



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 04:01 PM EDT

PDB ID : 2FT1  
Title : Bacteriophage HK97 Head II  
Authors : Gan, L.; Speir, J.A.; Conway, J.F.; Lander, G.; Cheng, N.; Firek, B.A.; Hendrix, R.W.; Duda, R.L.; Liljas, L.; Johnson, J.E.  
Deposited on : unknown  
Resolution : 3.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

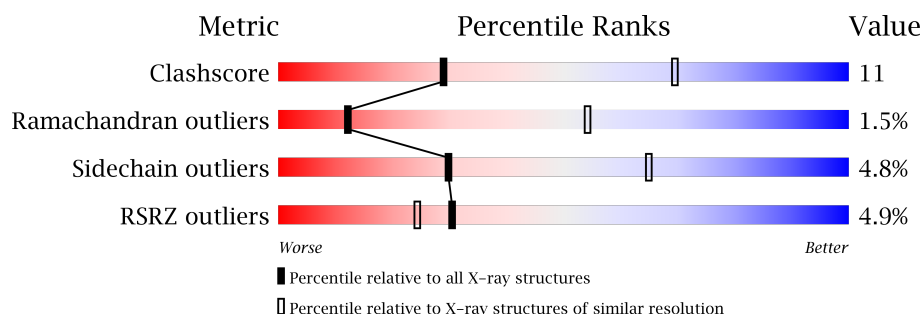
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	282	<div> <div>4%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	B	282	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	C	282	<div> <div>4%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	D	282	<div> <div>3%</div> <div>73%</div> <div>25%</div> <div>..</div> </div>
1	E	282	<div> <div>4%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	F	282	<div> <div>3%</div> <div>63%</div> <div>25%</div> <div>• 9%</div> </div>
1	G	282	<div> <div>10%</div> <div>74%</div> <div>18%</div> <div>• 7%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14777 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.

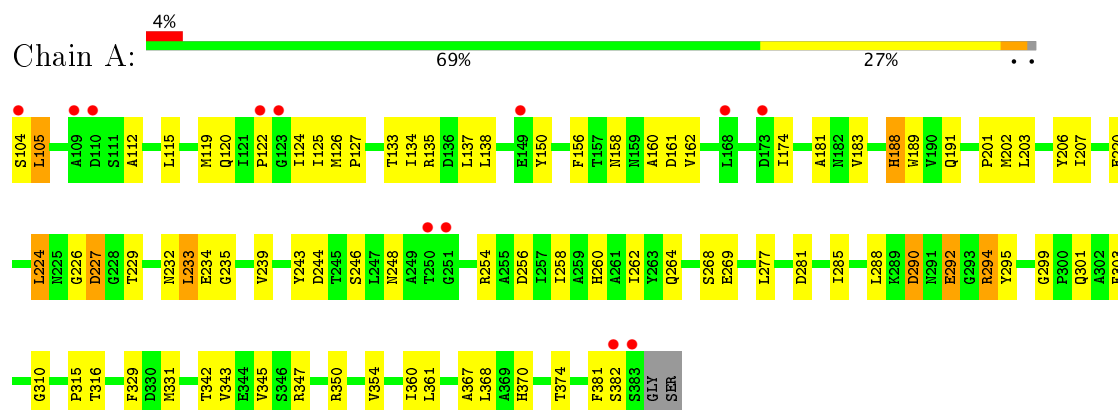
- Molecule 1 is a protein called major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	B	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	C	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	D	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	E	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	F	258	Total	C	N	O	S	0	0	0
			2001	1251	351	390	9			
1	G	261	Total	C	N	O	S	0	0	0
			2021	1265	354	393	9			

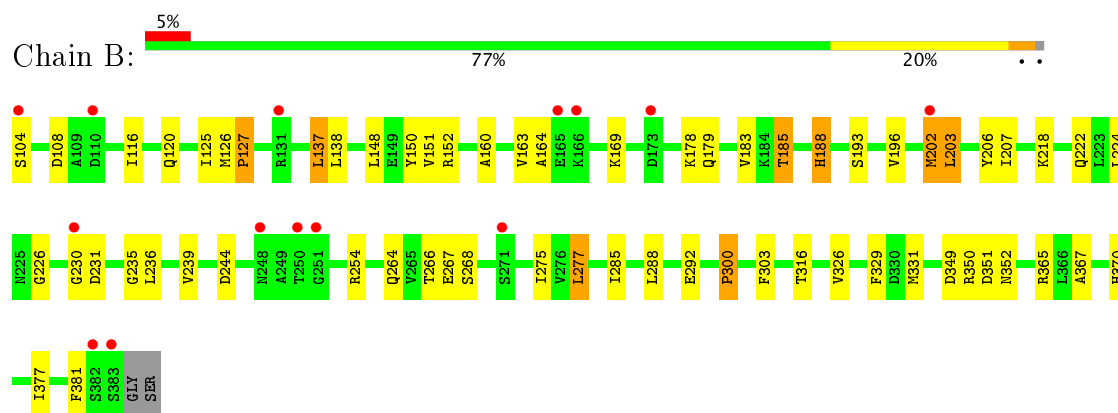
### 3 Residue-property plots [i](#)

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.

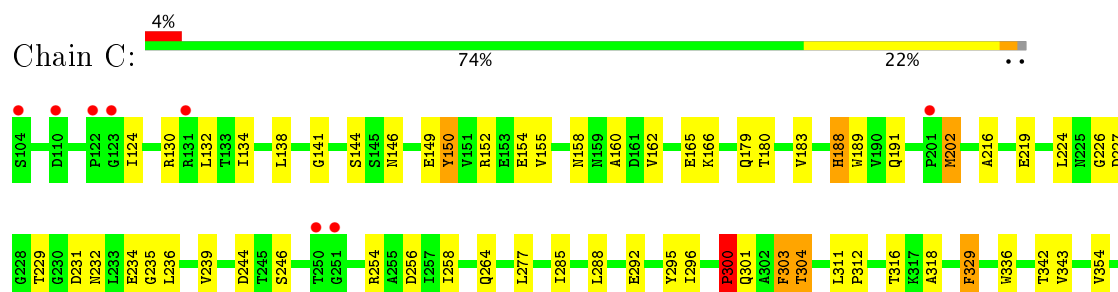
#### • Molecule 1: major capsid protein



#### • Molecule 1: major capsid protein



#### • Molecule 1: major capsid protein

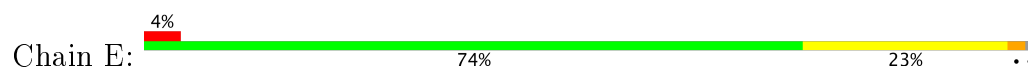




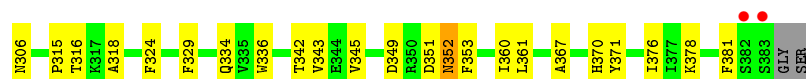
- Molecule 1: major capsid protein



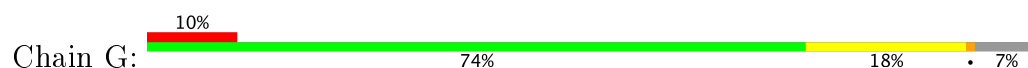
- Molecule 1: major capsid protein

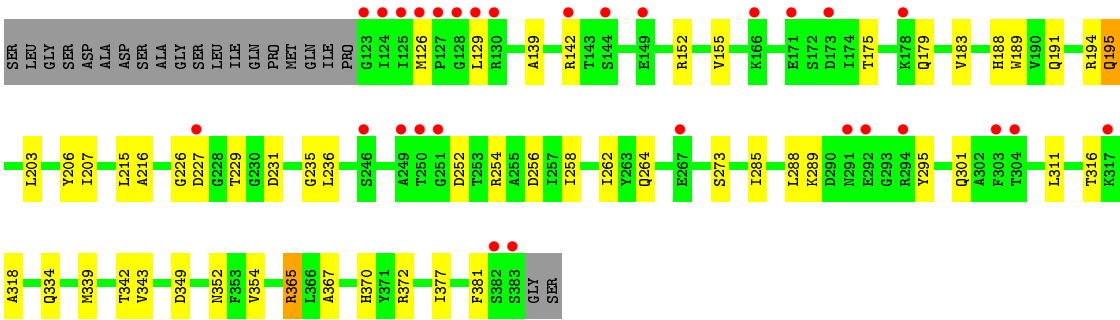


- Molecule 1: major capsid protein



- Molecule 1: major capsid protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	1009.80 Å   1009.80 Å   732.87 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 3.90 30.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	52.1 (30.00-3.90) 52.1 (30.00-3.90)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.86 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.297 , (Not available) 0.290 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.09	EDS
Total number of atoms	14777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/2188	0.52	0/2969
1	B	0.25	0/2188	0.51	0/2969
1	C	0.26	0/2188	0.52	0/2969
1	D	0.27	0/2188	0.51	0/2969
1	E	0.25	0/2188	0.53	0/2969
1	F	0.26	0/2036	0.52	0/2762
1	G	0.28	0/2056	0.51	0/2789
All	All	0.26	0/15032	0.52	0/20396

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 [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	2151	0	2119	62	0
1	B	2151	0	2119	47	0
1	C	2151	0	2119	61	0
1	D	2151	0	2119	44	0
1	E	2151	0	2119	51	0
1	F	2001	0	1967	61	0
1	G	2021	0	1992	34	0
All	All	14777	0	14554	320	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 11.

All (320) 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:D:229:THR:HG23	1:D:230:GLY:H	1.35	0.92
1:E:210:ARG:HH21	1:F:156:PHE:HD2	1.20	0.88
1:F:227:ASP:HB3	1:F:229:THR:HG22	1.54	0.88
1:E:116:ILE:HG21	1:F:146:ASN:HB2	1.59	0.82
1:D:193:SER:HB3	1:D:196:VAL:HG23	1.64	0.80
1:C:150:TYR:CE1	1:C:179:GLN:HB2	2.18	0.79
1:D:207:ILE:HG23	1:D:211:LEU:HD23	1.63	0.77
1:A:227:ASP:HB3	1:A:232:ASN:HB2	1.66	0.76
1:C:226:GLY:HA3	1:C:235:GLY:H	1.49	0.75
1:A:233:LEU:H	1:A:233:LEU:HD12	1.49	0.75
1:F:236:LEU:HD23	1:F:370:HIS:HE1	1.52	0.75
1:F:193:SER:HB3	1:F:195:GLN:HE21	1.52	0.75
1:E:194:ARG:HH11	1:E:347:ARG:HD3	1.52	0.74
1:F:150:TYR:CE1	1:F:179:GLN:HB2	2.23	0.73
1:C:149:GLU:HG2	1:C:180:THR:HG22	1.69	0.72
1:G:236:LEU:HD23	1:G:370:HIS:HE1	1.54	0.72
1:C:130:ARG:HH22	1:C:318:ALA:HB2	1.56	0.71
1:D:316:THR:HG22	1:D:318:ALA:H	1.55	0.70
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.72	0.69
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.06	0.69
1:F:316:THR:HG22	1:F:318:ALA:H	1.57	0.69
1:G:342:THR:HG22	1:G:343:VAL:H	1.57	0.69
1:A:134:ILE:HD12	1:A:220:GLU:HG2	1.75	0.68
1:C:150:TYR:HE1	1:C:179:GLN:HB2	1.59	0.68
1:A:244:ASP:HB2	1:A:264:GLN:NE2	2.09	0.67
1:F:183:VAL:HG22	1:F:367:ALA:HB2	1.77	0.67
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.30	0.66
1:A:226:GLY:HA3	1:A:235:GLY:H	1.59	0.65
1:E:222:GLN:HB3	1:E:233:LEU:HD11	1.79	0.65
1:A:254:ARG:HB3	1:A:381:PHE:HE2	1.62	0.65
1:F:138:LEU:HD23	1:F:329:PHE:HB3	1.78	0.65
1:G:189:TRP:HZ3	1:G:191:GLN:HG3	1.62	0.64
1:G:316:THR:HG22	1:G:318:ALA:H	1.62	0.64
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.61	0.63
1:D:148:LEU:HB2	1:D:181:ALA:HB3	1.81	0.63
1:G:273:SER:HA	1:G:311:LEU:HD22	1.81	0.62
1:G:339:MET:HB3	1:G:365:ARG:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HG21	1:C:146:ASN:HB2	1.80	0.62
1:A:191:GLN:HE22	1:A:350:ARG:HH21	1.46	0.62
1:B:349:ASP:O	1:B:352:ASN:HB2	1.99	0.61
1:F:254:ARG:HB3	1:F:381:PHE:CE2	2.36	0.61
1:E:183:VAL:HG22	1:E:367:ALA:HB2	1.82	0.61
1:C:295:TYR:HD1	1:C:300:PRO:HD3	1.65	0.61
1:E:202:MET:N	1:E:202:MET:SD	2.73	0.61
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.66	0.61
1:E:316:THR:HG22	1:E:318:ALA:H	1.65	0.60
1:C:124:ILE:HD12	1:C:124:ILE:H	1.65	0.60
1:B:244:ASP:HB2	1:B:264:GLN:NE2	2.16	0.60
1:G:226:GLY:H	1:G:235:GLY:HA3	1.67	0.59
1:A:244:ASP:HB2	1:A:264:GLN:HE22	1.67	0.59
1:F:130:ARG:HD2	1:F:133:THR:CG2	2.31	0.59
1:F:202:MET:N	1:F:202:MET:SD	2.76	0.59
1:F:139:ALA:O	1:F:334:GLN:HG3	2.03	0.59
1:C:244:ASP:HB2	1:C:264:GLN:HE22	1.67	0.59
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.18	0.58
1:A:191:GLN:NE2	1:A:350:ARG:HH21	2.02	0.58
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.68	0.58
1:F:281:ASP:O	1:F:285:ILE:HG12	2.03	0.58
1:E:345:VAL:HG12	1:E:360:ILE:HG12	1.85	0.58
1:F:244:ASP:HB2	1:F:264:GLN:HE22	1.68	0.58
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.67	0.58
1:G:183:VAL:HG22	1:G:367:ALA:HB2	1.86	0.58
1:F:226:GLY:H	1:F:235:GLY:HA3	1.69	0.57
1:B:226:GLY:HA3	1:B:235:GLY:H	1.68	0.57
1:D:229:THR:HG23	1:D:230:GLY:N	2.15	0.57
1:A:244:ASP:OD1	1:A:246:SER:HB3	2.05	0.57
1:E:349:ASP:O	1:E:352:ASN:HB2	2.04	0.57
1:F:244:ASP:HB2	1:F:264:GLN:NE2	2.19	0.57
1:A:234:GLU:HG2	1:A:239:VAL:HG23	1.86	0.57
1:B:116:ILE:HG21	1:C:146:ASN:CB	2.35	0.57
1:B:150:TYR:CE1	1:B:179:GLN:HB2	2.40	0.57
1:B:183:VAL:HG22	1:B:367:ALA:HB2	1.86	0.56
1:E:210:ARG:NH2	1:F:156:PHE:HD2	1.97	0.56
1:G:289:LYS:HE2	1:G:295:TYR:HE2	1.70	0.56
1:A:119:MET:HB3	1:B:148:LEU:CD2	2.35	0.56
1:C:124:ILE:HD12	1:C:124:ILE:N	2.20	0.56
1:D:185:THR:HG22	1:D:365:ARG:HG2	1.88	0.55
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ARG:HH11	1:F:133:THR:HG21	1.71	0.55
1:D:146:ASN:O	1:D:183:VAL:HG12	2.06	0.55
1:F:299:GLY:O	1:F:301:GLN:N	2.40	0.55
1:G:342:THR:HG22	1:G:343:VAL:N	2.21	0.54
1:A:294:ARG:HG3	1:F:294:ARG:HH21	1.71	0.54
1:A:189:TRP:CD1	1:B:169:LYS:HB2	2.43	0.54
1:G:229:THR:HG23	1:G:231:ASP:H	1.73	0.54
1:E:226:GLY:H	1:E:235:GLY:HA3	1.72	0.54
1:B:244:ASP:HB2	1:B:264:GLN:HE22	1.72	0.53
1:A:285:ILE:O	1:A:288:LEU:HG	2.08	0.53
1:G:139:ALA:O	1:G:334:GLN:HB2	2.08	0.53
1:G:254:ARG:HB3	1:G:381:PHE:CE2	2.44	0.53
1:C:219:GLU:HG3	1:C:366:LEU:HD11	1.91	0.53
1:A:104:SER:HA	1:C:166:LYS:NZ	2.24	0.53
1:C:227:ASP:OD1	1:C:229:THR:HB	2.08	0.53
1:C:295:TYR:CD1	1:C:300:PRO:HD3	2.43	0.53
1:D:268:SER:O	1:D:269:GLU:HB2	2.09	0.53
1:G:155:VAL:H	1:G:175:THR:HB	1.73	0.53
1:E:208:ASN:HD22	1:E:208:ASN:N	2.04	0.53
1:E:135:ARG:HG3	1:E:135:ARG:HH11	1.74	0.52
1:D:163:VAL:HG21	1:D:169:LYS:HG2	1.91	0.52
1:D:289:LYS:HE2	1:D:295:TYR:HE2	1.73	0.52
1:D:349:ASP:O	1:D:352:ASN:HB2	2.10	0.52
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.39	0.52
1:B:120:GLN:HE22	1:C:149:GLU:HB2	1.74	0.51
1:A:292:GLU:HG3	1:B:292:GLU:HG2	1.93	0.51
1:C:226:GLY:HA3	1:C:235:GLY:N	2.21	0.51
1:A:368:LEU:HD21	1:A:370:HIS:HE2	1.76	0.51
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.45	0.51
1:C:304:THR:HG23	1:C:304:THR:O	2.10	0.51
1:G:194:ARG:HH11	1:G:194:ARG:HG2	1.74	0.51
1:B:137:LEU:HD22	1:B:329:PHE:HB2	1.93	0.51
1:A:227:ASP:OD1	1:A:229:THR:HB	2.11	0.51
1:D:226:GLY:HA3	1:D:235:GLY:H	1.76	0.51
1:E:254:ARG:HB3	1:E:381:PHE:HE2	1.75	0.51
1:F:237:ASN:HB3	1:F:378:LYS:HD3	1.92	0.51
1:E:224:LEU:HG	1:E:237:ASN:ND2	2.25	0.51
1:F:342:THR:HG22	1:F:343:VAL:N	2.26	0.51
1:C:141:GLY:O	1:C:336:TRP:HA	2.11	0.51
1:F:127:PRO:HG2	1:F:210:ARG:HH11	1.77	0.51
1:F:239:VAL:HG21	1:F:370:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TYR:HB2	1:A:299:GLY:HA2	1.92	0.50
1:F:130:ARG:NH1	1:F:133:THR:HG21	2.26	0.50
1:F:127:PRO:HG2	1:F:210:ARG:NH1	2.26	0.50
1:D:193:SER:HB3	1:D:196:VAL:CG2	2.37	0.50
1:D:143:THR:HG23	1:D:338:ARG:HD3	1.93	0.50
1:D:272:ALA:HB3	1:D:311:LEU:HD11	1.92	0.50
1:E:211:LEU:HD23	1:E:362:CYS:HB3	1.94	0.50
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.46	0.50
1:C:132:LEU:HD12	1:C:132:LEU:H	1.76	0.50
1:G:139:ALA:HB3	1:G:334:GLN:HB2	1.94	0.50
1:C:189:TRP:HZ3	1:C:191:GLN:HB2	1.77	0.50
1:B:138:LEU:HD23	1:B:329:PHE:HB3	1.94	0.49
1:F:142:ARG:NH1	1:F:142:ARG:HB3	2.27	0.49
1:F:236:LEU:HD23	1:F:370:HIS:CE1	2.39	0.49
1:C:371:TYR:N	1:C:371:TYR:CD1	2.80	0.49
1:E:295:TYR:HD1	1:E:300:PRO:HD3	1.77	0.49
1:D:289:LYS:HA	1:D:294:ARG:O	2.12	0.49
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.94	0.49
1:B:226:GLY:H	1:B:235:GLY:HA3	1.78	0.49
1:C:254:ARG:HB3	1:C:381:PHE:HE2	1.76	0.49
1:C:138:LEU:CD2	1:C:329:PHE:HB3	2.42	0.49
1:E:277:LEU:O	1:E:315:PRO:HA	2.12	0.49
1:G:349:ASP:O	1:G:352:ASN:HB2	2.12	0.49
1:C:226:GLY:H	1:C:235:GLY:HA3	1.77	0.49
1:E:116:ILE:HG21	1:F:146:ASN:CB	2.38	0.49
1:F:349:ASP:O	1:F:352:ASN:HB2	2.13	0.49
1:C:371:TYR:N	1:C:371:TYR:HD1	2.11	0.49
1:G:195:GLN:H	1:G:195:GLN:HE21	1.60	0.49
1:F:324:PHE:CD2	1:F:381:PHE:HE1	2.31	0.48
1:E:126:MET:HG2	1:E:210:ARG:HH11	1.78	0.48
1:G:194:ARG:HG2	1:G:194:ARG:NH1	2.27	0.48
1:C:130:ARG:NH2	1:C:318:ALA:HB2	2.25	0.48
1:A:160:ALA:HB2	1:F:188:HIS:ND1	2.29	0.48
1:D:345:VAL:HG22	1:D:360:ILE:HA	1.95	0.48
1:G:183:VAL:HA	1:G:367:ALA:HB2	1.95	0.48
1:F:290:ASP:C	1:F:292:GLU:H	2.17	0.48
1:A:104:SER:HA	1:C:166:LYS:HZ3	1.79	0.48
1:D:120:GLN:O	1:D:122:PRO:HD3	2.14	0.48
1:A:124:ILE:HG12	1:A:125:ILE:N	2.28	0.48
1:B:120:GLN:NE2	1:C:149:GLU:HB2	2.28	0.48
1:D:354:VAL:O	1:D:354:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:THR:HG22	1:F:343:VAL:H	1.79	0.47
1:A:203:LEU:O	1:A:206:TYR:HB3	2.15	0.47
1:A:226:GLY:HA3	1:A:235:GLY:N	2.28	0.47
1:C:285:ILE:O	1:C:288:LEU:HG	2.15	0.47
1:A:134:ILE:O	1:A:137:LEU:HB2	2.15	0.47
1:A:156:PHE:CZ	1:A:158:ASN:HB2	2.49	0.47
1:G:254:ARG:HB3	1:G:381:PHE:HE2	1.80	0.47
1:A:258:ILE:HD12	1:A:258:ILE:H	1.80	0.47
1:D:141:GLY:O	1:D:336:TRP:HA	2.15	0.47
1:D:285:ILE:O	1:D:288:LEU:HG	2.15	0.46
1:D:339:MET:CE	1:D:363:GLU:HG3	2.45	0.46
1:E:325:THR:HA	1:E:377:ILE:O	2.15	0.46
1:F:351:ASP:O	1:F:353:PHE:N	2.47	0.46
1:G:354:VAL:O	1:G:354:VAL:HG12	2.15	0.46
1:E:295:TYR:CD1	1:E:300:PRO:HD3	2.50	0.46
1:A:226:GLY:H	1:A:235:GLY:HA3	1.81	0.46
1:B:163:VAL:HG12	1:B:164:ALA:O	2.16	0.46
1:B:266:THR:C	1:B:268:SER:H	2.19	0.46
1:C:138:LEU:HD23	1:C:329:PHE:HB3	1.98	0.46
1:D:188:HIS:CE1	1:E:160:ALA:HB2	2.50	0.46
1:A:342:THR:HG22	1:A:343:VAL:N	2.31	0.46
1:F:268:SER:O	1:F:269:GLU:HB2	2.13	0.46
1:F:236:LEU:HD22	1:F:376:ILE:HD13	1.98	0.46
1:A:258:ILE:N	1:A:258:ILE:HD12	2.30	0.46
1:A:160:ALA:HB2	1:F:188:HIS:CG	2.51	0.46
1:A:368:LEU:CD2	1:A:370:HIS:HE2	2.29	0.46
1:C:234:GLU:HG2	1:C:239:VAL:HG23	1.96	0.46
1:C:303:PHE:O	1:C:304:THR:HB	2.15	0.46
1:G:285:ILE:O	1:G:288:LEU:HG	2.16	0.46
1:G:142:ARG:HH11	1:G:142:ARG:HG2	1.81	0.46
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.51	0.46
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.97	0.46
1:B:285:ILE:O	1:B:288:LEU:HG	2.16	0.45
1:F:141:GLY:O	1:F:336:TRP:HA	2.14	0.45
1:A:120:GLN:O	1:A:122:PRO:HD3	2.16	0.45
1:B:183:VAL:HA	1:B:367:ALA:HB2	1.99	0.45
1:C:154:GLU:HG3	1:C:155:VAL:HG23	1.97	0.45
1:A:112:ALA:O	1:A:115:LEU:HB2	2.17	0.45
1:F:132:LEU:HB3	1:F:136:ASP:CG	2.36	0.45
1:E:138:LEU:HD23	1:E:329:PHE:HB3	1.97	0.45
1:A:183:VAL:HG22	1:A:367:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:CG2	1:B:365:ARG:HG2	2.47	0.45
1:B:264:GLN:HB3	1:B:377:ILE:HD13	1.98	0.45
1:C:202:MET:SD	1:C:202:MET:N	2.90	0.45
1:A:133:THR:O	1:A:135:ARG:N	2.49	0.45
1:C:292:GLU:OE2	1:C:292:GLU:HA	2.16	0.45
1:D:236:LEU:HD23	1:D:370:HIS:CE1	2.47	0.45
1:G:227:ASP:OD1	1:G:229:THR:HB	2.17	0.45
1:A:161:ASP:CG	1:A:162:VAL:H	2.19	0.45
1:D:339:MET:HE1	1:D:363:GLU:HG3	1.98	0.45
1:C:236:LEU:HD22	1:C:376:ILE:HD13	1.98	0.45
1:B:104:SER:HB2	1:D:166:LYS:NZ	2.31	0.45
1:F:266:THR:C	1:F:268:SER:H	2.19	0.45
1:B:203:LEU:O	1:B:206:TYR:HB3	2.17	0.44
1:D:234:GLU:HG2	1:D:239:VAL:HG23	1.97	0.44
1:B:236:LEU:HD23	1:B:370:HIS:CE1	2.48	0.44
1:B:218:LYS:HG2	1:C:158:ASN:HD21	1.82	0.44
1:C:227:ASP:HB3	1:C:232:ASN:HB2	1.98	0.44
1:A:354:VAL:O	1:A:354:VAL:HG12	2.18	0.44
1:F:252:ASP:HB3	1:F:256:ASP:HB2	1.99	0.44
1:A:203:LEU:O	1:A:207:ILE:HG13	2.18	0.44
1:C:244:ASP:OD2	1:C:246:SER:HB3	2.18	0.44
1:D:277:LEU:O	1:D:315:PRO:HA	2.18	0.44
1:E:119:MET:HB3	1:F:148:LEU:HD23	1.99	0.44
1:F:343:VAL:HA	1:F:361:LEU:O	2.17	0.44
1:C:342:THR:O	1:C:362:CYS:HA	2.18	0.44
1:A:254:ARG:HB3	1:A:381:PHE:CE2	2.46	0.44
1:B:277:LEU:HD12	1:B:277:LEU:N	2.33	0.44
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.99	0.44
1:C:354:VAL:HG12	1:C:354:VAL:O	2.18	0.44
1:G:189:TRP:CZ3	1:G:191:GLN:HG3	2.47	0.44
1:A:310:GLY:N	1:F:301:GLN:O	2.50	0.43
1:G:203:LEU:O	1:G:206:TYR:HB3	2.18	0.43
1:G:203:LEU:O	1:G:207:ILE:HG13	2.18	0.43
1:C:216:ALA:O	1:C:219:GLU:HB3	2.18	0.43
1:D:218:LYS:HG3	1:E:160:ALA:HB3	2.00	0.43
1:E:193:SER:HB3	1:E:196:VAL:HG23	2.00	0.43
1:E:371:TYR:CD2	1:E:371:TYR:N	2.86	0.43
1:B:275:ILE:HG22	1:B:277:LEU:HD11	1.99	0.43
1:D:254:ARG:NE	1:D:381:PHE:HD2	2.16	0.43
1:E:139:ALA:O	1:E:334:GLN:HG3	2.18	0.43
1:A:345:VAL:HG22	1:A:360:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:H	1:C:166:LYS:CE	2.32	0.43
1:A:260:HIS:HA	1:F:283:HIS:CE1	2.52	0.43
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.33	0.43
1:B:350:ARG:HG3	1:B:351:ASP:N	2.33	0.43
1:A:188:HIS:HB3	1:B:160:ALA:HA	1.99	0.43
1:E:322:GLY:O	1:E:380:THR:HA	2.19	0.43
1:C:236:LEU:HD23	1:C:370:HIS:CE1	2.49	0.43
1:E:223:LEU:O	1:E:236:LEU:HD23	2.19	0.43
1:G:264:GLN:HB3	1:G:377:ILE:HD13	2.00	0.43
1:A:281:ASP:O	1:A:285:ILE:HG13	2.18	0.43
1:E:380:THR:HG22	1:E:381:PHE:N	2.34	0.43
1:B:231:ASP:O	1:C:162:VAL:HG11	2.19	0.42
1:A:290:ASP:OD2	1:A:294:ARG:HG2	2.18	0.42
1:E:188:HIS:HB3	1:F:160:ALA:HA	2.00	0.42
1:F:193:SER:HB2	1:F:196:VAL:HG23	2.00	0.42
1:F:215:LEU:HD23	1:F:216:ALA:N	2.33	0.42
1:B:254:ARG:HB3	1:B:381:PHE:HE2	1.84	0.42
1:C:292:GLU:O	1:D:290:ASP:HB2	2.20	0.42
1:B:275:ILE:HG23	1:B:326:VAL:HG22	2.01	0.42
1:E:289:LYS:HG2	1:E:295:TYR:CE2	2.54	0.42
1:E:342:THR:O	1:E:362:CYS:HA	2.18	0.42
1:C:311:LEU:HA	1:C:312:PRO:HD3	1.89	0.42
1:F:277:LEU:O	1:F:315:PRO:HA	2.20	0.42
1:C:258:ILE:HD11	1:C:381:PHE:CZ	2.55	0.42
1:F:156:PHE:CD1	1:F:156:PHE:C	2.93	0.42
1:F:345:VAL:HG13	1:F:360:ILE:HD13	2.01	0.42
1:B:125:ILE:HB	1:C:152:ARG:CB	2.50	0.42
1:E:292:GLU:HA	1:E:292:GLU:OE2	2.20	0.42
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.35	0.42
1:A:343:VAL:HA	1:A:361:LEU:O	2.20	0.42
1:F:282:TRP:CZ2	1:F:306:ASN:HA	2.55	0.42
1:D:174:ILE:HG22	1:D:175:THR:N	2.35	0.41
1:E:285:ILE:O	1:E:288:LEU:HG	2.20	0.41
1:G:258:ILE:O	1:G:262:ILE:HG13	2.20	0.41
1:A:134:ILE:HD13	1:A:224:LEU:HD23	2.02	0.41
1:A:126:MET:HA	1:A:127:PRO:HD3	1.84	0.41
1:D:119:MET:HB3	1:E:148:LEU:CD2	2.51	0.41
1:B:350:ARG:HG3	1:B:351:ASP:H	1.85	0.41
1:B:300:PRO:HG2	1:C:296:ILE:HG21	2.02	0.41
1:C:342:THR:HG22	1:C:343:VAL:N	2.35	0.41
1:A:191:GLN:HE22	1:A:350:ARG:NH2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLY:O	1:A:227:ASP:HB2	2.20	0.41
1:G:252:ASP:HB2	1:G:256:ASP:CG	2.41	0.41
1:D:187:ALA:HB2	1:D:363:GLU:HB3	2.03	0.41
1:E:208:ASN:N	1:E:208:ASN:ND2	2.69	0.41
1:A:310:GLY:HA3	1:F:303:PHE:HB2	2.02	0.41
1:B:126:MET:HA	1:B:127:PRO:HD3	1.93	0.41
1:G:152:ARG:CZ	1:G:179:GLN:HG3	2.51	0.41
1:A:258:ILE:O	1:A:262:ILE:HG13	2.21	0.41
1:A:268:SER:O	1:A:269:GLU:HB3	2.20	0.41
1:B:188:HIS:CE1	1:C:160:ALA:HB2	2.56	0.41
1:B:222:GLN:O	1:B:226:GLY:N	2.53	0.41
1:D:222:GLN:O	1:D:226:GLY:N	2.54	0.41
1:F:371:TYR:N	1:F:371:TYR:CD2	2.87	0.41
1:A:150:TYR:HE2	1:A:181:ALA:HB2	1.85	0.41
1:B:193:SER:HB3	1:B:196:VAL:HG23	2.03	0.41
1:B:202:MET:N	1:B:202:MET:SD	2.94	0.41
1:C:165:GLU:O	1:C:166:LYS:HB2	2.20	0.41
1:C:316:THR:HG22	1:C:318:ALA:H	1.84	0.41
1:E:311:LEU:HA	1:E:312:PRO:HD3	1.91	0.41
1:E:381:PHE:CD1	1:E:381:PHE:N	2.89	0.41
1:B:151:VAL:HG12	1:B:178:LYS:HA	2.03	0.40
1:E:339:MET:CE	1:E:363:GLU:HG3	2.51	0.40
1:G:195:GLN:H	1:G:195:GLN:NE2	2.19	0.40
1:A:138:LEU:HD23	1:A:329:PHE:HB3	2.03	0.40
1:C:358:LEU:HD12	1:C:358:LEU:N	2.36	0.40
1:D:288:LEU:HD23	1:D:288:LEU:HA	1.95	0.40
1:E:153:GLU:OE1	1:E:156:PHE:HB2	2.22	0.40
1:A:294:ARG:NH2	1:F:292:GLU:HG2	2.36	0.40
1:B:203:LEU:O	1:B:207:ILE:HG13	2.22	0.40
1:D:213:TYR:CE2	1:D:217:LEU:HD12	2.56	0.40
1:D:184:LYS:NZ	1:D:231:ASP:HA	2.36	0.40
1:F:132:LEU:HB3	1:F:136:ASP:OD2	2.21	0.40
1:A:243:TYR:HE2	1:A:248:ASN:HD21	1.70	0.40
1:A:277:LEU:O	1:A:315:PRO:HA	2.21	0.40
1:E:243:TYR:HA	1:E:264:GLN:HE22	1.86	0.40
1:E:339:MET:HE1	1:E:363:GLU:HG3	2.04	0.40
1:G:215:LEU:HD23	1:G:216:ALA:N	2.37	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/282 (99%)	242 (87%)	33 (12%)	3 (1%)	17	60
1	B	278/282 (99%)	243 (87%)	31 (11%)	4 (1%)	13	55
1	C	278/282 (99%)	246 (88%)	26 (9%)	6 (2%)	8	47
1	D	278/282 (99%)	248 (89%)	25 (9%)	5 (2%)	10	51
1	E	278/282 (99%)	252 (91%)	21 (8%)	5 (2%)	10	51
1	F	256/282 (91%)	229 (90%)	22 (9%)	5 (2%)	9	49
1	G	259/282 (92%)	230 (89%)	29 (11%)	0	100	100
All	All	1905/1974 (96%)	1690 (89%)	187 (10%)	28 (2%)	12	54

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	C	134	ILE
1	C	304	THR
1	D	229	THR
1	E	134	ILE
1	E	298	GLY
1	F	134	ILE
1	F	300	PRO
1	F	352	ASN
1	A	201	PRO
1	A	227	ASP
1	B	230	GLY
1	D	134	ILE
1	E	300	PRO
1	C	144	SER
1	C	300	PRO
1	E	144	SER
1	B	300	PRO

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Mol	Chain	Res	Type
1	C	329	PHE
1	D	144	SER
1	F	132	LEU
1	B	267	GLU
1	C	303	PHE
1	D	201	PRO
1	D	300	PRO
1	E	329	PHE
1	F	201	PRO
1	B	127	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	230/231 (100%)	214 (93%)	16 (7%)	18	54
1	B	230/231 (100%)	218 (95%)	12 (5%)	27	63
1	C	230/231 (100%)	220 (96%)	10 (4%)	33	68
1	D	230/231 (100%)	220 (96%)	10 (4%)	33	68
1	E	230/231 (100%)	220 (96%)	10 (4%)	33	68
1	F	213/231 (92%)	202 (95%)	11 (5%)	27	63
1	G	215/231 (93%)	208 (97%)	7 (3%)	43	73
All	All	1578/1617 (98%)	1502 (95%)	76 (5%)	30	65

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	ILE
1	A	188	HIS
1	A	202	MET
1	A	224	LEU
1	A	233	LEU
1	A	256	ASP
1	A	290	ASP

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Mol	Chain	Res	Type
1	A	292	GLU
1	A	294	ARG
1	A	301	GLN
1	A	303	PHE
1	A	316	THR
1	A	331	MET
1	A	347	ARG
1	A	374	THR
1	A	382	SER
1	B	108	ASP
1	B	137	LEU
1	B	152	ARG
1	B	185	THR
1	B	188	HIS
1	B	202	MET
1	B	203	LEU
1	B	224	LEU
1	B	277	LEU
1	B	303	PHE
1	B	316	THR
1	B	331	MET
1	C	150	TYR
1	C	188	HIS
1	C	202	MET
1	C	224	LEU
1	C	231	ASP
1	C	256	ASP
1	C	277	LEU
1	C	300	PRO
1	C	301	GLN
1	C	371	TYR
1	D	115	LEU
1	D	156	PHE
1	D	188	HIS
1	D	194	ARG
1	D	202	MET
1	D	211	LEU
1	D	269	GLU
1	D	277	LEU
1	D	284	ASN
1	D	374	THR
1	E	137	LEU

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Mol	Chain	Res	Type
1	E	156	PHE
1	E	188	HIS
1	E	202	MET
1	E	211	LEU
1	E	233	LEU
1	E	297	PHE
1	E	300	PRO
1	E	303	PHE
1	E	354	VAL
1	F	126	MET
1	F	150	TYR
1	F	156	PHE
1	F	157	THR
1	F	188	HIS
1	F	194	ARG
1	F	195	GLN
1	F	202	MET
1	F	224	LEU
1	F	227	ASP
1	F	292	GLU
1	G	126	MET
1	G	129	LEU
1	G	188	HIS
1	G	195	GLN
1	G	301	GLN
1	G	365	ARG
1	G	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	301	GLN
1	A	334	GLN
1	B	120	GLN
1	B	191	GLN
1	B	334	GLN
1	B	352	ASN
1	C	158	ASN
1	C	248	ASN
1	C	334	GLN
1	D	291	ASN

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Mol	Chain	Res	Type
1	D	334	GLN
1	D	352	ASN
1	E	191	GLN
1	E	208	ASN
1	E	237	ASN
1	E	334	GLN
1	E	352	ASN
1	F	195	GLN
1	F	301	GLN
1	F	306	ASN
1	F	334	GLN
1	G	188	HIS
1	G	191	GLN
1	G	195	GLN
1	G	232	ASN
1	G	284	ASN
1	G	352	ASN

### 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 [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/282 (99%)	0.08	12 (4%) 36 28	1, 42, 106, 140	0
1	B	280/282 (99%)	0.02	14 (5%) 30 24	1, 36, 96, 150	0
1	C	280/282 (99%)	0.02	10 (3%) 43 34	1, 37, 100, 154	0
1	D	280/282 (99%)	0.02	9 (3%) 48 38	1, 37, 94, 133	0
1	E	280/282 (99%)	0.02	11 (3%) 40 32	1, 35, 93, 193	0
1	F	258/282 (91%)	0.06	9 (3%) 44 35	2, 38, 106, 201	0
1	G	261/282 (92%)	0.53	29 (11%) 6 6	2, 53, 136, 214	0
All	All	1919/1974 (97%)	0.10	94 (4%) 30 24	1, 39, 105, 214	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	383	SER	11.2
1	G	123	GLY	9.6
1	F	383	SER	8.3
1	G	383	SER	7.9
1	F	382	SER	7.5
1	F	126	MET	7.0
1	B	383	SER	6.3
1	G	126	MET	6.3
1	G	128	GLY	6.1
1	G	127	PRO	6.0
1	G	130	ARG	5.9
1	G	125	ILE	5.2
1	F	128	GLY	5.1
1	G	124	ILE	5.0
1	A	383	SER	4.8
1	A	123	GLY	4.4
1	F	127	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	382	SER	4.1
1	G	129	LEU	4.1
1	D	383	SER	4.0
1	B	250	THR	3.8
1	C	383	SER	3.8
1	G	304	THR	3.7
1	C	104	SER	3.6
1	A	251	GLY	3.5
1	A	110	ASP	3.4
1	C	250	THR	3.4
1	C	251	GLY	3.3
1	F	129	LEU	3.3
1	C	382	SER	3.3
1	G	291	ASN	3.3
1	G	250	THR	3.2
1	G	178	LYS	3.2
1	F	131	ARG	3.2
1	A	104	SER	3.2
1	D	250	THR	3.2
1	G	251	GLY	3.1
1	D	104	SER	3.1
1	E	104	SER	3.1
1	E	382	SER	3.0
1	B	382	SER	2.9
1	D	271	SER	2.9
1	D	251	GLY	2.9
1	B	251	GLY	2.9
1	A	250	THR	2.8
1	G	292	GLU	2.7
1	G	166	LYS	2.7
1	G	149	GLU	2.6
1	A	382	SER	2.5
1	B	104	SER	2.5
1	A	109	ALA	2.5
1	A	122	PRO	2.5
1	B	173	ASP	2.5
1	G	227	ASP	2.5
1	E	250	THR	2.5
1	G	317	LYS	2.4
1	C	110	ASP	2.4
1	E	168	LEU	2.4
1	B	131	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	173	ASP	2.3
1	B	202	MET	2.3
1	G	144	SER	2.3
1	B	248	ASN	2.3
1	A	149	GLU	2.3
1	E	166	LYS	2.3
1	E	251	GLY	2.3
1	A	168	LEU	2.3
1	B	271	SER	2.3
1	E	305	SER	2.3
1	C	123	GLY	2.3
1	G	294	ARG	2.3
1	B	166	LYS	2.2
1	C	131	ARG	2.2
1	D	110	ASP	2.2
1	G	249	ALA	2.2
1	D	382	SER	2.2
1	G	171	GLU	2.2
1	G	246	SER	2.2
1	G	142	ARG	2.1
1	A	173	ASP	2.1
1	B	165	GLU	2.1
1	B	110	ASP	2.1
1	F	201	PRO	2.1
1	B	230	GLY	2.1
1	G	303	PHE	2.1
1	G	267	GLU	2.1
1	C	201	PRO	2.1
1	E	110	ASP	2.1
1	D	344	GLU	2.1
1	G	173	ASP	2.1
1	E	123	GLY	2.1
1	F	250	THR	2.0
1	D	173	ASP	2.0
1	C	122	PRO	2.0

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

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.