 (1%)	65	52	55, 83, 146, 274	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	139	THR	6.5
1	D	216	GLN	5.1
3	O	139	THR	5.0
3	C	139	THR	4.9
3	L	136	ALA	4.4
1	D	215	LYS	4.4
3	I	28	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	217	GLU	4.2
3	I	139	THR	4.2
3	C	143	ASP	4.0
3	L	141	THR	4.0
3	F	139	THR	3.9
3	C	136	ALA	3.7
3	C	141	THR	3.7
1	M	215	LYS	3.7
1	A	216	GLN	3.7
3	O	141	THR	3.5
1	M	216	GLN	3.4
3	L	143	ASP	3.4
1	D	220	LEU	3.3
1	G	214	HIS	3.2
1	M	214	HIS	3.2
3	L	140	GLY	3.2
1	D	217	GLU	3.1
1	D	214	HIS	3.1
1	J	216	GLN	3.0
3	I	143	ASP	2.9
3	L	49	ALA	2.8
3	O	140	GLY	2.8
1	D	72	SER	2.7
1	J	72	SER	2.7
3	L	137	GLY	2.7
3	I	140	GLY	2.6
3	L	138	GLY	2.6
3	I	141	THR	2.6
3	O	143	ASP	2.6
1	G	213	GLU	2.6
1	D	219	ASP	2.6
3	L	46	ASP	2.6
3	O	45	SER	2.5
1	G	217	GLU	2.5
1	D	73	HIS	2.5
3	F	140	GLY	2.4
1	D	221	GLU	2.4
1	A	220	LEU	2.4
3	O	137	GLY	2.4
3	L	142	GLU	2.3
3	F	143	ASP	2.3
3	O	135	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	ASP	2.3
1	M	100	THR	2.3
1	D	210	THR	2.2
3	C	137	GLY	2.2
3	C	140	GLY	2.2
1	D	104	ASN	2.2
3	F	138	GLY	2.2
3	L	24	THR	2.2
1	J	217	GLU	2.1
3	O	136	ALA	2.1
3	F	148	TYR	2.1
1	J	215	LYS	2.1
3	I	61	ASN	2.1
1	D	98	GLU	2.0
1	M	72	SER	2.0
1	M	219	ASP	2.0
3	I	27	GLU	2.0
3	L	45	SER	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 monosaccharides 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.